INTERNATIONAL TABLES
FOR
X-RAY CRYSTALLOGRAPHY

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VOLUME
I

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VOL. I. SYMMETRY GROUPS

VOL. II. MATHEMATICAL TABLES

VOL. III. PHYSICAL AND CHEMICAL TABLES

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INTERNATIONAL TABLES

FOR

X-RAY CRYSTALLOGRAPHY

Volume I

SYMMETRY GROUPS

Edited by

NORMAN F. M. HENRY and KATHLEEN LONSDALE

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CONTENTS

PAGE

GENERAL PREFACE viii

PREFACE TO VOLUME I ix

SYMBOLS USED IN VOLUME I xi

1. HISTORICAL INTRODUCTION, *by M. von Laue* 1

2. CRYSTAL LATTICES
   2.1. The One- and Two-dimensional Lattices 6
   2.2. The 14 Three-dimensional Bravais Lattices 6
   2.3. Crystal Axes and Systems 10
   2.4. The Reciprocal Lattice 11
   2.5. Unit-cell Transformations 15

3. POINT-GROUP (CRYSTAL-CLASS) SYMMETRY
   3.1. Operations of Point-group Symmetry 22
   3.2. The 10 Two-dimensional Point Groups 24
   3.3. The 32 Three-dimensional Point Groups 25
   3.4. The 11 Laue-symmetry Groups 30
   3.5. Forms of Planes in the Laue Groups (Multiplicity Factors) 31
   3.6. Sub- and Super-groups of the Two-dimensional and the Three-dimensional Point Groups 35
   3.7. Projection Symmetries of the 32 Point Groups 38
   3.8. Point-group Symmetry and the Physical Properties of Crystals 41
   3.9. Names and Symbols of the Crystal Classes 44

4. SPACE-GROUP SYMMETRY
   4.1. Introduction to Space-group Symmetry and Possible Reflections 45
   4.2. The 17 Two-dimensional Space Groups: Equivalent Positions, Symmetry, and Possible Reflections 57
   4.3. The 230 Three-dimensional Space Groups: Equivalent Positions, Symmetry, and Possible Reflections 73
   4.4. Diffraction Symbols of the Space Groups 347
   4.5. Introduction to Structure Factor Tables 353
   4.6. Geometrical Structure Factors and Electron Density Formulae for the Two-dimensional Space Groups 367
   4.7. Geometrical Structure Factors and Electron Density Formulae for the Three-dimensional Space Groups 373
   4.8. Patterson and Patterson–Harker Functions 526
   4.9. Transformation of Co-ordinates 527

5. NOTES ON SPECIAL TOPICS
   5.1. Reduced cells 530
   5.2. Sub- and Super-groups of the Space Groups 536
   5.3. Space Group Determination by Methods outside the Friedel Law 539
   5.4. Inequalities arising from Symmetry Elements 540

6. INDEX OF SYMBOLS OF SPACE GROUPS
   6.1. Index of Symbols of Two-dimensional Space Groups 542
   6.2. Index of Three-dimensional Space-group Symbols for Various Settings 543

7. DICTIONARY OF TERMS IN ENGLISH, FRENCH, GERMAN, RUSSIAN AND SPANISH .. 554

GENERAL PREFACE

THE Editorial Commission of the International Union of Crystallography was originally charged with the task of preparing a new edition of the *International Tables for the Determination of Crystal Structures* published in 1935. Although much of the matter in the 1935 *Tables* has been preserved, the changes and the amount of new material are so considerable that the present work must be considered as being a separate publication: consequently it has received a new name which expresses the wider field embraced. Only the English language has been used, but a dictionary of crystallographic terms in English, French, German, Russian and Spanish is included in each of the three volumes.

The aim of the present compilation is to facilitate the work of three categories of scientists: those who are actually engaged in the determination of crystal structures, those who are using X-ray methods in the study of crystals in general, and students of crystallography. This aim has been borne in mind in deciding the contents. The Commission has tried to produce a definitive presentation of all the data which are firmly established as essential to the work of the X-ray crystallographer. In addition, some space has been given to topics which give promise of becoming essential during the next ten years, and provision has been made for the supplementary issue of tables of data for such topics if necessary.

That Commission members owe a debt to the pioneers of the 1935 *Tables* goes without saying, and in particular they owe much to the former editor, Dr. Carl Hermann. The Commission wishes also to express its gratitude to Dr. Wessenberger, of the firm of Borntraeger, Berlin, for permission to use and to reproduce parts of the 1935 *Tables*.

The work of the Editorial Commission has been greatly facilitated by the willingness of crystallographers in all parts of the world who have helped with the compilation of tables and lists of references, by careful checking of the data, and by giving advice on the selection of material. Although limitation of space prevented the publication of all the material which was received, the work of all has helped towards the shaping of the present publication. Specific reference to individual helpers is made in the prefaces to each volume. Since it would be too much to hope that all errors have been eliminated, the Commission would be grateful for notification of any mistakes which may be discovered, and indeed for any expressions of opinion or further suggestions regarding the present *Tables*. These should be sent to Professor Kathleen Lonsdale, Department of Chemistry, University College, Gower Street, London W.C.1, England.

Finally, the Commission would like to express thanks to The Kynoch Press, Birmingham, England, for the great care taken in the difficult work of printing.

PREFACE TO THE 1965 EDITION

The Commission for International Tables has been engaged in future planning for the Tables in view of the continuing demand for all three volumes. Since the complete revision and extension of the material of volume I would be a task of many years, it has been decided to reprint this volume with all corrections received to date.

PREFACE TO THE 1969 EDITION

In this edition the material forming the Additional Notes in the 1965 Edition has been incorporated in certain revised sections, particularly in 3.5, 3.7, and 4.4.

Section 4.7, which contained a number of errors not corrected in 1965, has been completely revised by Dr E. Schultze-Rhonhof.

Section 5.1 has been replaced by new material prepared by A. D. Mighell, A. Santoro, and J. D. H. Donnay, National Bureau of Standards, Washington, D.C., U.S.A.

No list of the corrections and changes made in 1965 or in the present edition has yet been published. It is intended to make good this lack by printing a complete list for both the 1965 and the 1969 editions in Acta Crystallographica early in 1970. This will acknowledge the help of all those who have kindly notified the Editor of errors in the 1952 and 1965 editions.

PREFACE TO VOLUME I

THIS Volume includes such information concerning the crystallographic symmetry groups in two and three dimensions as is currently used in X-ray crystallographic work. No attempt has been made by the editors to aim at theoretical completeness, their intention being rather to tabulate and display only essential material. Under the heading of Notes on Special Topics there is, however, discussion of several subjects (some of which may be included in Volumes II and III also) which are either in the process of development or which have not been much used since the publication of the 1935 *Tables*. If there is a sufficient demand for any of these, or for other subjects which may subsequently be developed, the Editorial Commission would be prepared to publish data tables as supplementary issues. This applies also to the field of semi-crystalline symmetry, where the methods of representation are still in the experimental stage.

A considerable amount of the material given here was included in the *International Tables for Crystal Structure Determination*, 1935, Volume I, which was edited by Dr. Carl Hermann, the contributing authors being W. T. Astbury, E. Brandenberger, C. Hermann, K. Lonsdale, C. Mauguin, P. Niggli and R. W. G. Wyckoff. The present editors wish to affirm their great debt to these original authors. To one of the two honorary chief editors of the 1935 *Tables*, Professor M. von Laue, they are indebted for the Historical Introduction which he has so kindly written for these new *Tables*. Sir Lawrence Bragg has also contributed to this introduction an account of the early work done by himself and by his father, Sir William Bragg, to whose inspiration the original *Tables* owed so much.

Use has been made of a considerable amount of published work and, where possible, references have been given to papers which should be consulted for further explanatory details. A number of crystallographers have helped greatly with the preparation of material and its arrangement for printing, with proof-reading or with general advice. Among these are, of course, our fellow-members of the Editorial Commission and especially Dr. R. C. Evans, the Secretary of the International Union of Crystallography, in his capacity as an *ex-officio* member of the Commission. It is impossible to name all those who have assisted in various ways, but we should like to record our thanks to the following, and to many others who have also helped in the preparation of this Volume.

Members of the *ad hoc* 1946 Committee

Members of the Nomenclature Commission of the International Union of Crystallography

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F. Laves	J. Wyart

The editors wish to thank Mr. Walkey of the Cambridge University Press, and Mr. Rickson of the Department of Mineralogy and Petrology, Cambridge, for preparation of the new diagrams. They also wish to thank the Managers of the Royal Institution for permission to use Lonsdale's *Simplified Structure Factor Tables*, which have been reproduced in modified form. All the material taken over from the 1935 *Tables* has also been rearranged, tabulated and displayed in new ways which, it is hoped, will make for greater convenience in use. The data on geometrical structure factors have been separated from the other data on the 230 space groups for convenience in printing layout.

Certain kinds of space-group symbols and class names no longer in use have been dropped. Enquiry has also shown that sufficient use was not actually made of data on sub-groups and lattice complexes to justify the space that would have been required to display them properly in the present *Tables*. If the need for them should ever develop, complete tables of these data could be published separately.

Data relating to two-dimensional lattices, point groups and space groups are included because of their importance in the development and teaching of systematic group theory, in the representation of projection symmetry and in work on certain types of layer structure.

A suggestion made to the Editorial and Nomenclature Commissions by Prof. M. J. Buerger, that the z-axis should be taken as the unique axis in the monoclinic system, was circulated to a number of crystallographers and crystallographic societies in as many countries as possible. So many favourable replies were received that it was agreed that the present *Tables* must include duplicate

descriptions of the monoclinic point groups and space groups. The description using the z-axis as the unique axis is taken as the "1st setting," that using the y-axis as the unique axis is called the "2nd setting."

At the Stockholm General Assembly of the International Union of Crystallography in 1951 it was agreed that the 2nd setting should be accepted as standard for morphological and structural crystallographic studies, but that the 1st setting could be used where there was a special reason for this alternative.

Various changes in nomenclature and layout have been made, to conform to modern usage and for the sake of consistency. The space groups have each been given a number, for reference purposes only. The use of the C and F settings in the tetragonal system has been dropped, P and I only being used. In the trigonal and hexagonal systems the use of the H setting has been dropped for systematic descriptions and the primitive hexagonal lattice is called P and not C.

This has necessitated the redrawing of a considerable number of tetragonal, trigonal and hexagonal diagrams. In addition, the outline of the hexagonal (triple) unit cell has been given in the diagrams of the 7 space groups with the R-lattice. The other non-cubic diagrams have been reproduced unchanged, except for the correction of errors. These diagrams have stood the test of time well, but it was felt that the cubic diagrams, if included, would have to be revised. Enquiry showed, however, that comparatively little use was being made of the cubic diagrams, and in the interests of economy and compactness it was decided that they should be omitted from the present publication. Again, it would be easy to publish these as a supplementary issue in the future if the demand were sufficient and if a more satisfactory method of representation could be devised.

The arrangement of material has been systematic as far as is consistent with the object of the *Tables*. The lattice is basic to the crystal structure, and the reciprocal lattice to the understanding of diffraction effects. These are considered in Section 2. The external form of the crystal indicates the point-group symmetry, and a systematic study of all the kinds of point-group symmetry that can be applied to a lattice is therefore next given in Section 3. The addition of translations to the rotations and rotatory inversions of point-group symmetry gives the space groups, which are fundamental in crystallographic group theory. The main part of Section 4 of this volume consists of data for the 230 three-dimensional space groups, and of tables used in the interpretation of diffraction effects from crystals belonging to any of these. Volume I, however, does not include such tables as atomic scattering factors for the different elements, or values of mathematical functions which occur in the intensity formulae.

The staff of The Kynoch Press have been most patient and tireless in rearranging these *Tables* in order to produce a result which shall be both pleasing to the eye and convenient in use. We believe that they have been most successful in achieving both objects, and we are exceedingly grateful to them.

SYMBOLS USED IN THIS VOLUME

a, b, c	Lengths of unit-cell edges.
a, b, c	Unit-cell vectors.
α, β, γ	Interaxial angles $y \wedge z$, $z \wedge x$, $x \wedge y$.
x-, y-, z-, (u-)	Directions of crystallographic axes of co-ordinates.
x, y, z	Co-ordinates of any point (equivalent position) in the unit cell, expressed in terms of a, b, c, except on rhombohedral axes.
x, y, z	Co-ordinates of equivalent position in the primitive rhombohedral unit cell, expressed in terms of rhombohedral axes.
x_r, y_r, z_r	Co-ordinates of an atom r, expressed in terms of a, b, c.
X, Y, Z / U, V, W	Co-ordinates of any one of a series of systematically spaced points (expressed as fractions of a, b, c), filling the unit cell at regular intervals (Fourier and Patterson analyses respectively).
u, v, w	Co-ordinates of any lattice point, expressed in terms of a, b, c as units.
$[u\ v\ w]$	Indices of a direction in the direct (real-space) lattice (zone axis).
$\langle u\ v\ w \rangle$	Indices of a "form" of zone axes (related by symmetry).
$(h\ k\ l)$	Indices of a crystal face, or of a single plane, or of a set of parallel planes.
$h\ k\ l$	Indices of the reflection from a set of parallel planes; co-ordinates of a reciprocal lattice point.
$\{h\ k\ l\}$	Indices of a form of planes, or of the reflections from a form of sets of parallel planes.
$\{h\ k\ i\ l\}$	Ditto for the hexagonal co-ordinate axes x-, y-, u-, z-.
a^*, b^*, c^*	Lengths of reciprocal-lattice unit-cell edges.
$\mathbf{a}^*\ \mathbf{b}^*\ \mathbf{c}^*$	Unit-cell vectors in reciprocal space.
$\alpha^*, \beta^*, \gamma^*$	Interaxial angles in reciprocal space.
d_{hkl}	Interplanar spacing of planes (hkl).
V or V_c; V^*	Unit-cell volume in direct and in reciprocal space.
p, c; p	Primitive and centred two-dimensional lattices; one-dimensional lattice.
P, R, A, B, C, F, I, H	Lattice symbols in three dimensions.
1, 2, 3, 4, 6	Rotation-axis symbols (X) (or rotation-point symbols in two dimensions).
$\bar{1}, \bar{2}, \bar{3}, \bar{4}, \bar{6}$	Inversion-axis symbols ($\bar{X}$).
$2_1, 3_1, 3_2, 4_1, 4_2, 4_3, 6_1, 6_2, 6_3, 6_4, 6_5$	Screw-axis symbols.
m	Mirror-reflection plane in three dimensions, mirror-reflection line in two dimensions, or mirror-reflection point in one dimension.
g	Glide-reflection line in two dimensions.
a, b, c, n, d	Glide-reflection planes in three dimensions.
$f(hkl)$	Atomic scattering factor for the particular value of $(\sin\theta)/\lambda$ corresponding to the Bragg reflection hkl.
$F(hkl)$	Structure factor for the unit cell, corresponding to the Bragg reflection hkl.
$\lvert F(hkl)\rvert$	Modulus of the structure factor for hkl (sometimes shortened to $\lvert F\rvert$).
$\alpha(hkl)$	Phase of the structure factor for hkl (sometimes shortened to α).
A, B	$\lvert F\rvert \cos\alpha$, $\lvert F\rvert \sin\alpha$ respectively.
$\rho(XYZ)$	Electron density at the point X, Y, Z.
$P(UVW)$	Patterson function at the point U, V, W.
n, m	Any integers.

1. HISTORICAL INTRODUCTION

by M. VON LAUE

THE science which the *International Tables* are intended to serve is concerned primarily with the atomic theory of crystals, and secondarily with optical theory as applied to the short wavelengths of X-radiation. Moreover, now that we know of electron and neutron diffraction by crystals, it must include quantum mechanical wave theory, which is also, as it happens, of importance in the branch of optics already mentioned. This introduction has to deal, therefore, with the history of these three branches of physics. Let us begin with the most important and the oldest branch, the theory of crystals.

We may take as a beginning the small pamphlet written in the year 1611 by the great astronomer Johannes Kepler, which bears the title *Strena seu de nive sexangula*, or in translation "A New Year's present; on hexagonal snow." It is dedicated to one of his patrons at the court of the Emperor Rudolph II, whose friendship Kepler enjoyed during his stay in Prague. Kepler's astronomical works show that throughout his life he believed that the material world was the creation of a Spirit delighting in harmony and mathematical order. Had he not tried in his youth to deduce the radii of the planetary orbits from the dimensions of certain regular polyhedra, and did not his principal work (1619) bear the title *Harmonice Mundi*? It need not surprise us, therefore, that it was the appearance of these regular and beautifully shaped snowflakes rather than the appearance of the crystals of the mineral world that inspired Kepler with the idea that this regularity might be due to the regular geometrical arrangement of minute and equal brick-like units. Thus he was led to think of close-packed spheres, and, although he did not coin the expression "space-lattice" and although his development of these ideas is not always correct, we can find among his illustrations the first pictures of space-lattices.

Nevertheless Kepler felt uneasy about these speculations. He realised, quite correctly, that his way would lead to an atomic theory; yet the idea of the atom, as handed down from the ancient Greeks, lacked an empirical foundation and therefore has often been the subject of excessively fanciful speculation even until well into the nineteenth century. Hence it was not without reason that the natural scientist in Kepler mistrusted this idea and would not take it seriously. He toyed with the double meaning of the word "nix," which in Latin means snow but in German dialect "nichts" —nothing. And so from beginning to end he repeatedly explained the whole idea away as a mere "nothing."

In these circumstances the little pamphlet, even though it was printed, naturally made no deep impression on his contemporaries, and was gradually forgotten. Crystallography took another direction, that of the description of the external form of crystals, after Niels Stensen had in 1669 pointed out the existence of characteristic angles between crystal faces. By devious ways this led eventually to the Millerian indexing of faces (1839), to the laws of symmetry and to the classification of crystals in 32 classes, which was accomplished in 1830 by Johann Friedrich Christian Hessel and in 1867, independently and rather more simply, by Axel Gadolin.

This consistently phenomenological approach was not abandoned, even though the crystal-optical discoveries made early in the nineteenth century by such men as Baptiste Biot, David Brewster, Augustin Fresnel and Frederick William Herschel had led to the development of the important idea that the same laws of symmetry which were valid for the positions of crystal faces also controlled the physical events inside the crystal. This was first made clear by Franz Neumann in 1833.

Apart from these trends of thought, however, ideas about the internal structure of crystals continued to appear. Thus Christiaan Huygens' fundamental work on the wave theory of optics, *Traité de la lumière*, which was published in 1690, contains among other things a wave-theoretical explanation of birefringence, and ascribes to calcite a structure made up of ellipsoidal particles; the threefold periodicity of this arrangement characterises it as a space-lattice, although Huygens, like Kepler, did not define it as such. It was the cleavage along three planes which led him to this idea. Like Kepler's pamphlet, however, this part of the otherwise famous work was soon forgotten. Independently of Huygens, crystal cleavage in general led Torbern Bergman in 1773 and René Just Haüy in 1782 to suppose that all crystals consist of a kind of masonry of equal, parallelepipedal building bricks. That these "molécules soustractives"

were often supposed to consist of "molécules intégrantes" of other shapes need not concern us here. A structure of this kind involves a space lattice, and Haüy could therefore easily go on from this idea to deduce the laws governing the geometry of crystal faces, already empirically known. But it would be premature to describe this as an atomic theory of crystals. No wonder! For the scientific theory of atoms had yet to be created, in its own good time, by the great chemists of the eighteenth century. The theorem that a lattice may be divided into unit cells, as we should say today, in an infinite number of different ways would have made no physical sense whatever to Haüy (although he would have admitted, of course, its geometrical correctness), since the shape of the "molécules soustractives" was fixed unambiguously by Nature.

Thus the true beginning of the atomic theory of crystals must be dated from a paper published in the year 1824 by Ludwig August Seeber, physicist in Freiburg, in Gilbert's *Annalen der Physik*, vol. 76, page 229. Seeber, who certainly knew of Haüy's works but probably did not know the part we have quoted from Huygens', was trying to find an explanation of the thermal expansion and the elasticity of solids, of which he quite rightly believed crystals to be the normal type. He found the bricklike structure unsuitable for his purpose, since, he argued, the only view compatible with this picture would be that the single bricks themselves possess these physical properties, which does not solve the problem but only pushes it one step farther back. Seeber, whose outlook was essentially modern, introduced instead the idea of a structure consisting of chemical atoms or molecules (at the time these two concepts were not strictly differentiated), whose mutual distances are determined by the balance of attractive and repulsive forces, thus forming a system of stable equilibrium. External disturbances cause certain changes of position—this is his explanation of elasticity—and possibly also elastic vibrations about the equilibrium positions. Seeber, of course, did not visualise thermal vibration: he explained thermal expansion in terms of the temperature dependence of the attractive and repulsive forces. In order to retain the sound parts of Haüy's postulate, Seeber placed each of his molecules, assumed by him to be spherical, at the midpoint of the cell which would have formed one of Haüy's "molécules soustractives"; he thus arrived at a "parallelepipedal arrangement of the indivisible parts of matter," as he describes it at the end of his paper. In our language such an arrangement implies a primitive translation lattice, and it is not far from this concept to the idea that each unit cell of the space lattice is occupied by several atoms.

This was the earliest application of the scientific atomic theory to a purely physical problem. The kinetic theory of gases, which is usually regarded as the beginning of atomic theory in physics, did not appear until thirty-two years later. Seeber was therefore far ahead of his time, and it was no wonder that his contemporary physicists failed to respond to his ideas, which were forgotten until Sohncke revived them in 1879. But at least one mathematical problem had been raised—the number of geometrically possible space lattices that correspond to the 32 crystal classes and to their symmetry operations. Moritz Ludwig Frankenheim and Auguste Bravais took up this problem, and in 1850 Bravais described the 14 pure translation lattices which have been named after him. Incidentally, his papers also contain the concept of the reciprocal lattice, which was later rediscovered and used in connection with the study of interference effects from crystals. This purely group-theoretical investigation was extended by Leonhard Sohncke in 1879 through the introduction of further symmetry operations, thus arriving at 65 different "space groups." The complete solution of the problem, taking into account *all* possible symmetry operations on a lattice, was given simultaneously in the year 1890 by Evgraph Stepanovitsch Fedorov and by Artur Schoenflies. They derived the 230 space groups which are used in modern structural research.

Investigations pursued by English scientists of the following decade were less systematic and far more hypothetical, but their ideas possessed the advantage that they could be visualised more easily. Inspired by the success of stereochemistry, they devised three-dimensional models of atomic structures based on lattices. Lord Kelvin published a paper on this subject in 1894. Reasoning along these lines was most fully expressed in a series of long papers by W. Barlow in the last decade of the nineteenth century. Barlow took up the idea of close packing, and distinguished for the first time correctly between the cubic and hexagonal forms of packing. He also considered the question of packing of spheres of two or three different sizes and described, for example, the sodium chloride structure, although neither in this nor in any other case did he in these early papers name a substance which might be expected to have one of the proposed structures. This was undoubtedly one of the reasons why the whole of his structure

theory at first attracted little attention. Moreover, the very reality of atoms was doubted again and again right up to the end of the nineteenth century. Even in the absence of such doubts, and even when collaboration with Pope had given the chemical application of Barlow's theory, there was still no way of bringing the hypothetical structures into relation with experiment. In order to establish structure theory on a firm basis, yet another set of ideas, those of physical optics, had to be brought in.

The diffraction of visible light by gratings, which mostly consisted of lines scratched on glass or metal, had already been described by Grimaldi in the seventeenth century, and again by Joseph Fraunhofer at the beginning of the nineteenth. The relevant theory can be found in the comprehensive treatise by Friedrich Magnus Schwerd: *Die Beugungserscheinungen, aus den Fundamentalgesetzen der Undulationstheorie analytisch entwickelt* (1835). The grating was and still is the most important instrument in spectroscopy. Later physicists engaged in work on optics have often returned to Schwerd's theory. In particular, Lord Rayleigh frequently emphasised that the essential characteristic of a grating is the periodic repetition of its elements and not the nature of those elements. Round about 1910 M. von Laue, in writing an article on wave theory for the *Encyklopädie der mathematischen Wissenschaften*, set himself the task of elaborating, as clearly as possible, this idea of Rayleigh's, and arrived at an equation for the position of the diffraction maxima which could be extended without difficulty to the case of double periodicity as it exists in cross-gratings; in the latter case two such equations had to be formulated.

In the meantime the science of optics had been extended far beyond the limits of the visible spectrum. The farthest extension on the short-wave side had come about in 1895 through Röntgen's discovery of X-rays; soon afterwards (1896) Emil Wiechert and George Gabriel Stokes concluded from the way in which X-rays are produced that they must be short waves consisting of electromagnetic pulses. This was confirmed by the observation of their polarisation, made by C. G. Barkla in 1906. Wilhelm Wien in 1907 estimated their wavelength to be 7×10^{-9} cm. on the basis of their observed photoelectric effect, while A. Sommerfeld in 1912 calculated a value of 4×10^{-9} cm. from their diffraction by a slit. On the other hand, they showed such strong quantum effects that some very eminent physicists held firmly to the corpuscular theory of X-rays.

Both these questions and that of the fine structure of crystals were decided by the researches of W. Friedrich and P. Knipping, which were published in the summer of 1912 in the *Sitzungsberichte der Bayerischen Akademie*. Von Laue's diffraction theory, which had provided the inspiration for these experiments and which had indeed been confirmed by their results, simply consisted of the diffraction conditions for a cross-grating, with the addition of a third condition to take account of the three-dimensional periodicity of a space lattice. Admittedly von Laue had expected, in accordance with the Stokes–Wiechert pulse theory, that many more interference spots would appear on the photographs than were actually observed, and he could only explain their absence by ascribing to the atoms of the crystal a strongly selective scattering power for X-rays: this idea, though it later proved to be mistaken, was not altogether unreasonable in view of the characteristic X-ray emission of the elements which had been found by Barkla. Towards the end of 1913, at the second Solvay Congress, von Laue used the rediscovered reciprocal-lattice theory to extend to the general case of any crystal the geometrical construction for the interference maxima from cubic crystals that had been given by P. P. Ewald. He thus provided the foundation for a simple "geometrical" theory of X-ray diffraction.

Meanwhile the experiments of Friedrich and Knipping, and von Laue's interpretation of them, had become known in England, and had inspired much discussion and further investigation, particularly by W. H. and W. L. Bragg. The story of what happened is here continued by Sir Lawrence Bragg:

"In the summer of 1912 my father showed me von Laue's paper, which had aroused his intense interest because of his work on the exciting of cathode rays by X-rays, which pointed to the projectile-like properties of X-rays, and he discussed with me possible alternative explanations for the effects which von Laue had found. I undertook some experiments at Leeds that summer to see whether we could explain von Laue's spots by the shooting of particles down avenues in the crystal lattice rather than by the diffraction of waves, experiments which were of course abortive.

"On returning to Cambridge in the autumn of 1912 I studied von Laue's photographs very intensively, and was very naturally forced to the conclusion that they must be due to diffraction. I also concluded at the same time that one must modify the explanation of them which von Laue had given.

Von Laue had remarked that one did not get all the spots one would expect from a simple cubic lattice, but only a selection of the whole range. He ascribed this to the existence in the X-radiation of five characteristic wavelengths chosen so that they approximately satisfied the diffraction conditions for the spots which actually appeared in the photographs. I, on the other hand, concluded that von Laue's spots were due to the diffraction of 'white' X-radiation, representing a continuous band of wavelengths over a certain range. I was led to this first by noting the changing shape of the Laue spots when the distance from the photographic plate to the crystal was altered. This in turn led me to consider the diffraction effect as a reflection of X-ray pulses by the lattice planes of the crystal. I pointed out that this was equivalent to the selection from the continuous spectrum of a wavelength determined by the lattice spacing of the crystal. I tested this by reflecting the X-rays from a mica plate set at a series of angles, getting in every case a spot in the reflected position and so showing, as I believed, that all wavelengths were represented over a certain range in the X-rays. The problem then remained to explain why only certain spots appeared in the Laue photographs, and I ascribed this to the fact that the essential underlying lattice of the crystal was face-centred and not simple cubic. I communicated these results to the Cambridge Philosophical Society in November 1912. The 'Bragg equation' appeared in this paper (p. 46) in the form $\lambda = 2d \cos \theta$, but in later papers θ was defined as the glancing angle and not the angle of incidence.

"Professor Pope at Cambridge was very interested in these results, because the close-packed lattices which he and Barlow had devised for atoms which they believed to be of equal size were face-centred cubic. He procured crystals of potassium chloride and sodium chloride for me, and I took their Laue photographs. I showed that these could be explained by an arrangement of alternate scattering centres in two interleaved face-centred lattices, the NaCl structure in fact, and that these centres must be equal in scattering power in KCl but different in scattering power in NaCl.

"This work was done at Cambridge before I collaborated with my father. We worked along divergent lines at first, which came together later. My father was very interested in my explanation of the diffraction effect as a reflection, and he set up at Leeds the first X-ray spectrometer. He was primarily interested in the nature of X-rays. He checked that the reflected rays were really X-rays, a point on which he wished to satisfy himself because of his speculations about the corpuscular nature of X-rays. He found as I did that there appeared to be a continuous spectrum, but his spectrum also showed some peaks superimposed upon this continuous range, and by improving the apparatus he soon narrowed these down so much that it was clear that they were monochromatic components characteristic of the target. Incidentally I think it is not often realised how much work he did on characteristic X-rays before Moseley made his brilliant generalisations. My father constructed tubes with about a dozen different anticathodes and identified Barkla's K and L radiation, showing that the K contained two peaks and the L three peaks. He related the wavelengths to the atomic weights of the metals in each anticathode (the idea of atomic number had not yet come to the fore) by a simple law. In fact he gave the first hint of Moseley's relations, and it was his work which inspired Moseley to his broader generalisations.

"My father then examined with his spectrometer crystals of KCl and NaCl such as I had used for my Laue photographs, and found the reflections of the characteristic peaks from the (100), (111) and (110) faces. It was clear at once that the spectrometer was a far more powerful way of investigating crystal structure than the Laue photographs, which I had used. It was only at this stage that we joined forces. In particular, I had been trying to analyse the diamond structure by Laue methods without success, but my father mounted it on the spectrometer and the structure became immediately obvious. We wrote a paper on the diamond structure together, but the results which gave the clue to it were obtained by him. I was able, however, to work along with him with the spectrometer in the summer of 1913, and so to work out the structures of zincblende, fluorspar, pyrites and some of the carbonates, which showed how powerful the spectrometer could be. My father was at first principally interested in X-ray spectra and X-ray absorption edges, but crystal structures also fascinated him, and from that point on we both mainly devoted ourselves to crystal structure analysis."

These experiments, together with those of Friedrich and Knipping, not only confirmed von Laue's diffraction theory but gave a direct proof of the existence of the space-lattice, and provided a simple expression (the Bragg law) for the relationship between the wavelength of the X-rays used and the lattice spacings of the crystal. The ionisation

curves obtained by means of the Bragg spectrometer showed clearly that the "mirror-image reflection" postulated by Bragg is selective and is conditioned by multiple interference. The Bragg equation was first published in its usual form in a paper by W. H. and W. L. Bragg in the *Proceedings of the Royal Society*, vol. 88, page 428 (1913). Soon afterwards von Laue [*Physikalische Zeitschrift*, **14**, 421 (1913)] was able to show that this equation was only another way of expressing the results of the geometrical space-lattice theory.

Ionisation spectrometer measurements also revealed another reason for the absence of many of the interference spots at first expected by von Laue. The pulse theory of X-rays predicted much too wide an extension of their spectrum in the short-wave direction. In fact, as W. Duane and F. L. Hunt established in 1915, this spectrum ends abruptly at the short-wavelength limit given by the now well-known quantum rule.

Still further credit is due, however, to W. H. and W. L. Bragg. X-ray diffraction patterns had made it possible to compare the wavelengths of X-rays with the three lattice constants, whose axial ratios were already known. Absolute measurements, however, remained impossible without a knowledge of the absolute value of the lattice constant of at least one substance. It was necessary for this purpose to know the number of atoms in the unit cell, and this was impossible without a knowledge of the structure. The Braggs' measurements, however, had shown that sodium chloride really did possess one of the hypothetical structures postulated by Barlow. Thus it was possible to obtain the absolute value of the lattice constant of this salt; this in turn provided an absolute measure of the wavelengths of X-rays, and hence the absolute lattice constants of all other crystals investigated. Rarely has the value of hypothesis in research been so strikingly demonstrated.

This brings us to the end of the historical introduction as far as X-rays are concerned, since all that has followed is merged into present-day practice. Yet the space lattice has had another most important part to play in physics.

In 1924 L. de Broglie put forward in his *Thèses* the basic idea of wave mechanics. In the summer of 1925 Walter Elsasser, in a letter to the editor of *Naturwissenschaften*, pointed out that the de Broglie waves of electrons must cause space-lattice interference effects, and that experiments by Davisson and Kunzman on the reflection of electrons from a platinum sheet had actually shown maxima of the expected kind. When in 1926 E. Schrödinger published his communications on *Quantisierung als Eigenwertproblem*, C. J. Davisson and L. H. Germer began systematically to look for these effects. In March 1927 they were able to publish a note in *Nature* to say that their efforts, made on a single crystal of nickel, had been crowned with success. In May of the same year G. P. Thomson and A. Reid announced that an electron beam of several thousand volts had, on passing through a celluloid film, produced Debye–Scherrer rings, and G. P. Thomson found the same effect even more clearly with metal foils. Thus Elsasser's prediction was confirmed and the plainest of all proofs had been given of the connection of a wave with the movement of a corpuscle.

Admittedly the geometrical theory of space-lattice interference does not apply so well to electrons as it does to X-rays, especially not to low-energy electrons. But it has enjoyed further triumphs in the diffraction of neutrons, observed first by D. P. Mitchell and P. M. Powers, then since 1946 by W. H. Zinn, E. Fermi, C. Shull and other American physicists using the cyclotron or the uranium pile as a source. Here a new possibility has to be taken into account: the atomic structure factor, which is characteristic for the scattering of single atoms, may be negative as well as positive. This branch of research is, however, still in its infancy. It appears to be capable of great development.

2. CRYSTAL LATTICES

2.1. The One- and Two-dimensional Lattices

There is only one one-dimensional lattice. This consists of a single row of equally spaced points, the lattice being completely specified by one vector. The lattice symbol is p

The general two-dimensional lattice is an infinite array of points which obey the lattice condition that every point should have the same environment in the same orientation. The unit cell of this lattice is a general parallelogram which can be outlined in several different ways. It is conventional in drawing the unit cell to take the origin at the top left corner; the positive direction of the y-axis points horizontally to the right, and the positive direction of the x-axis points down the page, either straight down or to the left.

Specialisation of the two vectors needed to specify the lattice gives rise to four other lattices, described in Table 2.1.1. Small italic letters are used in the nomenclature for the two-dimensional lattices in order to distinguish their symbols from those of the three-dimensional lattices, for which capital italic letters are used. The symbol p is used when the conventionally chosen unit cell is "primitive," i.e. has points at the corners only. The symbol c is used when the conventional choice of unit cell produces a centring point. There is only one centred two-dimensional lattice, and it would be easy to select a primitive unit cell in this also, but only if the conventional rule for the choice of unit cell were disregarded. This conventionally chosen unit cell is related to the symmetry elements of the lattice, and this relation is discussed in section 2.3; but here the rules are given in terms of the vectors chosen as axes.

TABLE 2.1.1

The 5 Two-dimensional Lattices

Shape of unit cell	Lattice symbol	Conventional rule for choice of axes	Nature of axes and angles[1]	Name of corresponding system
General parallelogram (rhomboid)	p	None	$a \neq b$ $\gamma \neq 90°$	Oblique
Rectangle	p c	Two shortest, mutually perpendicular vectors	$a \neq b$ $\gamma = 90°$	Rectangular
Square	p	Two shortest, mutually perpendicular vectors	$a = b$ $\gamma = 90°$	Square
60° angle rhombus	p	Two shortest vectors at 120° to each other	$a = b$ $\gamma = 120°$	Hexagonal

(1) The symbol $\neq$ implies non-equality by reason of symmetry; accidental equality may, of course, occur.

It is not necessary to add to the lattice symbol p a mark to distinguish one primitive lattice from the other three primitive ones, because this is done by the rest of the space-group symbol which follows the lattice symbol (see section 4.1).

It should be noted that the four different shapes of unit cell given in the above table can be referred to four "systems" of co-ordinate axes analogous to the systems in three dimensions.

2.2. The 14 Three-dimensional Bravais Lattices

A one-dimensional lattice may be called a "row." An evenly spaced array of rows forms a two-dimensional lattice, that is, a "net." An evenly spaced array of nets forms a three-dimensional lattice, which is an infinite array of points such that each point has the same environment in the same orientation. A "unit cell" may be defined in an infinite number of ways, and it will be characterised by three vectors, not in one plane, which are the edges of a parallelepiped.

2.2. THE 14 THREE-DIMENSIONAL BRAVAIS LATTICES

The Bravais lattices may be taken as arrangements of points in real space, the repeat distance between the points in any direction being proportional, in any particular case, to the corresponding repeat distance in the real crystal under study. Consequently the magnitude of the vectors of the Bravais lattice may be expressed in Å units and the lattices drawn to an appropriate scale. The general symbols for the unit-cell vectors are **a**, **b**, **c** and for their magnitudes a, b, c; while the co-ordinate axes, or directions of the sides of the unit cell, are referred to in general as the x-, y- and z-axes. The interaxial angles $y \wedge z$, $z \wedge x$, $x \wedge y$ are denoted by α, β, γ.

When one or more of the vectors is specialised in a non-trivial way the lattice possesses symmetry (other than identity symmetry). In such cases it is much more convenient to select the unit-cell vectors in such a way that they are closely related to the symmetry elements of the lattice, even though the unit cell may not then be primitive (i.e. with one lattice point only). This sometimes results in the conventional choice of a unit cell centred in various ways.

TABLE 2.2.1 **The 14 Bravais Lattices and Conventional Unit Cells**

System	Number of lattices in system	Lattice symbols	Nature of unit-cell axes and angles[1]	Lengths and angles to be specified	Symmetry of lattice[2]
Triclinic	1	P	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	a, b, c α, β, γ	$\bar{1}$
Monoclinic[3]	2	1st setting $\begin{cases} P \\ B \end{cases}$	$a \neq b \neq c$ $\alpha = \beta = 90° \neq \gamma$	a, b, c γ	$2/m$
		2nd setting $\begin{cases} P \\ C \end{cases}$	$a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$	a, b, c β	
Orthorhombic	4	P C[4] I F	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	a, b, c	mmm
Tetragonal	2	P[5] I	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	a, c	$4/mmm$
Cubic	3	P I F	$a = b = c$ $\alpha = \beta = \gamma = 90°$	a	$m3m$
Trigonal	1	R[6]	$a = b = c$ $\alpha = \beta = \gamma$ $< 120°, \neq 90°$	a α	$\bar{3}m$
Hexagonal	1	P[7]	$a = b \neq c$ $\alpha = \beta = 90°$ $\gamma = 120°$	a, c	$6/mmm$

(1) The symbol $\neq$ implies non-equality by reason of symmetry; accidental equality may, of course, occur.
(2) For explanation of the symmetry symbols see section 3.1.
(3) The side-centred monoclinic lattice is conventionally taken as B in the 1st setting (z-axis unique) and as C in the 2nd setting (y-axis unique). It would be an equally correct description to take A in either case, but this would not distinguish which setting had been chosen. (See Preface to Volume I for the reason for listing alternative settings in the monoclinic system.)
(4) When referring to lattices alone, it is conventional to call the side-centred orthorhombic lattice C. In the space groups of the point group $mm2$, the "z-axis unique" convention requires that the side-centred lattice shall sometimes be called C, and sometimes A (or B).
(5) The tetragonal lattices P and I may also be described as C and F, but only if the **a**, **b** vectors chosen are not the shortest ones perpendicular to **c**.
(6) The R-lattice is here described on rhombohedral axes, but it may also be referred to hexagonal axes. Where it is necessary to distinguish these the symbols R_{obv} or R_{rev} (see p. 20) are used for the description on rhombohedral axes and R_{hex} for that on hexagonal axes.
(7) In the 1935 *Tables* the symbol C was used to denote the hexagonal lattice. The reasons for this, although valid, do not outweigh the confusion caused. The lattice is, in fact, primitive and is therefore called P. It is common to both the trigonal and hexagonal systems (see pp. 10, 11).

The different types of lattice are as follows:

A, *B* or *C* Centred on one pair of opposite faces of the unit cell [*A* (100), *B* (010), *C* (001)] as well as having points at the corners.

F All faces centred, in addition to points at the corners.

I Body centred, in addition to points at the corners.

P Primitive (points only at the corners); except rhombohedral.

R Primitive rhombohedral.

The relationships between the magnitudes of the axes and the interaxial angles in the conventional unit cell are given in Table 2.2.1. But it must be emphasised that in every lattice it is possible to choose a primitive unit cell, although this is not always convenient. Such a primitive unit cell (the vectors of which are known as a "primitive triplet") may be found from the analysis of diffraction data and may have to be 'reduced' to the corresponding conventional unit cell (see section 5.1). It should be noted that in choosing the primitive unit cell various alternatives are possible, although sometimes one of these might be obviously more convenient than another. The relationships of axes and angles in *some* of these non-conventional unit cells corresponding to conventional but non-primitive unit cells are shown in Table 2.2.2. These are listed as (1), (2), (3), etc. It will be noticed that although symmetry is *ignored* in choosing these primitive cells, it is always, if present, *revealed* by axis or angle relationships.

The 14 Bravais lattices can be referred to seven different co-ordinate systems on the basis of the specialisation of their vectors. These systems are discussed in section 2.3. In each of the systems, with the exception of the trigonal, the shape of the unit cell (see column 4, Table 2.2.1) of the lattice is characteristic of the system. In the trigonal system two kinds of primitive unit cell are possible; and it is found in practice that some trigonal crystals have a structure based on the hexagonal lattice while others have a structure based on the rhombohedral lattice.

TABLE 2.2.2

Relationships between Axes and Angles in some Primitive Unit Cells and in the Conventional Non-primitive Unit Cells to which they Correspond

NOTE. See section 5.1 for systematic reduction of the general primitive unit cell to the corresponding conventional Bravais lattice unit cell, and for the complete list of 24 possible "reduced cells" defined there.
The symbol $\neq$ implies non-equality by reason of symmetry; accidental equality may, of course, occur.

Conventional unit cell (symmetry considered)	Primitive unit cell (symmetry ignored)
Triclinic $a\neq b\neq c$; $\alpha\neq\beta\neq\gamma$ (including all non-primitive unit cells)	*Triclinic* $a\neq b\neq c$; $\alpha\neq\beta\neq\gamma$ α,β,γ not satisfying any of the restrictive conditions given below, except in an accidental way.
Monoclinic 1st setting (z-axis unique) Lattice *A* or *B* $a\neq b\neq c$; $\alpha=\beta=90°\neq\gamma$ 2nd setting (y-axis unique) Lattice *A* or *C* $a\neq b\neq c$; $\alpha=\gamma=90°\neq\beta$ 1st or 2nd setting Lattice *I* or *F*	*Monoclinic* (1) $a\neq b\neq c$, $\alpha=90°\neq\beta\neq\gamma$: $\beta=\cos^{-1}\frac{c}{2a}$; $\gamma\neq\cos^{-1}\frac{b}{2a}$ (2) $a\neq b\neq c$, $\alpha\neq\beta\neq\gamma\neq 90°$: $\alpha\neq\cos^{-1}\frac{b^2+c^2-a^2}{2bc}$; $\beta=\cos^{-1}\frac{c^2+a^2-b^2}{2ca}$; $\gamma=\cos^{-1}\frac{a^2+b^2-c^2}{2ab}$ (3) $a=b\neq c$, $\alpha=\beta\neq\gamma\neq 90°$: $\alpha\neq\cos^{-1}\frac{c}{2a}\neq\cos^{-1}\left[\frac{a}{2c}(1+\cos\gamma)\right]$ etc.

TABLE 2.2.2 (*continued*)

Relationships between Axes and Angles in some Primitive Unit Cells and in the Conventional Non-primitive Unit Cells to which they Correspond

NOTE. See section 5.1 for systematic reduction of the general primitive unit cell to the corresponding conventional Bravais lattice unit cell, and for the complete list of 24 possible "reduced cells" defined there.
The symbol $\neq$ implies non-equality by reason of symmetry; accidental equality may, of course, occur.

Conventional unit cell (symmetry considered)	Primitive unit cell (symmetry ignored)
Orthorhombic	*Orthorhombic*
Lattice A or B or C $a \neq b \neq c$ $\alpha=\beta=\gamma=90°$	(1) $a \neq b \neq c$; $\alpha=\beta=90°$; $\gamma=\cos^{-1}\frac{a}{2b}$ (2) $a=b \neq c$; $\alpha=\beta=90° \neq \gamma \neq 120°$ etc.
Lattice I $a \neq b \neq c$ $\alpha=\beta=\gamma=90°$	(1) $a \neq b \neq c$; $4a^2 \neq 2b^2+c^2$ $\alpha=90°$; $\beta=\cos^{-1}\frac{c}{2a}$; $\gamma=\cos^{-1}\frac{b}{2a}$ (2) $a=b \neq c$; $\alpha=\beta \neq \gamma \neq 90°$; $\alpha=\cos^{-1}\frac{c}{2a}$ (3) $a=b=c$; $\alpha \neq \beta \neq \gamma$; $1+\cos\alpha=\cos\beta+\cos\gamma$ etc.
Lattice F $a \neq b \neq c$ $\alpha=\beta=\gamma=90°$	(1) $a \neq b \neq c$; $\alpha=\cos^{-1}\frac{b^2+c^2-a^2}{2bc}$ $\beta=\cos^{-1}\frac{c^2+a^2-b^2}{2ca}$ $\gamma=\cos^{-1}\frac{a^2+b^2-c^2}{2ab}$ (2) $a=b \neq c$; $\alpha=\beta \neq \gamma$; $\alpha=\cos^{-1}\left[\frac{a}{2c}(1+\cos\gamma)\right]$ etc.
Tetragonal	*Tetragonal*
Lattice I or F $a=b \neq c$ $\alpha=\beta=\gamma=90°$	(1) $a \neq b \neq c$; $4a^2=2b^2+c^2$ $\alpha=90°$; $\beta=\cos^{-1}\frac{c}{2a}$; $\gamma=\cos^{-1}\frac{b}{2a}$ (2) $a=b \neq c$; $\alpha=\beta=\cos^{-1}\frac{a}{2c}$; $\gamma=90°$ (3) $a=b=c$; $\alpha=\beta \neq \gamma$ etc.
Cubic	*Cubic*
$a=b=c$; $\alpha=\beta=\gamma=90°$	
Lattice I	(1) $a=b=c$; $\alpha=\beta=\gamma=\cos^{-1}(-\frac{1}{3})=109°\ 28'$; etc.
Lattice F	(1) $a=b=c$; $\alpha=\beta=\gamma=\cos^{-1}\frac{1}{2}=60°$; etc.

Note on Nomenclature

If any point of the lattice is taken as origin, the vectors corresponding to any other lattice point may be expressed as $u\mathbf{a}$, $v\mathbf{b}$, $w\mathbf{c}$, where u, v, and w are integers. The co-ordinates of the lattice point are then said to be u, v, w (no brackets).

The direction joining the origin to the points u, v, w; $2u, 2v, 2w$; . . . defines a row of points $[u\ v\ w]$ (square brackets); the same symbol stands for any line parallel to the given direction, since the lattice is infinite and the origin may be taken at any point. $[u\ v\ w]$ is the symbol for a single zone axis; a form of zone axes (directions related by symmetry) is denoted by the use of angular brackets $\langle u\ v\ w\rangle$.

Any position whatever in space may be given co-ordinates in terms of a lattice point taken as origin and the edges of the unit cell as axes. If the vectors corresponding to the required position are $(u+x)\mathbf{a}$, $(v+y)\mathbf{b}$, $(w+z)\mathbf{c}$, where u, v, w are integers and x, y, z are all less than unity, then the co-ordinates of the position are said to be x, y, z (no brackets).

The lattice may be intersected by sets of equally spaced parallel planes, in an infinite number of ways. If the plane in any set nearest to, but not passing through, the origin, intersects the unit-cell vectors at $\mathbf{a}/h$, $\mathbf{b}/k$, $\mathbf{c}/l$, then the set of planes is said to have the indices $(h\ k\ l)$ (in parentheses). The same symbol stands for the indices of a single crystal face parallel to the set of planes. A form of faces (or sets of planes, related by symmetry) is denoted by the use of braces $\{h\ k\ l\}$.

In the hexagonal lattice the equilateral nature of the nets perpendicular to the unique axis is often emphasised by the use of indices $(h\ k\ i\ l)$, where the three indices h, k and i refer to the directions x-, y- and u-, all at 120° to each other. In this case the relationship holds that $i=-(h+k)$.

2.3. Crystal Axes and Systems

The morphological study of crystals of different symmetry showed that they could be referred to seven different sets of crystallographic axes of reference, each set possessing characteristic symmetry. A more fundamental division, however, was that into 32 crystal classes, on the basis of point-group symmetry (see section 3). The grouping of the 32 point groups into the seven systems is shown in Table 2.3.1.

The 14 Bravais lattices may also be referred to the same seven systems (see Table 2.2.1) because the sets of axes of reference are simply the edges of the unit cells of the Bravais lattices.

The seven systems were originally taken as follows: Triclinic, Monoclinic, Orthorhombic, Tetragonal, Rhombohedral, Hexagonal and Cubic (or Isometric).

It had long been known, of course, that crystals belonging to the "Rhombohedral" system could be described equally well on hexagonal (Miller–Bravais) axes as on rhombohedral (Miller) axes. The later development of space-group theory, and then of X-ray diffraction methods of crystal structure investigation, showed that there was a complication in the case of crystals with 3-fold symmetry but lacking a symmetry plane normal to the 3-fold axis. The 230 space groups (see section 4) are obtained by adding the point-group symmetry, with possible translations, to appropriate lattices. Five point groups possess 3-fold symmetry but no perpendicular symmetry plane. A given crystal belonging to any one of the five crystal classes so defined might, it was discovered, have a space group based either on a primitive hexagonal lattice or on a primitive rhombohedral lattice. This is the basis of the use of alternative hexagonal or rhombohedral axes of reference for crystals belonging to these five classes (as in Tables 2.2.1 and 2.3.1). Consequently it is not possible to make an altogether satisfactory grouping of crystal classes into systems. The five classes mentioned above can be grouped as the Trigonal system; alternatively they can be grouped as a subdivision of the Hexagonal system. It is not satisfactory to call them Rhombohedral.

TABLE 2.3.1

Crystallographic Axial and Angular Relationships, and Characteristic Symmetry of the Crystal Systems

Point groups[1]	System	Axial and angular relationships[2]	Axial ratios and angles to be specified for each substance	Characteristic symmetry
1, $\bar{1}$	Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90°$	$a : b : c$ α, β, γ	1-fold (identity or inversion) symmetry only.
2, m, $2/m$	Monoclinic[3]	1st setting $a \neq b \neq c$ $\alpha = \beta = 90° \neq \gamma$ ——— 2nd setting $a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$	$a : b : c$ γ ——— $a : b : c$ β	2-fold axis (rotation or inversion) in one direction only, this being taken as the z-axis in the first setting and as the y-axis in the second setting.
222, $mm2$, mmm	Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	$a : b : c$	2-fold axes (rotation or inversion) in three mutually perpendicular directions.
4, $\bar{4}$, $4/m$, 422, $4mm$, $\bar{4}2m$, $4/mmm$	Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	$c : a$	4-fold axis (rotation or inversion) along the z-axis.
23, $m3$, 432, $\bar{4}3m$, $m3m$	Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90°$	None	Four 3-fold axes each inclined at 54° 44′ to the crystallographic axes.
3, $\bar{3}$, 32, $3m$, $\bar{3}m$	Trigonal (may be taken as subdivision of hexagonal)	(Rhombohedral axes) $a = b = c$ $\alpha = \beta = \gamma < 120° \neq 90°$ ——— (Hexagonal axes)[4] $a = b \neq c$ $\alpha = \beta = 90°, \gamma = 120°$	α ——— $c : a$	3-fold axis (rotation or inversion) along [111] using rhombohedral axes, or along the z-direction using hexagonal axes.
6, $\bar{6}$, $6/m$, 622, $6mm$, $\bar{6}m2$, $6/mmm$	Hexagonal	$a = b \neq c$ [4] $\alpha = \beta = 90°$ $\gamma = 120°$	$c : a$	6-fold axis (rotation or inversion) along the z-axis.

(1) For explanation of point-group symbols see section 3.1.
(2) The sign $\neq$ implies non-equality by reason of symmetry; accidental equality may, of course, occur.
(3) See Preface to Volume I for explanation of alternative settings.
(4) In drawing the hexagonal axes, it is customary to take three axes, x-, y- and u-, at 120° to each other, and normal to the z-axis.

2.4. The Reciprocal Lattice

To each direct (or real-space) lattice there is a corresponding lattice in "reciprocal" space, which has the same symmetry and can therefore be referred to the same type of co-ordinate axes of reference (system). Rows of points (zone axes) in the direct lattice are normal to nets (planes) of points in the reciprocal lattice, and vice versa. The repeat distance between successive points along a row in reciprocal space is inversely proportional to the interplanar spacing between nets of points in real space normal to the row of points in question, and vice versa. It should be noticed that the interplanar spacing is the perpendicular distance between successive planes (nets) of lattice points, and is not, in general, an actual distance between points, but that it reciprocates into a distance between points.

2.4. THE RECIPROCAL LATTICE

The lattice reciprocal to a given primitive direct lattice may be obtained by taking any point as origin and from it drawing normals to all sets of direct-lattice planes (hkl), (h, k, and l integral, but not necessarily prime to each other). Points are then placed along these normals at distances K/d_{hkl} from the origin, where K is a constant and d_{hkl} is the interplanar spacing of the planes (hkl). The array of points thus obtained forms a lattice as defined in section 2.2. Each reciprocal lattice point is denoted by the symbol hkl (without brackets) of the set of direct-lattice planes to which it is thus related, and h, k, l (always integral) are the co-ordinates of the lattice point in reciprocal space (Fig. 2.4.1, p. 14).

In applying reciprocal lattice methods in X-ray diffraction problems it is common to take the constant $K=\lambda$ (the wavelength used); in this case the distance of the reciprocal lattice point hkl from the origin, λ/d_{hkl}, is given in dimensionless units. Alternatively, K may be taken as unity. In all representations of the reciprocal lattice it is therefore necessary to give the value of K and also the scale on which the lattice is drawn. Scales such as 5 or 10 cm. to 1 unit (dimensionless, or Å^{-1}) are convenient in practice.

Table 2.4.1 gives the relationships between the unit-cell axes and angles in real space and in reciprocal space, for primitive unit cells only. The unit cell in the reciprocal lattice which corresponds to a primitive unit cell chosen in the direct lattice may be constructed as follows. Any lattice point is taken as origin and from this point normals are drawn to the axial planes (100), (010), (001) of the primitive direct-lattice unit cell. Along each of these normals a point is placed at distances from the origin respectively $a^*=K/d_{100}$, $b^*=K/d_{010}$, $c^*=K/d_{001}$. The three vectors, $\mathbf{a}^*$, $\mathbf{b}^*$ and $\mathbf{c}^*$, defined in this way are the edges or axes of the reciprocal-lattice unit cell (also primitive) which corresponds to the primitive direct-lattice unit cell originally chosen. The repetition of this unit cell produces the lattice which is reciprocal to the original direct lattice. The reversal of this procedure will give the direct lattice corresponding to the reciprocal lattice. Since a primitive unit cell can be outlined (in an infinite number of ways) in any direct lattice, the above procedure can always be used to find the direct lattice from the reciprocal lattice and vice versa. Use may be made here of Table 2.2.2.

If, however, the direct lattice is such that the conventional choice of unit cell is non-primitive, then the above procedure must not be applied without modification to the *conventional* unit cell in order to obtain the reciprocal lattice. The necessary modification required is shown in Table 2.4.2. It will be seen in this table that if the conventional unit cell in the direct lattice is non-primitive, then that in the reciprocal lattice will also be non-primitive, although not necessarily of the same kind.

Fig. 2.4.2 (p. 14) shows, two-dimensionally, the relationship between direct and reciprocal-lattice cells when both are primitive, and Fig. 2.4.3 shows the relationship (again two-dimensionally) in the case where the net is centred, the actual values of the direct unit-cell vectors $\mathbf{a}$ and $\mathbf{b}$ being the same in the two figures. The conventional unit cell in the reciprocal lattice is now centred also, and the lengths of its sides are $2a^*$, $2b^*$, its area being four times that of the primitive cell shown in Fig. 2.4.2.

TABLE 2.4.1

Relation between Axes and Angles of Direct-lattice and Reciprocal-lattice Primitive Unit Cells for the Various Systems

Symbols	
a, b, c	Lengths of edges of direct-lattice unit cell.
α, β, γ	Inter-axial angles of direct-lattice unit cell.
a^*, b^*, c^*	Lengths of edges of reciprocal-lattice unit cell.
α^*, β^*, γ^*	Inter-axial angles of reciprocal-lattice unit cell.
K	Reciprocal constant.
V; V^*	Volume of direct-lattice unit cell; of reciprocal-lattice unit cell.

TABLE 2.4.1 (*continued*)

For symbols see previous page.

Triclinic

$$a^*=\frac{Kbc\sin\alpha}{V};\quad b^*=\frac{Kca\sin\beta}{V};\quad c^*=\frac{Kab\sin\gamma}{V}$$

where $V=abc\{1+2\cos\alpha\cos\beta\cos\gamma-\cos^2\alpha-\cos^2\beta-\cos^2\gamma\}^{\frac{1}{2}}$

$=2\,abc\{\sin s.\ \sin(s-\alpha).\ \sin(s-\beta).\ \sin(s-\gamma)\}^{\frac{1}{2}};\quad V^*=\frac{1}{V}$

$2s=\alpha+\beta+\gamma$

$$\cos\alpha^*=\frac{\cos\beta\cos\gamma-\cos\alpha}{\sin\beta\sin\gamma};\quad \cos\beta^*=\frac{\cos\gamma\cos\alpha-\cos\beta}{\sin\gamma\sin\alpha};\quad \cos\gamma^*=\frac{\cos\alpha\cos\beta-\cos\gamma}{\sin\alpha\sin\beta}$$

Monoclinic

1st setting $\quad a^*=\frac{K}{a\sin\gamma};\ b^*=\frac{K}{b\sin\gamma};\ c^*=\frac{K}{c};\ \alpha^*=\beta^*=90°;\ \gamma^*=180°-\gamma$

2nd setting $\quad a^*=\frac{K}{a\sin\beta};\ b^*=\frac{K}{b};\ c^*=\frac{K}{c\sin\beta};\ \alpha^*=\gamma^*=90°;\ \beta^*=180°-\beta$

Orthorhombic	**Tetragonal**	**Cubic**
$a^*=\frac{K}{a};\ b^*=\frac{K}{b};\ c^*=\frac{K}{c}$	$a^*=b^*=\frac{K}{a};\ c^*=\frac{K}{c}$	$a^*=b^*=c^*=\frac{K}{a}$
$\alpha^*=\beta^*=\gamma^*=90°$	$\alpha^*=\beta^*=\gamma^*=90°$	$\alpha^*=\beta^*=\gamma^*=90°$

Hexagonal	**Rhombohedral**
$a^*=b^*=\frac{2K}{a\sqrt{3}};\ c^*=\frac{K}{c}$	$a^*=b^*=c^*=\frac{K.a^2\sin\alpha}{V}$ where $V=a^3[1-3\cos^2\alpha+2\cos^3\alpha]^{\frac{1}{2}}$
$\alpha^*=\beta^*=90°;\ \gamma^*=60°$	$\cos\alpha^*=\cos\beta^*=\cos\gamma^*=\frac{\cos^2\alpha-\cos\alpha}{\sin^2\alpha}=-\frac{\cos\alpha}{(1+\cos\alpha)}$

TABLE 2.4.2

Modification of Table 2.4.1 required to include Non-primitive Unit Cells

Direct lattice		Reciprocal lattice		
Unit cell edges	Type	Type	Unit cell edges	Volume
a, b, c	*P* and *R*	*P* and *R*	a^*, b^*, c^*	V^*
	A	*A*	$a^*, 2b^*, 2c^*$	$4V^*$
	B	*B*	$2a^*, b^*, 2c^*$	$4V^*$
	C	*C*	$2a^*, 2b^*, c^*$	$4V^*$
	I	*F*	$2a^*, 2b^*, 2c^*$	$8V^*$
	F	*I*	$2a^*, 2b^*, 2c^*$	$8V^*$

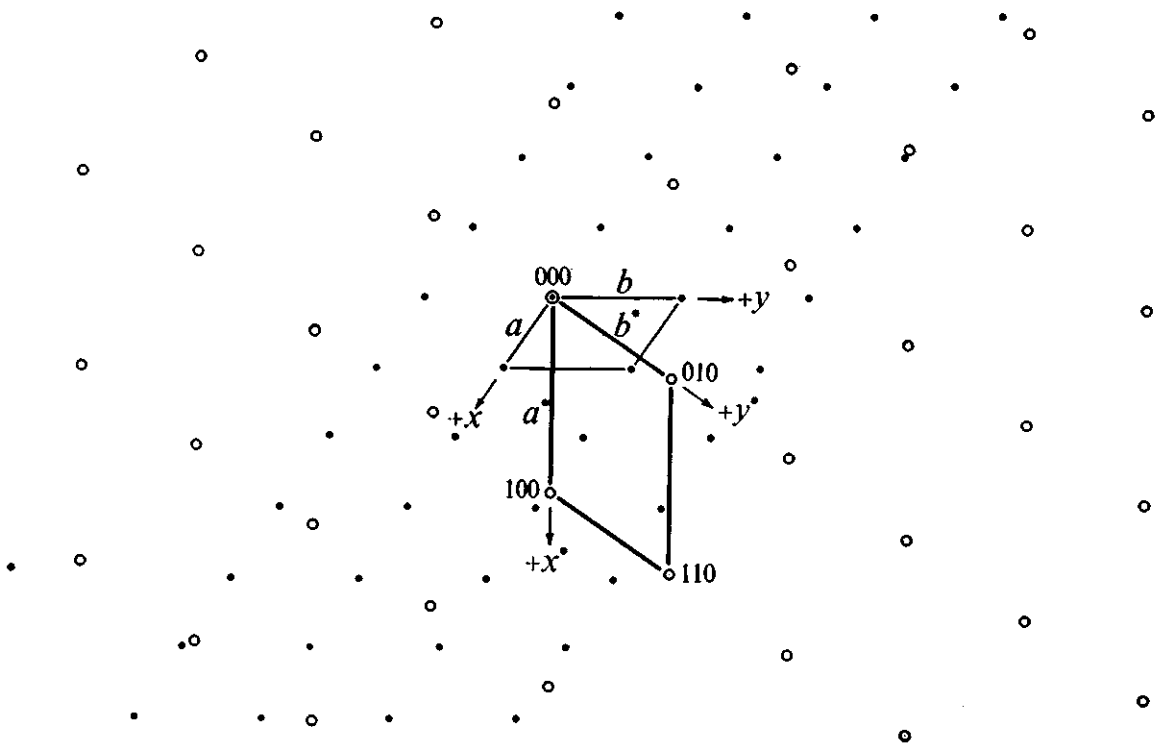


Fig. 2.4.1.
Oblique direct lattice and the reciprocal lattice.

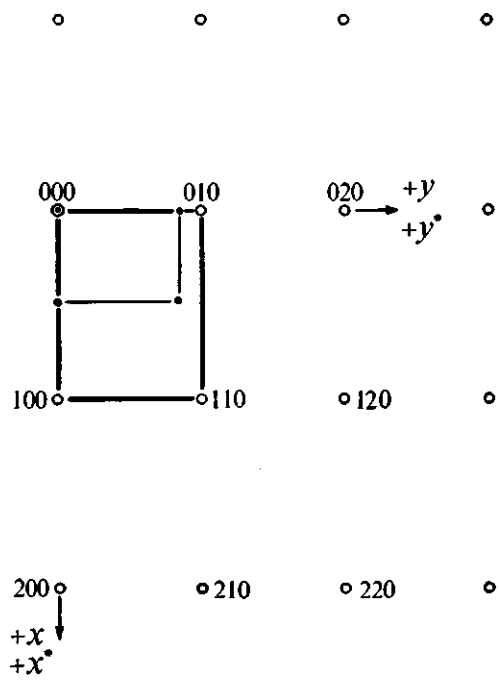


Fig. 2.4.2.
Primitive rectangular direct lattice and the reciprocal lattice.

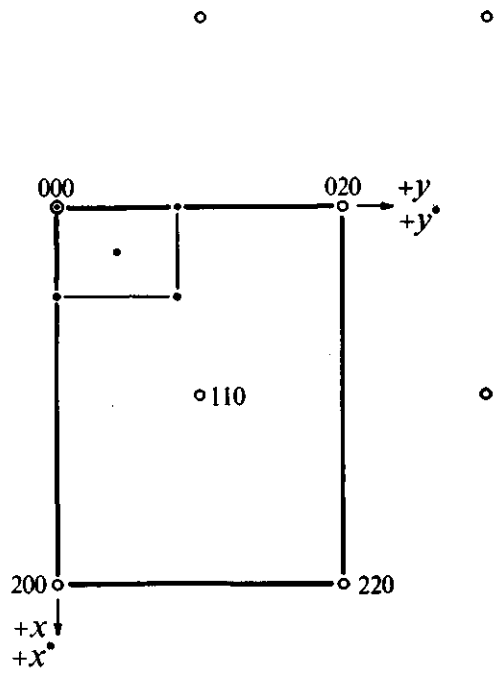


Fig. 2.4.3.
Centred rectangular direct lattice and the reciprocal lattice.

2.5. Unit-cell Transformations

In the study of crystals different choices of unit cell are often made, and it is necessary to be able to transform data relative to one unit cell into data relative to another. Even where the choice of unit cell is fixed by convention it is often useful to be able to transform to another choice of unit cell (possibly from a primitive into a non-primitive, or vice versa) in order to make comparison with other crystals. Thus we may wish to transform

Direct-lattice unit-cell vectors.
Indices of faces or sets of parallel planes.
Reciprocal-lattice unit-cell vectors.
Zone-axis symbols.
Co-ordinates of positions in the unit cell.

The co-ordinates of positions in the unit cell transform like zone-axis symbols, and the transformations of these co-ordinates, including those consequent simply upon change of origin, are studied further in section 4.9. Change of space-group symbol consequent upon change of unit cell is studied in section 6.

If we have two choices of unit cell in a direct lattice with vectors respectively $\mathbf{a}_1$, $\mathbf{b}_1$, $\mathbf{c}_1$ and $\mathbf{a}_2$, $\mathbf{b}_2$, $\mathbf{c}_2$, we can write down the unit vectors of the second set in terms of the first set, and vice versa:

$$\begin{aligned} \mathbf{a}_2&=s_{11}\mathbf{a}_1+s_{12}\mathbf{b}_1+s_{13}\mathbf{c}_1 \\ \mathbf{b}_2&=s_{21}\mathbf{a}_1+s_{22}\mathbf{b}_1+s_{23}\mathbf{c}_1 \\ \mathbf{c}_2&=s_{31}\mathbf{a}_1+s_{32}\mathbf{b}_1+s_{33}\mathbf{c}_1 \end{aligned} \quad \text{and} \quad \begin{aligned} \mathbf{a}_1&=t_{11}\mathbf{a}_2+t_{12}\mathbf{b}_2+t_{13}\mathbf{c}_2 \\ \mathbf{b}_1&=t_{21}\mathbf{a}_2+t_{22}\mathbf{b}_2+t_{23}\mathbf{c}_2 \\ \mathbf{c}_1&=t_{31}\mathbf{a}_2+t_{32}\mathbf{b}_2+t_{33}\mathbf{c}_2 \end{aligned} \qquad \ldots\ldots 2.5.1$$

The coefficients s_{ik} and t_{ik} ($i=1, 2, 3$; $k=1, 2, 3$) are second-order tensors related as follows:

$$s_{1i}t_{k1}+s_{2i}t_{k2}+s_{3i}t_{k3}=0 \text{ (if } i\neq k) \text{ or } 1 \text{ (if } i=k)$$
$$s_{i1}t_{1k}+s_{i2}t_{2k}+s_{i3}t_{3k}=0 \text{ (if } i\neq k) \text{ or } 1 \text{ (if } i=k)$$

Similar transformation equations to those given above apply also, just as they stand, to the indices of planes or faces:

$$\begin{aligned} h_2&=s_{11}h_1+s_{12}k_1+s_{13}l_1 \\ k_2&=s_{21}h_1+s_{22}k_1+s_{23}l_1 \\ l_2&=s_{31}h_1+s_{32}k_1+s_{33}l_1 \end{aligned} \quad \text{and} \quad \begin{aligned} h_1&=t_{11}h_2+t_{12}k_2+t_{13}l_2 \\ k_1&=t_{21}h_2+t_{22}k_2+t_{23}l_2 \\ l_1&=t_{31}h_2+t_{32}k_2+t_{33}l_2 \end{aligned} \qquad \ldots\ldots 2.5.2$$

In order to transform reciprocal-lattice vectors (and zone-axis symbols or co-ordinates of positions in the unit cell) the related set of equations given below must be used:

$$\begin{aligned} \mathbf{a}_2^*&=t_{11}\mathbf{a}_1^*+t_{21}\mathbf{b}_1^*+t_{31}\mathbf{c}_1^* \\ \mathbf{b}_2^*&=t_{12}\mathbf{a}_1^*+t_{22}\mathbf{b}_1^*+t_{32}\mathbf{c}_1^* \\ \mathbf{c}_2^*&=t_{13}\mathbf{a}_1^*+t_{23}\mathbf{b}_1^*+t_{33}\mathbf{c}_1^* \end{aligned} \quad \text{and} \quad \begin{aligned} \mathbf{a}_1^*&=s_{11}\mathbf{a}_2^*+s_{21}\mathbf{b}_2^*+s_{31}\mathbf{c}_2^* \\ \mathbf{b}_1^*&=s_{12}\mathbf{a}_2^*+s_{22}\mathbf{b}_2^*+s_{32}\mathbf{c}_2^* \\ \mathbf{c}_1^*&=s_{13}\mathbf{a}_2^*+s_{23}\mathbf{b}_2^*+s_{33}\mathbf{c}_2^* \end{aligned} \qquad \ldots\ldots 2.5.3$$

It will be noted that not only are the coefficients interchanged as a whole, but the rows and columns of coefficients are interchanged separately within each set of equations.

For convenience the actual vectors or indices being transformed are not repeated in practice; it is sufficient to write the coefficients in the form of a square matrix. The symbol 2→1 means the expression for vectors or indices of the second unit cell *in terms of* those of the first unit cell, and vice versa for the symbol 1→2.

$$\begin{array}{c|ccc|} & & \longrightarrow 1 & \\ \hline 2 & s_{11} & s_{12} & s_{13} \\ & s_{21} & s_{22} & s_{23} \\ & s_{31} & s_{32} & s_{33} \\ \hline \end{array} \quad \text{and} \quad \begin{array}{c|ccc|} & & \longrightarrow 2 & \\ \hline 1 & t_{11} & t_{12} & t_{13} \\ & t_{21} & t_{22} & t_{23} \\ & t_{31} & t_{32} & t_{33} \\ \hline \end{array}$$

In printing, these are often arranged for convenience as follows:

$$s_{11}\ s_{12}\ s_{13}/s_{21}\ s_{22}\ s_{23}/s_{31}\ s_{32}\ s_{33} \quad \text{and} \quad t_{11}\ t_{12}\ t_{13}/t_{21}\ t_{22}\ t_{23}/t_{31}\ t_{32}\ t_{33}$$

A single layout of transformation coefficients can be used both for axes and plane indices in the direct lattice and for reciprocal-lattice axes, zone-axis symbols and co-ordinates, if the following arrangement is used:

I

$$\begin{array}{ccccc|ccc}
 & & & & & x_1 & y_1 & z_1 \\
 & & & & & u_1 & v_1 & w_1 \\
 & & & & & \mathbf{a}_1^* & \mathbf{b}_1^* & \mathbf{c}_1^* \\
 & & & & & h_1 & k_1 & l_1 \\
 & & & & & \mathbf{a}_1 & \mathbf{b}_1 & \mathbf{c}_1 \\
\hline
x_2 & u_2 & \mathbf{a}_2^* & h_2 & \mathbf{a}_2 & s_{11} & s_{12} & s_{13} \\
y_2 & v_2 & \mathbf{b}_2^* & k_2 & \mathbf{b}_2 & s_{21} & s_{22} & s_{23} \\
z_2 & w_2 & \mathbf{c}_2^* & l_2 & \mathbf{c}_2 & s_{31} & s_{32} & s_{33}
\end{array}$$

and

II

$$\begin{array}{ccccc|ccc}
 & & & & & x_2 & y_2 & z_2 \\
 & & & & & u_2 & v_2 & w_2 \\
 & & & & & \mathbf{a}_2^* & \mathbf{b}_2^* & \mathbf{c}_2^* \\
 & & & & & h_2 & k_2 & l_2 \\
 & & & & & \mathbf{a}_2 & \mathbf{b}_2 & \mathbf{c}_2 \\
\hline
x_1 & u_1 & \mathbf{a}_1^* & h_1 & \mathbf{a}_1 & t_{11} & t_{12} & t_{13} \\
y_1 & v_1 & \mathbf{b}_1^* & k_1 & \mathbf{b}_1 & t_{21} & t_{22} & t_{23} \\
z_1 & w_1 & \mathbf{c}_1^* & l_1 & \mathbf{c}_1 & t_{31} & t_{32} & t_{33}
\end{array}$$

Matrix I gives the **a**, **b**, **c** or h, k, l transformation 2→1, and matrix II gives the **a**, **b**, **c** or h, k, l transformation 1→2, when read *from left to right* (denoted by the arrow ⌐→) in each case (see equations 2.5.1 and 2.5.2). Matrix I gives the $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ or u, v, w or x, y, z transformation 1→2, and matrix II gives the corresponding 2→1 transformations, when read *from top to bottom* (denoted by the arrow ↓⌐) in each case (compare equations 2.5.3).

The symmetrical form of these matrixes provides a useful mnemonic rule.

The generalised expression for the direct-lattice axes transformation is taken as $\mathbf{a}_i' = s_{ik}\mathbf{a}_k$ and for the reciprocal-lattice axes transformation as $\mathbf{a}_i^* = s_{ki}\mathbf{a}_k'^*$ where the primed symbols represent the second choice of unit cell.

Table 2.5.1 (p. 21) gives some transformation matrices which may be useful, but it is important to realise that (compare Table 2.2.2) there are other ways of choosing a primitive cell (or a body-centred cell) in a face-centred lattice, and vice versa, if symmetry is ignored, and that therefore the matrices given as applying to "all systems" are not unique.

Examples

1. In Fig. 2.5.1 two unit cells are shown with a common z-axis (this is merely in order to simplify the figure). We express the unit axes of the second unit cell vectorially in terms of those of the first, and vice versa, as follows:

$$\begin{aligned}
\mathbf{a}_2 &= +1\mathbf{a}_1 + 2\mathbf{b}_1 + 0 \\
\mathbf{b}_2 &= -2\mathbf{a}_1 - 1\mathbf{b}_1 + 0 \\
\mathbf{c}_2 &= +0 \quad +0 \quad +1\mathbf{c}_1
\end{aligned}
\qquad \text{and} \qquad
\begin{aligned}
\mathbf{a}_1 &= -\tfrac{1}{3}\mathbf{a}_2 - \tfrac{2}{3}\mathbf{b}_2 + 0 \\
\mathbf{b}_1 &= +\tfrac{2}{3}\mathbf{a}_2 + \tfrac{1}{3}\mathbf{b}_2 + 0 \\
\mathbf{c}_1 &= +0 \quad +0 \quad +1\mathbf{c}_2
\end{aligned}$$

or in matrix form:

I

$$\begin{array}{c|ccc|}
 & & \longrightarrow 1 & \\
\hline
2 & 1 & 2 & 0 \\
 & \bar{2} & \bar{1} & 0 \\
 & 0 & 0 & 1 \\
\hline
\end{array}$$

and

II

$$\begin{array}{c|ccc|}
 & & \longrightarrow 2 & \\
\hline
1 & \bar{\tfrac{1}{3}} & \bar{\tfrac{2}{3}} & 0 \\
 & \tfrac{2}{3} & \tfrac{1}{3} & 0 \\
 & 0 & 0 & 1 \\
\hline
\end{array}$$

Taking the indices (210) of the plane MN (Fig. 2.5.1) relative to the first unit cell and operating the matrix 2→1 on it, we get the indices of MN relative to the second unit cell from matrix I:

$$\left.\begin{aligned}
1\times2+2\times1+0\times0&=4 \\
\bar{2}\times2+\bar{1}\times1+0\times0&=\bar{5} \\
0\times2+0\times1+1\times0&=0
\end{aligned}\right\} \quad \ldots \quad (4\bar{5}0)$$

Transforming back by operating the matrix 1→2 on the indices $(4\bar{5}0)$ we get from matrix II:

$$\left.\begin{array}{l}\bar{\tfrac{1}{3}}\times 4+\bar{\tfrac{2}{3}}\times\bar{5}+0\times 0=2\\ \tfrac{2}{3}\times 4+\tfrac{1}{3}\times\bar{5}+0\times 0=1\\ 0\times 4+0\times 5+1\times 0=0\end{array}\right\}\quad\ldots\ (210)$$

In order to transform reciprocal-lattice axes, zone-axis symbols or co-ordinates, however, we use the matrices in reverse order and read from top to bottom:

II

$$\begin{array}{c|ccc|}\hline & & 2 & \\ \hline \downarrow & \bar{\tfrac{1}{3}} & \bar{\tfrac{2}{3}} & 0\\ 1 & \tfrac{2}{3} & \tfrac{1}{3} & 0\\ & 0 & 0 & 1\\ \hline\end{array}$$

I

$$\begin{array}{c|ccc|}\hline & & 1 & \\ \hline \downarrow & 1 & 2 & 0\\ 2 & \bar{2} & \bar{1} & 0\\ & 0 & 0 & 1\\ \hline\end{array}$$

For example, in Fig. 2.5.1 the direction OP has indices $[\tfrac{3}{2},2,0]$ on the first set of axes; the transformation by the reciprocal matrix gives:

$$\left.\begin{array}{l}\bar{\tfrac{1}{3}}\times\tfrac{3}{2}+\tfrac{2}{3}\times 2+0\times 0=\tfrac{5}{6}\\ \bar{\tfrac{2}{3}}\times\tfrac{3}{2}+\tfrac{1}{3}\times 2+0\times 0=-\tfrac{1}{3}\\ 0\times\tfrac{3}{2}+0\times 2+0\times 1=0\end{array}\right\}\quad\ldots\ [\tfrac{5}{6},\bar{\tfrac{1}{3}},0]$$

and it can be seen from the figure that $[\tfrac{5}{6},\bar{\tfrac{1}{3}},0]$ are the indices of the direction OP expressed in terms of the second set of axes.

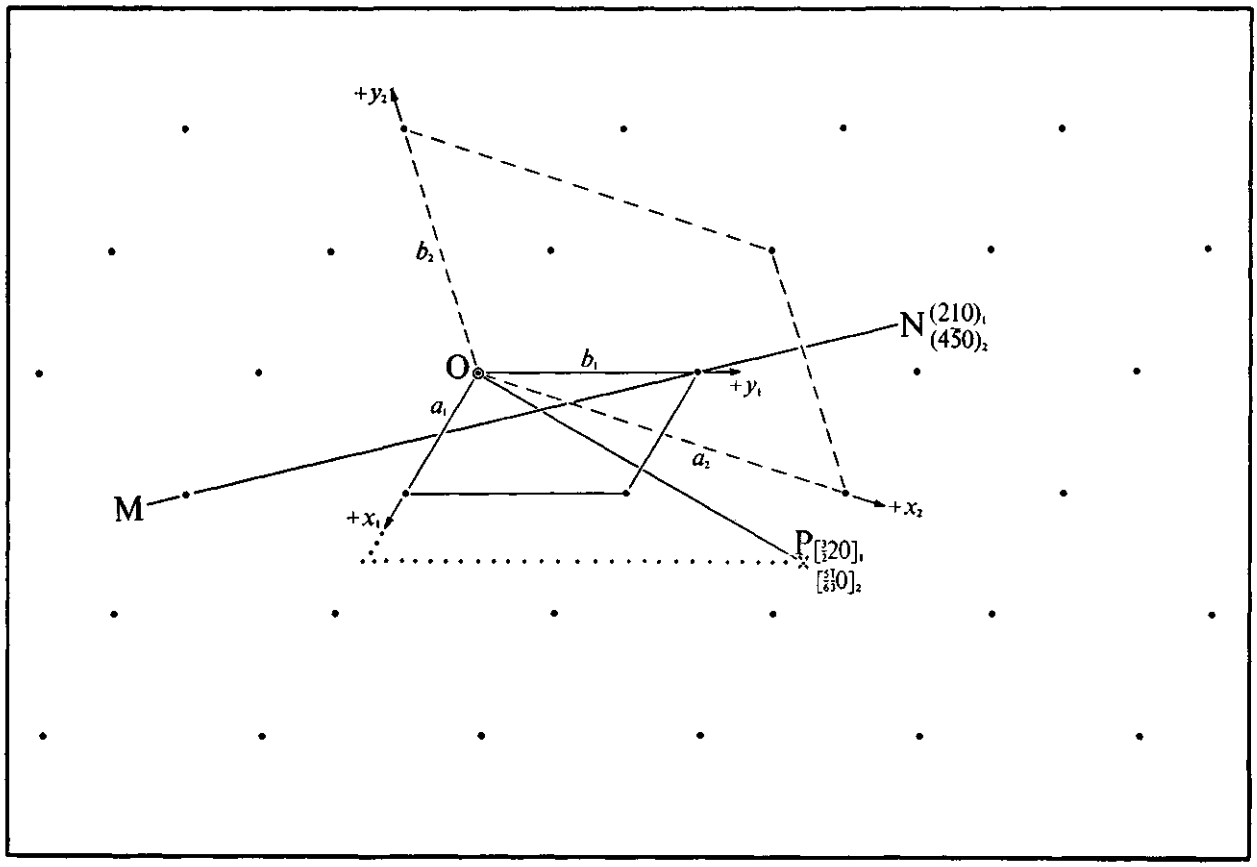


Fig. 2.5.1. Diagram to illustrate unit-cell transformation

c

2. When hexagonal axes are used, whether in the hexagonal lattice or in the rhombohedral lattice, it is usual to select the smallest unit cell, although in the rhombohedral lattice the smallest hexagonal unit cell will be non-primitive, with lattice points at 0,0,0; $\frac{2}{3},\frac{1}{3},\frac{1}{3}$; $\frac{1}{3},\frac{2}{3},\frac{2}{3}$. If the specimen possesses faces and has been set previously from morphological study, the setting thus chosen may not correspond to the choice of the smallest hexagonal unit cell. In classes 3 and $\bar{3}$ the morphologist has to make an arbitrary choice of directions normal to the z-axis as the x-, y- and u-axes. In class 32 he selects the diad rotation axes and in $3m$ and $\bar{3}m$ the normals to the reflection planes (the diad inversion axes) as the x-, y- and u-axes. In some of the space groups belonging to these classes (e.g. $P31m$, $P312$, $P\bar{3}1c$, etc.) the unit cell corresponding to this conventional choice of axes will not be the smallest hexagonal cell, but will be one of three times the volume (see Fig. 2.5.2*a*, and note the choice of three such cells). This kind of unit cell, which has the same z-axis as the smallest unit cell P, was called H in the 1935 *International Tables*. The matrices for the transformation $P \rightleftarrows H$ (H to P and vice versa) are shown in Table 2.5.1 for the three alternative cases.

For H_1, we have
$$\left.\begin{aligned} h_{H1} &= h_P - k_P \\ k_{H1} &= h_P + 2k_P \\ l_{H1} &= l_P \end{aligned}\right\} \text{and } (h-k)_{H1} = -3k_P = 3n, \text{ since } k \text{ is integral.}$$

As will be seen from Table 4.1.8, this is the condition for reflection in a non-primitive hexagonal cell with points at

$$0,0,0;\ \tfrac{1}{3},\tfrac{2}{3},0;\ \tfrac{2}{3},\tfrac{1}{3},0.$$

If the lattice is really rhombohedral, then the choice of axes corresponding to the H_1 hexagonal unit cell will give points at

$$\begin{array}{lll} 0,0,0; & \tfrac{1}{3},\tfrac{2}{3},0; & \tfrac{2}{3},\tfrac{1}{3},0; \\ 0,\tfrac{1}{3},\tfrac{2}{3}; & \tfrac{1}{3},0,\tfrac{2}{3}; & \tfrac{2}{3},\tfrac{2}{3},\tfrac{2}{3}; \\ \tfrac{1}{3},\tfrac{1}{3},\tfrac{1}{3}; & \tfrac{2}{3},0,\tfrac{1}{3}; & 0,\tfrac{2}{3},\tfrac{1}{3}. \end{array}$$

For some purposes it is convenient to use orthogonal axes for the hexagonal lattice, and Fig. 2.5.2*b* shows how this can be done in three ways also, the unit cell in this case having a volume twice that of the primitive cell. The corresponding matrices are listed in Table 2.5.1.

3. As another example we may take the relations between the primitive rhombohedral unit cell (in the obverse position; see Fig. 2.5.3, p. 20) in the rhombohedral lattice, and the triple hexagonal unit cell which corresponds to it. From Fig. 2.5.3 we can derive the vectorial relationships between the direct-lattice vectors, and form the transformation matrices shown in Table 2.5.1 (p. 21).

Thus we have, for example

$$\begin{aligned} h_{\mathrm{hex}} &= \mathrm{h}_{\mathrm{obv}} - \mathrm{k}_{\mathrm{obv}} \\ k_{\mathrm{hex}} &= \phantom{\mathrm{h}_{\mathrm{obv}}} - \mathrm{k}_{\mathrm{obv}} - \mathrm{l}_{\mathrm{obv}} \\ l_{\mathrm{hex}} &= \mathrm{h}_{\mathrm{obv}} + \mathrm{k}_{\mathrm{obv}} + \mathrm{l}_{\mathrm{obv}} \end{aligned}$$

and it will be noted that $(-h+k+l)_{\mathrm{hex}} = 3\mathrm{k}_{\mathrm{obv}}$. Since k is necessarily an integer, this means that the condition for reflection in the hexagonal setting which corresponds to the obverse rhombohedron is $-h+k+l=3n$ (see section 4.3 and Table 4.1.8).

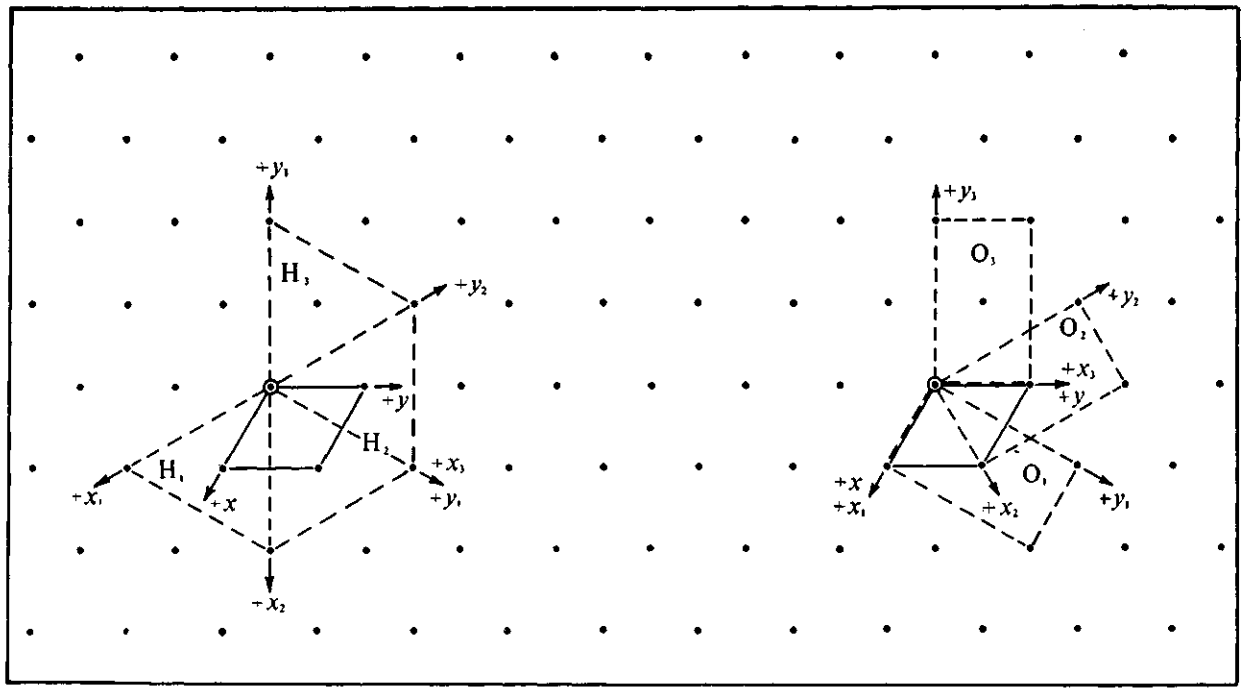


Fig. 2.5.2. Hexagonal lattice, showing (*a*) the three H unit cells and (*b*) the three O (orthohexagonal) unit cells

Volume Relationships

The ratio of the volumes V of unit cell 1 and unit cell 2 can be obtained by evaluation of the modulus of the appropriate determinant:

$$V_1 : V_2 = 1 : \begin{vmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \end{vmatrix} = \begin{vmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{vmatrix} : 1$$

Thus in example 1:

$$V_1 : V_2 = 1 : [1(\bar{1} \times 1) + 2(-\bar{2} \times 1) + 0] = 1 : 3$$

so that $V_2 = 3V_1$

In example 3 of the rh$\rightleftarrows$hex transformation:

$$V_{\text{hex}} : V_{\text{rh}} = [1(1+1)+1] : 1 = 3 : 1$$

$$V_{\text{hex}} = 3V_{\text{rh}}$$

The modulus, when evaluated, should never give a negative result, as this would indicate the choice of a left-handed set of axes in one of the unit cells, and this is contrary to convention.

Sometimes in tables the transformation of a unit cell into itself is given; this is called the identity transformation and is easily recognised.

$$\begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix}$$

NOTE. Rhombohedral axes can be orientated in two ways relative to the corresponding hexagonal axes. Different terms have been used to define these two orientations, but the terms used in the present tables are "obverse" and "reverse." These terms are defined by the appropriate transformation matrices given in Table 2.5.1 under the heading Rhombohedral, and by the diagrams of Fig. 2.5.3. Other terms such as "positive" or "direct" have been used for the orientation here called "obverse", with "negative" or "inverse" used for the orientation here called "reverse". In section 4, the obverse orientation is adopted as standard.

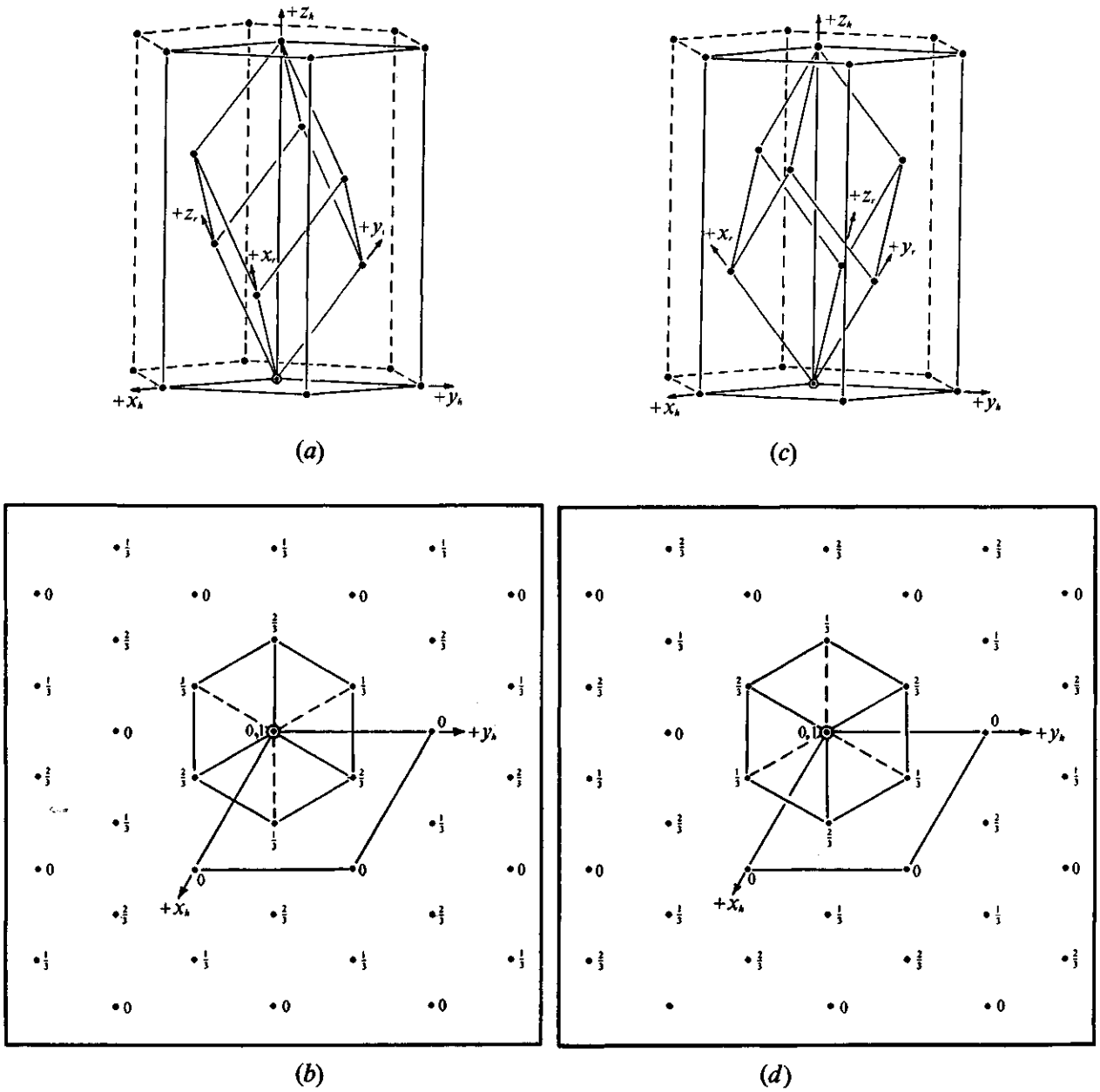


Fig. 2.5.3. Unit cells in the rhombohedral lattice

(*a*) Obverse setting of rhombohedron and corresponding hexagonal non-primitive unit cell, R_{obv} and R_{hex}.
(*b*) Plan of obverse setting (– – – – – lower edges, ——— upper edges of rhombohedron).
(*c*) Reverse setting of rhombohedron and corresponding hexagonal non-primitive unit cell, R_{rev} and R_{hex}.
(*d*) Plan of reverse setting (– – – – – lower edges, ——— upper edges of rhombohedron).

TABLE 2.5.1

Table of Selected Transformation Matrices

All lattices

$$\begin{array}{c|c} & I \\ \hline P & \begin{matrix} \bar{\tfrac{1}{2}} & \tfrac{1}{2} & \tfrac{1}{2} \\ \tfrac{1}{2} & \bar{\tfrac{1}{2}} & \tfrac{1}{2} \\ \tfrac{1}{2} & \tfrac{1}{2} & \bar{\tfrac{1}{2}} \end{matrix} \end{array} \qquad \begin{array}{c|c} & P \\ \hline I & \begin{matrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{matrix} \end{array}$$

$$\begin{array}{c|c} & F \\ \hline P & \begin{matrix} 0 & \tfrac{1}{2} & \tfrac{1}{2} \\ \tfrac{1}{2} & 0 & \tfrac{1}{2} \\ \tfrac{1}{2} & \tfrac{1}{2} & 0 \end{matrix} \end{array} \qquad \begin{array}{c|c} & P \\ \hline F & \begin{matrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{matrix} \end{array}$$

$$\begin{array}{c|c} & F \\ \hline I & \begin{matrix} \tfrac{1}{2} & \bar{\tfrac{1}{2}} & 0 \\ \tfrac{1}{2} & \tfrac{1}{2} & 0 \\ 0 & 0 & 1 \end{matrix} \end{array} \qquad \begin{array}{c|c} & I \\ \hline F & \begin{matrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{matrix} \end{array}$$

Monoclinic (1st and 2nd settings)

$$\begin{array}{c|c} & P_2 \\ \hline P_1 & \begin{matrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{matrix} \end{array} \qquad \begin{array}{c|c} & P_1 \\ \hline P_2 & \begin{matrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{matrix} \end{array}$$

Rhombohedral (Fig. 2.5.3)

$$\begin{array}{c|c} & R_{\text{hex}} \\ \hline R_{\text{obv}} & \begin{matrix} \tfrac{2}{3} & \tfrac{1}{3} & \tfrac{1}{3} \\ \bar{\tfrac{1}{3}} & \tfrac{1}{3} & \tfrac{1}{3} \\ \bar{\tfrac{1}{3}} & \bar{\tfrac{2}{3}} & \tfrac{1}{3} \end{matrix} \end{array} \qquad \begin{array}{c|c} & R_{\text{obv}} \\ \hline R_{\text{hex}} & \begin{matrix} 1 & \bar{1} & 0 \\ 0 & 1 & \bar{1} \\ 1 & 1 & 1 \end{matrix} \end{array}$$

$$\begin{array}{c|c} & R_{\text{hex}} \\ \hline R_{\text{rev}} & \begin{matrix} \tfrac{1}{3} & \bar{\tfrac{1}{3}} & \tfrac{1}{3} \\ \tfrac{1}{3} & \tfrac{2}{3} & \tfrac{1}{3} \\ \bar{\tfrac{2}{3}} & \bar{\tfrac{1}{3}} & \tfrac{1}{3} \end{matrix} \end{array} \qquad \begin{array}{c|c} & R_{\text{rev}} \\ \hline R_{\text{hex}} & \begin{matrix} 1 & 0 & \bar{1} \\ \bar{1} & 1 & 0 \\ 1 & 1 & 1 \end{matrix} \end{array}$$

Hexagonal (Fig. 2.5.2*a*)

$$\begin{array}{c|c} & P \\ \hline H_1 & \begin{matrix} 1 & \bar{1} & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 1 \end{matrix} \end{array} \qquad \begin{array}{c|c} & H_1 \\ \hline P & \begin{matrix} \tfrac{2}{3} & \tfrac{1}{3} & 0 \\ \bar{\tfrac{1}{3}} & \tfrac{1}{3} & 0 \\ 0 & 0 & 1 \end{matrix} \end{array}$$

$$\begin{array}{c|c} & P \\ \hline H_2 & \begin{matrix} 2 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{matrix} \end{array} \qquad \begin{array}{c|c} & H_2 \\ \hline P & \begin{matrix} \tfrac{1}{3} & \bar{\tfrac{1}{3}} & 0 \\ \tfrac{1}{3} & \tfrac{2}{3} & 0 \\ 0 & 0 & 1 \end{matrix} \end{array}$$

$$\begin{array}{c|c} & P \\ \hline H_3 & \begin{matrix} 1 & 2 & 0 \\ \bar{2} & \bar{1} & 0 \\ 0 & 0 & 1 \end{matrix} \end{array} \qquad \begin{array}{c|c} & H_3 \\ \hline P & \begin{matrix} \bar{\tfrac{1}{3}} & \bar{\tfrac{2}{3}} & 0 \\ \tfrac{2}{3} & \tfrac{1}{3} & 0 \\ 0 & 0 & 1 \end{matrix} \end{array}$$

Hexagonal (Fig. 2.5.2*b*)

$$\begin{array}{c|c} & P \\ \hline O_1 & \begin{matrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 1 \end{matrix} \end{array} \qquad \begin{array}{c|c} & O_1 \\ \hline P & \begin{matrix} 1 & 0 & 0 \\ \bar{\tfrac{1}{2}} & \tfrac{1}{2} & 0 \\ 0 & 0 & 1 \end{matrix} \end{array}$$

$$\begin{array}{c|c} & P \\ \hline O_2 & \begin{matrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{matrix} \end{array} \qquad \begin{array}{c|c} & O_2 \\ \hline P & \begin{matrix} \tfrac{1}{2} & \bar{\tfrac{1}{2}} & 0 \\ \tfrac{1}{2} & \tfrac{1}{2} & 0 \\ 0 & 0 & 1 \end{matrix} \end{array}$$

$$\begin{array}{c|c} & P \\ \hline O_3 & \begin{matrix} 0 & 1 & 0 \\ \bar{2} & \bar{1} & 0 \\ 0 & 0 & 1 \end{matrix} \end{array} \qquad \begin{array}{c|c} & O_3 \\ \hline P & \begin{matrix} \bar{\tfrac{1}{2}} & \bar{\tfrac{1}{2}} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{matrix} \end{array}$$

3. POINT-GROUP (CRYSTAL-CLASS) SYMMETRY

3.1. Operations of Point-group Symmetry

A point group is a group of symmetry operations all of which leave one point unmoved, translation operations thus being excluded. In one dimension there can only be "reflection" across the point. In two dimensions there can be "rotation" about a point and also the more limited operation of reflection across a line. In three dimensions there can be "inversion" about a point, rotation about a line and reflection across a plane. These possible types of point-group symmetry are summarised in Table 3.1.1.

TABLE 3.1.1

Types of Point-group Symmetry

One-dimensional	Two-dimensional	Three-dimensional
Reflection (point)	Rotation (point) Reflection (line)	Inversion (point) Rotation (line) Reflection (plane)

Increasing freedom of symmetry operation ↑	INVERSION ROTATION REFLECTION	POINT LINE PLANE	↓	Increasing geometric extension

The concept of a point group is convenient for the analysis of the symmetry of a finite body. If we confine ourselves to the crystallographic point groups, we have the limitation that only those symmetry elements are permitted which can operate on lattices, that is, which can give rise to parallelepipeds which can be stacked together in the same orientation to fill space (see section 2.2). This condition limits us to axes of 1-, 2-, 3-, 4- and 6-fold rotation symmetry, with or without inversion in the three-dimensional case.

In two dimensions inversion reduces to rotation, but in three dimensions, interaction between the three types of possible operation listed in Table 3.1.1 may give rotatory-inversion or rotatory-reflection axes of symmetry. The rotatory-inversion operation consists of rotation through $2\pi/X$ (where $X=1, 2, 3, 4$ or 6 in crystallographic operations) about a line (the symmetry axis) combined with inversion about a definite point on that line. The rotatory-reflection operation combines rotation about a line with reflection across a plane normal to the line. Rotatory-reflection axes (alternating axes) were formerly used in crystallographic work, but have now been superseded in use by the rotatory-inversion axes (usually called simply "inversion axes").

Table 3.1.2 gives the symmetry operators used in systematic crystallography. The equivalence of certain operators are shown in the table and in the notes attached to it. The table also shows that symmetry operators in three dimensions can be divided into two kinds. Operators of the first kind (rotation axes) do not involve a change of hand; that is, they do not change a right- into a left-hand. Those of the second kind (inversion axes; among which are included the mirror plane and the centre of symmetry) do make a change of hand. Two crystals whose structural arrangement, morphology or optical activity show that they are identical except for being respectively right- and left-handed are said to be "enantiomorphous" to each other. Such crystals must have point-group symmetry which lacks any operation of the second kind.

TABLE 3.1.2

Symmetry Operators of Point Groups

Kind of operation	Nature of operation		Symmetry operator		Written symbols	Graphical symbols
	Two-dimensional					
First kind[1]	The original direction is repeated by being turned through the given angle until the original is again reached	$\frac{2\pi}{1}$	1-fold (monad)	Rotation points[2]	1	None
		$\frac{2\pi}{2}$	2-fold (diad)		2	⬮
		$\frac{2\pi}{3}$	3-fold (triad)		3	▲
		$\frac{2\pi}{4}$	4-fold (tetrad)		4	◆
		$\frac{2\pi}{6}$	6-fold (hexad)		6	⬢
Second kind	Reflection across the line		Mirror line[3]		m	—
	Three-dimensional					
First kind	The original direction is repeated by being turned through the given angle until the original is again reached	$\frac{2\pi}{1}$	1-fold (monad)	Rotation axes	1	None
		$\frac{2\pi}{2}$	2-fold (diad)		2	⬮
		$\frac{2\pi}{3}$	3-fold (triad)		3	▲
		$\frac{2\pi}{4}$	4-fold (tetrad)		4	◆
		$\frac{2\pi}{6}$	6-fold (hexad)		6	⬢
Second kind	The original direction is turned through the given angle and is then inverted through the point; this procedure is repeated until the original is again reached	$\frac{2\pi}{1}$	1-fold (monad)	Rotatory-inversion axes[6][7]	$\bar{1}$ (≡centre)	See note[4]
		$\frac{2\pi}{2}$	2-fold (diad)		$\bar{2}$ (≡m)	See note[5]
		$\frac{2\pi}{3}$	3-fold (triad)		$\bar{3}$ (≡3 plus centre)	▲
		$\frac{2\pi}{4}$	4-fold (tetrad)		$\bar{4}$	◆
		$\frac{2\pi}{6}$	6-fold (hexad)		$\bar{6}$ (≡$3/m$)	⬢
	Reflection across the plane		Mirror plane[8]		m	—
	Inversion through the centre		Centre[8]		$\bar{1}$	See note[4]

Two-dimensional Symmetry Operators

(1) Inversion becomes rotation in two dimensions; the question of "hand" (enantiomorphy) arises only with reflection.
(2) Rotation points of even symmetry include two-fold rotation (centro-symmetry about a point); those of odd symmetry do not.
(3) Operation about a mirror line of symmetry is not equivalent to any form of rotation in two dimensions.

Three-dimensional Symmetry Operators

(4) The centre of symmetry is shown in writing only by the symbol for the inverse monad axis ($\bar{1}$). Since the symmetry centre occurs at the centre of the sphere of projection, its presence cannot properly by shown by a symbol on a stereogram; but its presence or absence is easily detected from the arrangement of the poles of equivalent directions.
(5) No graphical symbol is used for $\bar{2}$ other than that of the mirror plane equivalent to it.
(6) All inversion axes except the inverse tetrad are equivalent to some other operator or combination of operators. Since the inverse tetrad axis is necessary, the whole set of inversion axes is used systematically.
(7) Inversion axes of odd symmetry give rise to centro-symmetry, while inversion axes of even symmetry do not.
(8) The mirror plane and centre of symmetry are mentioned separately, although they are included also among the inversion axes listed systematically, being equivalent to $\bar{2}$ and $\bar{1}$ respectively; this separate mention is justified by their fundamental importance in space-group theory. In stereograms a mirror plane is represented by a thick-line great circle.
By the direction of a mirror plane, we mean the direction of its normal, which is the direction of the $\bar{2}$ axis to which it is equivalent.

3.2. The 10 Two-dimensional Point Groups

The symmetry operations used in the two-dimensional "crystallographic" point groups are the 1-, 2-, 3-, 4- and 6-fold rotations about a point (denoted by the number) and mirror-reflection across a line (denoted by the symbol *m*). The various combinations of these give rise to 10 different two-dimensional point groups, the full symbols of which, with short symbols in parentheses where these are different, are as follows:

1, 2, 1*m* (*m*), 2*mm* (*mm*), 4, 4*mm* (4*m*), 3, 3*m*, 6, 6*mm* (6*m*)

In the full symbol the principal position, which comes first, refers to the rotation about the point. The secondary position refers to a mirror line (normal to the *x*-axis) and to the other mirror lines of the same "form" (directions related by symmetry). In 2-fold symmetry there is only one mirror line in this form because the 2-fold rotation merely relates the positive and negative directions of the same line. In 3-, 4-, and 6-fold symmetry there are respectively 3, 2 and 3 mirror lines in each form owing to the effect of the rotation about the point. But the combination of an even-order rotation and a mirror line produces another form of mirror lines different from the first form. The symbol for this is given in the tertiary position.

1. The interaction of 2 and *m* produces a second mirror line at 90° to the first one.
2. The interaction of 4 and *m* produces a pair of mirror lines at 45° to the pair of the first form.
3. The interaction of 6 and *m* produces a second form of three mirror lines at 30° to the three of the first form.

Thus the presence of a second *m* in the full point-group symbol shows the presence of a second form of mirror lines. It should be noted that this does not occur with odd-order rotation points.

In the short symbols the rotation symmetry is left out when it is either 1 or 2, so that in two symbols the principal position is left vacant. In the even-order symbols with mirror planes, other than 2-fold, the second *m* is omitted. It would be quite correct to use 2*m* as the short symbol for the point group 2*mm*, but the more symmetrical short symbol *mm* is preferred.

It can be seen that the exact connotation of the secondary and tertiary symbols depends on the number of the rotation symmetry. In Table 3.2.1 the order of the positions is given, along with the division of the point groups into systems based on the most convenient set of axes of reference or, what amounts to the same thing, on the shape of the conventional unit cell of the lattice with which the point group can be associated. It should be noted that the point group 2 falls into the oblique system, while the point group 1*m* falls into the rectangular system along with 2*mm*.

In the groups with only rotation about the point all directions are general. But in the groups with mirror lines a direction parallel to such a line has a special relation to this symmetry operator and is consequently a special direction. The total number in the form of such special directions is half the number in the general form of directions in the same point group.

TABLE 3.2.1. **Order of Positions in the Full Symbols of the Two-dimensional Point Groups**

System	Oblique	Rectangular	Square	Hexagonal
Point groups	1, 2	1*m*, 2*mm* (*m*)[1][2] (*mm*)	4, 4*mm* (4*m*)	3, 3*m*, 6, 6*mm* (6*m*)
Principal position	*X*, denoting *X*-fold rotation about the point			
Secondary position	None	Mirror line normal to the *x*-axis	Mirror lines normal to the *x*- and *y*-axes	Mirror lines normal to the *x*-, *y*- and *u*-axes
Tertiary position	None	Mirror line normal to the *y*-axis	Mirror lines at 45° to the *x*- and *y*-axes	Mirror lines at 60° to the *x*-, *y*- and *u*-axes

(1) The short symbols are given in parentheses.
(2) In class *m* the symbol 1 in the principal position is omitted because of confusion that might occur in later two-dimensional space-group nomenclature, in which 1 may occur in a secondary or tertiary position (section 4.2).

3.3. The 32 Three-dimensional Point Groups

The crystallographic point groups are those groups of symmetry operations which can operate on infinite three-dimensional lattices so as to leave one point unmoved. They are derived by combining the elements of symmetry listed in section 3.1. They may be grouped into systems according to the set of co-ordinate axes to which they are most conveniently referred or, which is the same thing, according to the group of Bravais lattices on which they can operate. This grouping is shown in Table 3.3.1 together with the point-group order adopted in the present volume, which is different from that used in the 1935 *Tables*. The symbol X here stands for the order of the rotation symmetry (a single symmetry operation being rotation through $2\pi/X$ about the axis), and the arrangement across the page is 1, 2, 4, 3, 6, $X3$ (cubic). The close relation between trigonal and hexagonal symmetry makes this more convenient than the direct numerical order would be. The notation is as follows:

Rotation axis X Inversion axis $\bar{X}$

Rotation axis with mirror plane normal to it X/m $\left(\frac{X}{m}\right)$

Rotation axis with diad axis (axes) normal to it $X2$

Rotation axis with mirror plane (planes) parallel to it Xm

Inversion axis with diad axis (axes) normal to it $\bar{X}2$

Inversion axis with mirror plane (planes) parallel to it $\bar{X}m$

Rotation axis with a mirror plane normal to it and mirror planes parallel to it X/mm $\left(\frac{X}{m}m\right)$

TABLE 3.3.1. **Symbols of the 32 Three-dimensional Point Groups**

General symbol	Triclinic	Monoclinic (1st setting)	Tetragonal	Trigonal	Hexagonal	Cubic
X	1	2	4	3	6	23
$\bar{X}$ (of even order)	—	$\bar{2}$ ($\equiv m$)	$\bar{4}$	—	$\bar{6}$	—
X plus centre (includes $\bar{X}$ of odd order)	$\bar{1}$	$2/m$	$4/m$	$\bar{3}$	$6/m$	$2/m\ \bar{3}$ ($m3$)
	Monoclinic (2nd setting)	Orthorhombic				
$X2$	2 ($\equiv 12$)	222	422 {42}	32	622 {62}	432 {43}
Xm	m ($\equiv 1m$)	$mm2$ {mm}	$4mm$	$3m$	$6mm$	—
$\bar{X}2$ and $\bar{X}m$ (of even order)	—	—	$\bar{4}2m$	—	$\bar{6}m2$	$\bar{4}3m$
$X2$ plus centre, Xm plus centre (includes $\bar{X}m$ of odd order)	$2/m$	$2/m\ 2/m\ 2/m$ (mmm)	$4/m\ 2/m\ 2/m$ ($4/mmm$)	$\bar{3}\ 2/m$ ($\bar{3}m$)	$6/m\ 2/m\ 2/m$ ($6/mmm$)	$4/m\ \bar{3}\ 2/m$ ($m3m$)

NOTES

1. Although it is convenient to use the concept of centro-symmetry in deriving the above arrangement of the symbols, the centre is not used in systematic symbolism, being replaced by its equivalent inversion axis $\bar{1}$.
2. The symbols given in parentheses, e.g. (mmm), are the short forms of the symbols where these differ from the full symbols.
3. The symbols given in braces, e.g. {42}, are the short symbols used in earlier space-group nomenclature. They are still used where *direction* is unspecified, as in the point symmetry corresponding to the various sets of equivalent positions (section 4.3).
4. The order of the point groups in the following tables (sections 4.3, 4.7 in particular) is that obtained by reading down each column in Table 3.3.1, taking the columns in turn from left to right, the two monoclinic settings being taken together.

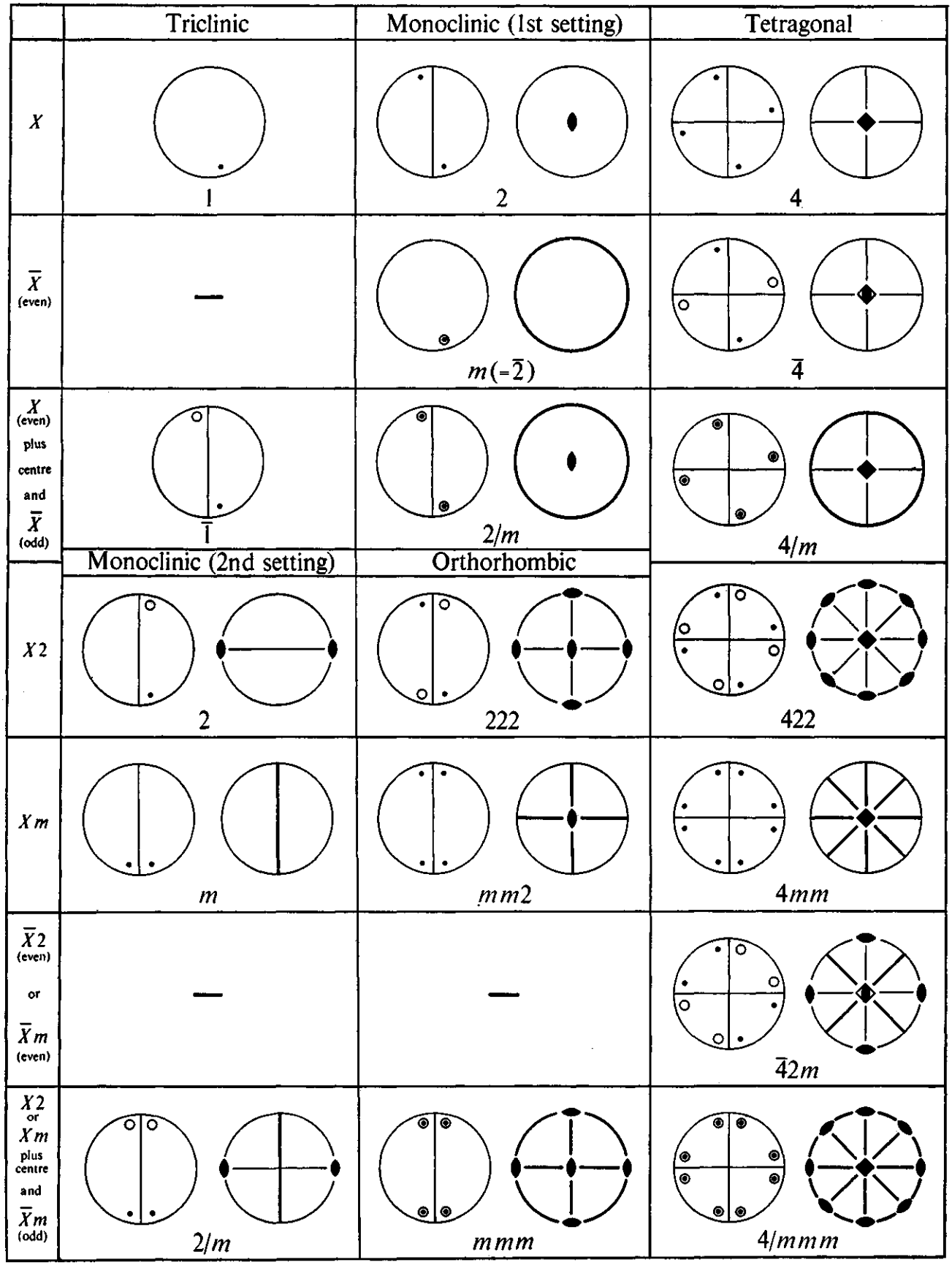
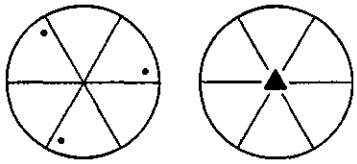
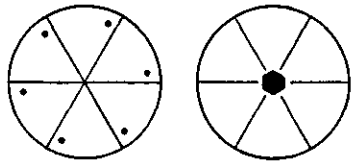
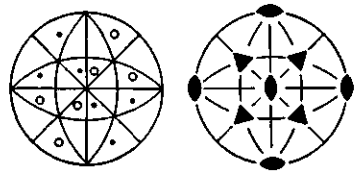
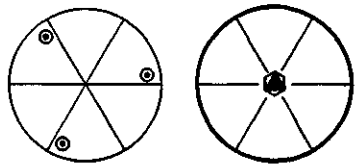
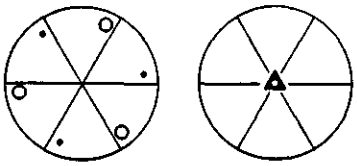
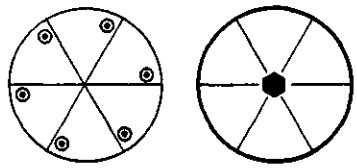
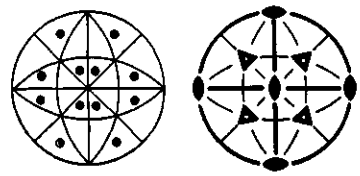
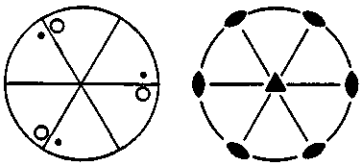
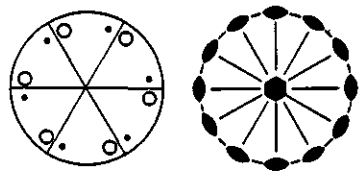
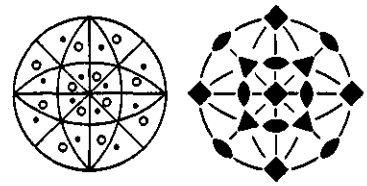
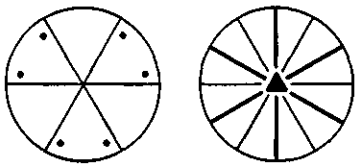
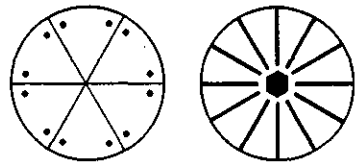
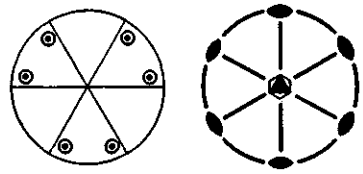
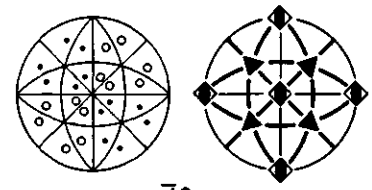
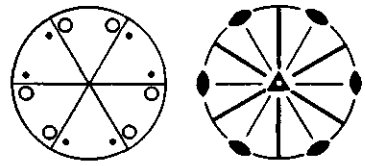
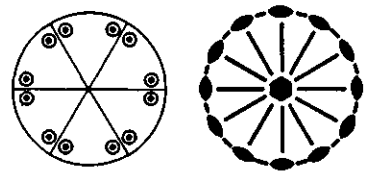
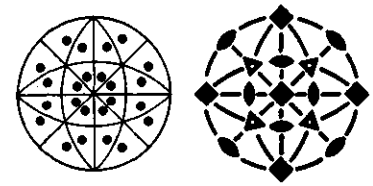


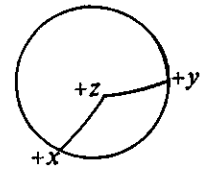
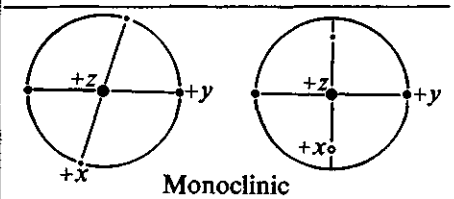
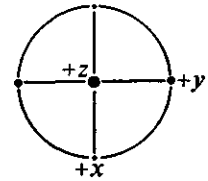
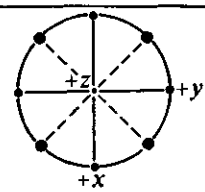
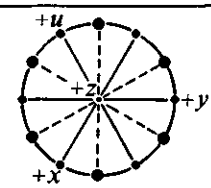
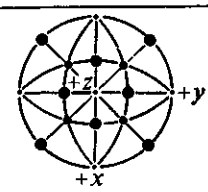
Fig. 3.3.1. Stereograms of poles of general equivalent directions, and symmetry

Trigonal	Hexagonal	Cubic	
 3	 6	 23	X
—	 $\bar{6}$	—	$\bar{X}$ (even)
 $\bar{3}$	 $6/m$	 $m3$	X (even) plus centre and $\bar{X}$ (odd)
 32	 622	 432	$X2$
 $3m$	 $6mm$	—	Xm
—	 $\bar{6}m2$	 $\bar{4}3m$	$\bar{X}2$ (even) or $\bar{X}m$ (even)
 $\bar{3}m$	 $6/mmm$	 $m3m$	$X2$ or Xm plus centre and $\bar{X}m$ (odd)

elements of each of the 32 point groups (z-axis normal to the paper in all drawings)

TABLE 3.3.2

Order of Positions in the Symbols of the Three-dimensional Point Groups as applied to Lattices

System and point groups	Position in point-group symbol			Stereographic representation • Poles of directions for primary position • secondary ditto • tertiary ditto
	Primary	Secondary	Tertiary	
Triclinic 1, $\bar{1}$	Only one symbol which denotes all directions in the crystal.			 Triclinic
Monoclinic 2, m, $2/m$	The symbol gives the nature of the unique diad axis[1] (rotation and/or inversion). 1st setting: z-axis unique[2] 2nd setting: y-axis unique			 Monoclinic 1st setting 2nd setting
Orthorhombic 222, $mm2$, mmm	Diad (rotation and/or inversion) along x-axis	Diad (rotation and/or inversion) along y-axis	Diad (rotation and/or inversion) along z-axis	 Orthorhombic
Tetragonal 4, $\bar{4}$, $4/m$; 422, $4mm$, $\bar{4}2m$, $4/mmm$	Tetrad (rotation and/or inversion) along z-axis	Diads (rotation and/or inversion) along x- and y-axes	Diads (rotation and/or inversion) along [110] and [1$\bar{1}$0] axes	 Tetragonal
Trigonal and hexagonal[3] 3, $\bar{3}$; 32, $3m$, $\bar{3}m$; 6, $\bar{6}$, $6/m$; 622, $6mm$, $\bar{6}m2$, $6/mmm$	Triad or hexad (rotation and/ or inversion) along z-axis	Diads (rotation and/or inversion) along x-, y- and u-axes	Diads (rotation and/or inversion) normal to x-, y-, u-axes in the plane (0001)	 Trigonal and hexagonal
Cubic 23, $m3$; 432, $\bar{4}3m$, $m3m$	Diads or tetrads (rotation and/ or inversion) along ⟨100⟩ axes	Triads (rotation and/ or inversion) along ⟨111⟩ axes	Diads (rotation and/ or inversion) along ⟨110⟩ axes	 Cubic

(1) The monoclinic symmetries are a diad rotation axis and/or a mirror plane normal to that axis. The latter is equivalent to a diad inversion axis along the normal to the plane.
(2) See Preface to Volume I. The 2nd setting is usual for crystallographic work.
(3) Both on hexagonal axes. If referred to rhombohedral axes, the unique axis is [111] and the diads (rotation and/or inversion) are along the three ⟨1$\bar{1}$0⟩ and the three ⟨11$\bar{2}$⟩ directions, respectively.

The written and graphical symbols used for operators have been explained in section 3.1. Here it is necessary to note the different kinds of symbol used for certain point groups.

1. *The Full Symbol.* This gives all the different kinds of symmetry elements present excepting those which are necessarily involved in each separate symbol shown. (Thus 6 involves 2 and 3; $\bar{3}$ involves $\bar{1}$ and 3; $\bar{4}$ involves 2, and so on.) For example, the full symbol of the most symmetrical point group of the cubic system is $4/m\bar{3}2/m$. This means that there are:

3 tetrads parallel to the ⟨100⟩ axes

3 mirror planes normal to the ⟨100⟩ axes

4 inversion triads parallel to the ⟨111⟩ axes

6 diads parallel to the ⟨110⟩ axes

6 mirror planes each normal to the ⟨110⟩ axes

The symbol $\bar{6}$ is never written as $3/m$ because point groups containing this operator belong to the hexagonal rather than to the trigonal system. They cannot operate on the rhombohedral lattice.

2. *The Short Symbol.* This need only be sufficient to determine the point-group symmetry unambiguously. The short symbol of the most symmetrical point group described above is $m3m$, since these operations, about the directions indicated in Table 3.3.2, involve all the rest. However, in practice it is sometimes advisable for the short symbol to be longer than is strictly necessary for the definition of the point group, if it is desired to show the orientation of the point group relative to the lattice on which it operates. Thus in $\bar{4}2m$ one of the two last symbols is, strictly speaking, superfluous. The usual morphological setting is for the diad rotation axes to lie along x- and y-, which necessarily involves mirror planes normal to the ⟨110⟩ directions. There is, however, an alternative setting (equally probable structurally) in which the diad axes would be along the ⟨110⟩ directions and the mirror planes normal to x- and y-. In this setting the point-group symbol would be $\bar{4}m2$. Similarly when $\bar{6}m2$ operates on a simple hexagonal lattice to give space groups (see section 4.1) it may do so in either of two ways:

1. The planes may be normal to x-, y-, u-; in which case there are diad axes also normal to x-, y-, u- (and z-). The symbol would then be $\bar{6}m2$, which is the conventional point-group symbol.
2. The planes may be parallel to x-, y-, u- (and z-); in which case there are diad axes also parallel to x-, y-, u-. The symbol would then be $\bar{6}2m$.

The object of putting in both symbols, m and 2, is to allow the distinction to be made later in respect of this orientation.

In the 1935 *Tables* the short symbol for the second point group of the orthorhombic system was mm. The symbol used in the present work is $mm2$. This has the advantage of showing clearly the conventional setting of the point group, with the diad axis parallel to the z-axis (compare 222 and mmm, where the three symbols also refer to the three crystallographic directions taken in alphabetical order). Moreover it allows the nature of the diad axis (rotation or screw) to be clearly shown in the space-group symbols which come later. This is, indeed, the reason also for giving the third diad symbol in the point group 222, which has always been common practice. For the sake of completeness, the tertiary symbols in 422, 622 and 432 are now inserted, to show that there are always rotation axes in the directions corresponding to the tertiary position.

NOTE

Crystals having any particular point-group symmetry are said to belong to a particular "class." The word "class," therefore, denotes a classificatory pigeon-hole and should not be used as synonymous with "point group."

3.4. The 11 Laue-symmetry Classes

The Friedel law states that the intensity of X-ray reflection from a set of crystal planes (hkl) is the same as that from $(\bar{h}\bar{k}\bar{l})$, as long as the wave-crystal interaction is not in the neighbourhood of a resonance level. Provided that this condition is fulfilled, all coherent diffraction effects appear to be centrosymmetrical, even from non-centrosymmetrical crystals. In other words, crystals of any class give the diffraction effects characteristic of that point-group symmetry which is obtained by adding a centre of symmetry to their actual symmetry elements where these are themselves non-centrosymmetrical.

There are 11 centrosymmetrical point groups and therefore there are 11 Laue classes of point groups which become identical when a centre of symmetry is added to those which lack it. The point group of highest symmetry in each Laue class is the centro-symmetrical point group, and the symbol of this is used for the Laue class. The Laue classes are shown in Table 3.4.1.

In practice Laue symmetry is best studied by allowing a continuous wavelength X-ray beam to be incident along or normal to a rotation or rotatory-inversion axis of the stationary crystal. The symmetry of the diffraction pattern obtained must be that of one of the 10 two-dimensional point groups (section 3.2), but, by repeating the procedure for different directions of projection, all 11 Laue classes can be distinguished. This distinction may also be made on the basis of moving-film diffraction patterns. New methods of distinguishing the full point-group symmetry from a statistical study of diffraction intensities have been developed, and are briefly indicated in section 5.3. References are also given in section 5.3 to the use of vector sets (Patterson analysis) for this purpose.

TABLE 3.4.1

The 11 Laue-symmetry classes

Triclinic	Monoclinic	Tetragonal	Trigonal	Hexagonal	Cubic
1 $\bar{1}$	2 m $\mathbf{2/m}$	4 $\bar{4}$ $\mathbf{4/m}$	3 $\bar{3}$	6 $\bar{6}$ $\mathbf{6/m}$	23 $\mathbf{m3}$
	Orthorhombic				
	222 $(mm2$ $m2m$ $2mm)$ $\mathbf{mmm}$	422 $4mm$ $(\bar{4}2m$ $\bar{4}m2)$ $\mathbf{4/mmm}$	321 or 312 $3m1$ or $31m$ $\mathbf{3m1}$ or $\mathbf{31m}$	622 $6mm$ $(\bar{6}m2$ $\bar{6}2m)$ $\mathbf{6/mmm}$	432 $\bar{4}3m$ $\mathbf{m3m}$

NOTES
1. Point groups belonging to the same Laue class are enclosed in a rectangle, and the symbol of the Laue class is in bold type, this being the symbol of the centric point group in the Laue class.
2. For three point groups there are alternative settings which, however, correspond to a single Laue symmetry, and these three point groups are put within large parentheses.
3. In the di-trigonal Laue-symmetry class each of the three point groups has two settings. These are distinguishable by the setting of the Laue symmetry relative to the shortest repeat in the lattice normal to the triad axis; hence the appropriate form of the Laue-symmetry symbol should be used, depending on the particular space group.

By analogy the two-dimensional Laue classes may be defined as classes of point groups that become identical when a point of inversion (two-fold rotation) is added to those that lack it. The six Laue classes divide up the two-dimensional point groups as follows, the Laue-symmetry symbol being in bold type:

(1, **2**); (m, **2mm**); (**4**); (**4mm**); (3, **6**); (3m, **6mm**).

3.5. Forms of Planes in the Laue Classes (Multiplicity Factors)

The "form" of a plane in a crystal is the complete set of similar planes related to the initial one by the symmetry operations of the point group. Thus, in the cubic system, the cube is a form consisting of the six planes (100), (010), (001), ($\bar{1}$00), (0$\bar{1}$0), (00$\bar{1}$). A table can be drawn up giving the number of planes in the general form, and in each of the different special forms, for any given crystal class. These numbers of planes for different values of *hkl* in the 11 Laue classes have significance in connection with all X-ray methods of crystal examination where more than one set of parallel planes contributes to a particular diffraction line or spot.

In a powder photograph any given line is built up by diffraction from all the planes of a single form, leaving out the cases in certain systems where identical spacings occur for unrelated values of *hkl*. Consequently, other things being equal, the density of a line will be proportional to the number of planes in the form. It should be noted that, since reflection may occur from both sides of the same set of planes, both *hkl* and $\bar{h}\bar{k}\bar{l}$ must always be counted in the number. Such numbers are called General Multiplicity Factors and they are equivalent to the number of morphological faces in the form. Certain single-crystal methods also involve multiplicity factors, and these may be submultiples of the general multiplicity factors applicable to the powder method, so that they must be separately determined for the particular method used.

In Table 3.5.1 are given the general multiplicity factors for the 11 Laue classes for all values of *hkl*. The three systems with no higher than 2-fold symmetry can be grouped together; the cubic and the tetragonal systems must be taken separately, while the trigonal system (for both the rhombohedral and the hexagonal lattice) is compared with the hexagonal system. In addition, the relations of the trigonal system based on the rhombohedral lattice and the cubic system are shown. In each of these parts of the table the Laue class of highest symmetry has a 7-fold division of types of form. We can imagine on a stereogram the unit spherical triangle which fills the whole surface of the sphere when all the symmetry elements of the point group operate on it. When the initial pole of a form is placed in turn at each of the apices of the unit spherical triangle, three forms with fixed values of *hkl* result. If the initial pole is placed in turn on the sides of the triangle, three forms result with special relations between *h* and *k* and *l*. Finally, when the initial pole is placed inside the triangle, the general form *hkl* results. The influence of this 7-fold grouping diminishes as one goes from higher to lower symmetry, but it provides the best framework for a table of forms of planes.

The table also shows the forms, in a lower-symmetry Laue class, which have the same spacing because of the same geometrical relation to the underlying lattice, even though, being unconnected by symmetry, their intensities of reflection are different. Such forms would give rise to the same line in a powder photograph, but the intensity of the line would be due to the sum of the reflections from the two forms.

TABLE 3.5.1

General Multiplicity Factors (for Notes see p. 34)

	Laue class	$h00$	$0k0$	$00l$	$k \not\equiv l$		$h \not\equiv l$		$h \not\equiv k$		$h \not\equiv k \not\equiv l$			
					$0kl$	$0\bar{k}l$	$h0l$	$\bar{h}0l$	$hk0$	$h\bar{k}0$	hkl	$hk\bar{l}$	$h\bar{k}l$	$\bar{h}kl$
Triclinic	$\bar{1}$	2	2	2	2	2	2	2	2	2	2	2	2	2
(z-axis unique) Monoclinic	$2/m$	2	2	2	4		4		2	2	4		4	
(y-axis unique)		2	2	2	4		2	2	4		4		4	
Orthorhombic	mmm	2	2	2	4		4		4		8			

	Laue class	$h00$ $0h0$	$00l$	$h \not\equiv l$ $\left\{\begin{matrix} h0l \\ \bar{h}0l \\ 0hl \\ 0\bar{h}l \end{matrix}\right\}$	$hk0$ $k\bar{h}0$	$h\bar{k}0$ $kh0$	$hh0$ $\bar{h}h0$	$h \not\equiv l$ $\left\{\begin{matrix} hhl \\ \bar{h}hl \\ h\bar{h}l \\ hh\bar{l} \end{matrix}\right\}$	$l \not\equiv h$ or k $\left\{\begin{matrix} hkl \\ hk\bar{l} \\ k\bar{h}l \\ k\bar{h}\bar{l} \end{matrix}\right\}$	$\left\{\begin{matrix} h\bar{k}l \\ h\bar{k}\bar{l} \\ khl \\ kh\bar{l} \end{matrix}\right\}$
Tetragonal	$4/m$	4	2	8	4	4	4	8	8	8
	$4/mmm$	4	2	8	8		4	8	16	

	Laue class	$h00$ ↻	$\left\{\begin{matrix} hh0 \\ h\bar{h}0 \end{matrix}\right\}$ ↻	$\left\{\begin{matrix} hhh \\ \bar{h}hh \\ h\bar{h}h \\ hh\bar{h} \end{matrix}\right\}$	$\left\{\begin{matrix} hk0 \\ \bar{h}k0 \end{matrix}\right\}$ ↻		↻ $\left\{\begin{matrix} hhl \\ \bar{h}hl \\ h\bar{h}l \\ hh\bar{l} \end{matrix}\right\}$		↻ $\left\{\begin{matrix} hkl \\ \bar{h}kl \\ h\bar{k}l \\ hk\bar{l} \end{matrix}\right\}$	
					$(h>k)$	$(h<k)$	$(h>l)$	$(h<l)$	$(h>k>l)$	$(h<k<l)$
Cubic	$m3$	6	12	8	12	12	24	24	24	24
	$m3m$	6	12	8	24		24	24	48	

	Laue class	$h00$ ↻	$hh0$ ↻	$h\bar{h}0$ ↻	hhh	$h\bar{h}h$ ↻	$hk0$ ↻	$kh0$ ↻	$\bar{h}k0$ ↻	$\bar{k}h0$ ↻	hkk ↻	$\bar{h}kk$ ↻	$h\bar{k}k$ ↻	$hk\bar{k}$ ↻
													$(h>k)$	
Trigonal (with rhombohedral lattice)	$\bar{3}m$	6	6	6	2	6	12		12		6	6	12	
	$\bar{3}$	6	6	6	2	6	6	6	6	6	6	6	6	6
Cubic	$m3$	6	12		8		12		12		24			
	$m3m$	6	12		8		24				24			

TABLE 3.5.1 (*continued*)

General Multiplicity Factors (for Notes see p. 34)

	Laue class	*hhh*	Sum zero (prism zone)				Sum not zero							
			Any one of the symbols may be zero and any two may be equal				*hhl*↻ $l>h$ same sign $l<h$; $l>2\bar{h}$ opp. sign $l\leq\bar{h}$ or $\bar{h}<l<2\bar{h}$		Any one symbol may be zero; $k\not\equiv l$					
									One symbol is the mean of the other two		*h*, *k*, *l* otherwise independent			
			hhl̄ ↻	*h*0*h̄* ↻	*hkl* ↻	*hlk* ↻	*h* may be zero	*l* may be zero	*hkl* ↻	*hlk* ↻	*hkl* ↻	*hlk* ↻	*h′k′l′* ↻	*h′l′k′* ↻
Trigonal (with rhombohedral lattice)	$\bar{3}$	2	6	6	6	6	6	6	6	6	6	6	6	6
	$\bar{3}m$	2	6	6	12		6	6	12		12		12	
							$l\not\equiv h$ or *k* or *i*							
		000*l*	*h*0$\bar{h}$0 ↻ (*h*0$\bar{h}$)	*hh*2$\bar{h}$0 ↻ (*hh*2$\bar{h}$)	*hki*0 ↻ (*hki*)	*hik*0 ↻ (*hik*)	*h*0$\bar{h}$*l* ↻ (*h*0$\bar{h}$)	*h*0$\bar{h}\bar{l}$ ↻ (*h*0$\bar{h}$)	*hh*2$\bar{h}$*l* ↻ (*hh*2$\bar{h}$)	*hh*2$\bar{h}\bar{l}$ ↻ (*hh*2$\bar{h}$)	*hkil* ↻ (*hki*)	*hik*$\bar{l}$ ↻ (*hik*)	*hikl* ↻ (*hik*)	*hki*$\bar{l}$ ↻ (*hki*)
Trigonal (with hexagonal lattice)	$\bar{3}$	2	6	6	6	6	6	6	6	6	6	6	6	6
	$\bar{3}m1$	2	6	6	12		6	6	12		12		12	
	$\bar{3}1m$	2	6	6	12		12		6	6	12		12	
											hkil ↻(*hki*) ± *l*		*hikl* ↻(*hik*) ± *l*	
Hexagonal	6/*m*	2	6	6	6	6	12		12		12		12	
	6/*mmm*	2	6	6	12		12		12		24			

	6	6	12		12		12		12		12		12	
	6	6	6	6	6	6	6	6	6	6	6	6	6	6
	hkk ↻	$\bar{h}$*kk* ↻	*h*$\bar{k}$*k* ↻	*hk*$\bar{k}$ ↻	*hkl* ↻	*hlk* ↻	$\bar{h}$*kl* ↻	$\bar{h}$*lk* ↻	*hk*$\bar{l}$ ↻	*h*$\bar{l}$*k* ↻	*h*$\bar{k}$*l* ↻	*hl*$\bar{k}$ ↻		
			(*h*<*k*)											
	24				24									
	24				48									

NOTES TO TABLE 3.5.1 (pp. 32, 33)

1. The symbol hkl includes $\bar{h}\bar{k}\bar{l}$.
2. The symbol $\circlearrowright$ means cyclic interchange; when followed by parentheses it applies only to the part within the parentheses.
3. Where a different letter, h or k or l, is used, this implies a corresponding difference in the numerals except where equalities are expressly permitted, as, for example, by the symbol $(h \not\equiv l)$. Also, the use of h, k or l implies a non-zero numeral except where the possibility of a zero value is expressly permitted. Also, the use of the same letter h, k or l twice or thrice in the same symbol implies equality of the corresponding numerals.
4. In groups of adjacent columns different arrangements of the same letters may occur; this implies that if numerical values were assigned to these, then the indices appropriate to the different forms would be as shown.
5. Where use is made of primed symbols $h'k'l'$, this indicates that the numerical values of these symbols bear no relation to those corresponding to hkl (unprimed) in the adjacent column.
6. Where two or more different forms have the same spacing, owing to their having the same geometrical relation to the underlying lattice, their multiplicity factors are enclosed in a dotted rectangle. Such forms do not have the same value of structure amplitude.
7. In the trigonal system the multiplicity factors given for the hexagonal lattice apply only where the lattice is hexagonal in a primitive sense and do not apply to the case of a rhombohedral crystal described on hexagonal axes. The same, *mutatis mutandis*, applies to the factors for the rhombohedral lattice.
8. This table applies to the powder method. Special multiplicity factors must be deduced for other methods.
9. For the di-trigonal Laue-symmetry class two settings are given; these can be distinguished by the different relation between the symmetry planes and the shortest lattice repeat normal to the triad axis.

3.6. Sub- and Super-groups of the Two-dimensional and the Three-dimensional Point Groups

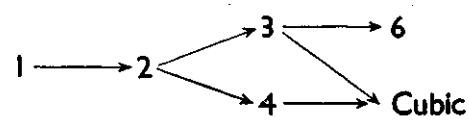
If, after subtracting from a point group certain symmetry elements, there remains a point group of reduced symmetry, then the latter is a sub-group of the former. Every point group except that of the lowest symmetry (1) has at least one sub-group, namely the one of lowest symmetry. Correspondingly, if, by adding certain symmetry elements to a point group we obtain a point group of higher symmetry, then the latter is a super-group of the former. Every point group except the two of highest symmetry ($6/mmm$ and $m3m$) has at least one crystallographic super-group.

TABLE 3.6.1. **Two-dimensional Sub- and Super-groups**

Point groups	Sub-groups									
	1	2	m	$2mm$	4	$4mm$	3	$3m$	6	$6mm$
1										
2	1									
m	1									
$2mm$	1	2	m							
4	1	2								
$4mm$	1	2	m	$2mm$	4					
3	1									
$3m$	1		m				3			
6	1	2					3			
$6mm$	1	2	m	$2mm$			3	$3m$	6	
Super-groups	Point groups									

In Table 3.6.1 the sub-groups of any given point group in the left-hand column are shown in the horizontal line opposite to it. The super-groups of a given point group are to be found in the left-hand column opposite to the symbols of the given point group in the body of the table.

Table 3.6.2 gives the sub- and super-groups of the 32 three-dimensional point groups. In the lower left-hand part of the table are listed the sub-groups of the 1-, 2- and 4-fold symmetry groups (that is, of point groups in the triclinic, monoclinic, orthorhombic and tetragonal systems). The point groups are given vertically on the left side, and the sub-groups corresponding to each point group are on the horizontal line. On the upper part of the left-hand page are given in the same way those sub-groups of the 3- and 6-fold and cubic symmetry groups (that is, of point groups in the trigonal, hexagonal and cubic systems) which have 1-, 2- and 4-fold symmetry. To obtain the remaining sub-groups of these systems, namely the 3-fold ones of the trigonal and cubic systems and the 3- and 6-fold ones of the hexagonal systems, the table on the right-hand page must be used. Consequently, to obtain all the sub-groups of a point group belonging to the trigonal, hexagonal or cubic systems it is necessary to include all the symbols in the horizontal line right across both pages. This layout of the groups is necessitated by the forking which occurs as one goes from the lowest towards high symmetry. The total number of sub-groups is given in each case in order to act as a check.



The super-groups of a given point group can be obtained from the same table. The symbols in the body of the table must now be treated as point groups. All the super-groups corresponding to a given point group are to be found in the vertical columns, opposite to the symbols of the given point group in the body of the table. For super-groups of point groups in the trigonal, hexagonal and cubic systems the right-hand table alone is used. For super-groups of point groups in the triclinic, monoclinic, orthorhombic and tetragonal systems the left-hand page is used; but the super-groups of a given point group must be counted using both tables on this page.

TABLE 3.6.2

Sub-groups and Super-groups of the 32 Point Groups

		1	3	2	3	2	5	6	4	10	11	8	17	24	10	31	Total No. of super-groups	Total No. of sub-groups
		4/mmm	**$\bar{4}2m$**	**4mm**	**422**	**4/m**	**$\bar{4}$**	**4**	**mmm**	**mm2**	**222**	**2/m**	**m**	**2**	**$\bar{1}$**	**1**	Sub-groups / Point groups	
		4/mmm	$\bar{4}2m$	4mm	422	4/m	$\bar{4}$	4	mmm	mm2	222	2/m	m	2	$\bar{1}$	1	**m3m**	24
			$\bar{4}2m$				$\bar{4}$			mm2	222		m	2		1	**$\bar{4}3m$**	10
					422			4			222			2		1	**432**	8
									mmm	mm2	222	2/m	m	2	$\bar{1}$	1	**m3**	11
											222			2		1	**23**	4
0	**1**								mmm	mm2	222	2/m	m	2	$\bar{1}$	1	**6/mmm**	19
1	**$\bar{1}$**	1								mm2			m	2		1	**$\bar{6}m2$**	8
1	**2**	1								mm2			m	2		1	**6mm**	7
1	**m**	1									222			2		1	**622**	6
4	**2/m**	1	$\bar{1}$	2	m							2/m	m	2	$\bar{1}$	1	**6/m**	9
2	**222**	1		2									m			1	**$\bar{6}$**	3
3	**mm2**	1		2	m									2		1	**6**	3
7	**mmm**	1	$\bar{1}$	2	m	2/m	222	mm2				2/m	m	2	$\bar{1}$	1	**$\bar{3}m$**	9
2	**4**	1		2									m			1	**3m**	3
2	**$\bar{4}$**	1		2										2		1	**32**	3
7	**4/m**	1	$\bar{1}$	2	m	2/m					4	$\bar{4}$			$\bar{1}$	1	**$\bar{3}$**	3
4	**422**	1		2			222				4					1	**3**	1
5	**4mm**	1		2	m			mm2			4							
6.	**$\bar{4}2m$**	1		2	m		222	mm2				$\bar{4}$						
14	**4/mmm**	1	$\bar{1}$	2	m	2/m	222	mm2	mmm		4	$\bar{4}$	4/m	422	4mm	$\bar{4}2m$		
Total No. of sub-groups	Point groups / Sub-groups	**1**	**$\bar{1}$**	**2**	**m**	**2/m**	**222**	**mm2**	**mmm**		**4**	**$\bar{4}$**	**4/m**	**422**	**4mm**	**$\bar{4}2m$**	**4/mmm**	

TABLE 3.6.2. (*continued*)

Sub-groups and Super-groups of the 32 Point Groups

Total No. of super-groups	16	5	6	6	2	4	3	1	1	1	1	0	4	1	1	1	0
Point groups \ Sub-groups	3	$\bar{3}$	32	$3m$	$\bar{3}m$	6	$\bar{6}$	$6/m$	622	$6mm$	$\bar{6}m2$	$6/mmm$	23	$m3$	432	$\bar{4}3m$	$m3m$
$m3m$	3	$\bar{3}$	32	$3m$	$\bar{3}m$								23	$m3$	432	$\bar{4}3m$	
$\bar{4}3m$	3			$3m$									23				
432	3		32										23				
$m3$	3	$\bar{3}$											23				
23	3																
$6/mmm$	3	$\bar{3}$	32	$3m$	$\bar{3}m$	6	$\bar{6}$	$6/m$	622	$6mm$	$\bar{6}m2$						
$\bar{6}m2$	3		32	$3m$			$\bar{6}$										
$6mm$	3			$3m$		6											
622	3		32			6											
$6/m$	3	$\bar{3}$				6	$\bar{6}$										
$\bar{6}$	3																
6	3																
$\bar{3}m$	3	$\bar{3}$	32	$3m$													
$3m$	3																
32	3																
$\bar{3}$	3																
3																	

Examples

The following examples will illustrate the use of Table 3.6.2.

1. To find the sub-groups of point group $4mm$.
   Answer: 1, 2, m, $mm2$, 4. (5)
2. To find the sub-groups of point group $\bar{6}m2$.
   Answer: 1, 2, m, $mm2$, 3, 32, $3m$, $\bar{6}$. (8)
3. To find the super-groups of point group $mm2$.
   Answer: mmm, $4mm$, $\bar{4}2m$, $4/mmm$, $6mm$, $\bar{6}m2$, $6/mmm$, $m3$, $\bar{4}3m$, $m3m$. (10)
4. To find the super-groups of point group 32.
   Answer: $\bar{3}m$, 622, $\bar{6}m2$, $6/mmm$, 432, $m3m$. (6)

3.7. Projection Symmetries of the 32 Point Groups

The point groups of symmetry operations can be projected on to any of the various types of lattice plane, and the resulting projected symmetry can be described by the appropriate two-dimensional point-group symbol. This is done in Table 3.7.1, where the various types of lattice plane are arranged in seven columns for the reason given in section 3.5. It should be noted that in the centrosymmetrical point groups the projected symmetry can belong only to one of the six two-dimensional point groups which have evenfold symmetry. Table 3.7.1 is not suitable for use with either of the two practical methods of obtaining symmetry information by using projected symmetry (Laue photographs or etch tests).

In a Laue photograph each spot is produced by diffraction from a single set of parallel lattice planes, and consequently, as with other X-ray methods governed by the Friedel law (page 30), the presence or absence of a centre of symmetry in the specimen cannot be deduced from such photographs. Although we are restricted to dealing with the 11 Laue classes, the Laue-photograph method does give useful information about symmetry. If the photograph is taken on a flat plate normal to the incident beam, the photograph will reveal directly the presence of symmetry planes containing the incident beam and the nature of any symmetry axis parallel to the beam. The resulting projection symmetry is included in Table 3.7.2, for different directions of incident beam, for the 11 Laue classes. If a cylindrical film with its axis normal to the incident beam is used, the amount of directly observable symmetry information is reduced owing to the lower symmetry of the cylinder as compared with the flat plate; but, by plotting the normals to reflecting planes on a stereographic projection, even more information is derivable. The projection will reveal all the information obtained directly from the flat plate, and in addition it will show the presence of symmetry planes other than those containing the incident beam and the nature of any symmetry axes other than that parallel to the incident beam. Such a projection could, of course, be made also from the flat-plate photograph, but much less data would be obtained than from a cylindrical film.

When a face of a crystal is etched with a suitable reagent, an "etch pit" consisting of small faces is produced, these being parallel to the lattice planes along which solution has taken place most readily (section 3.8). Now the readiness with which solution takes place on a given lattice plane will not be the same, in general, on opposite sides of the plane in a non-centrosymmetrical crystal. Hence etch tests can be used to distinguish between the presence and the absence of centrosymmetry, and are also very useful for the detection of twinning. The projection symmetry appropriate for etch tests is given in Table 3.7.2. The Laue projection symmetry can be obtained from Table 3.7.2 by selecting only those rows corresponding to the Laue classes $\bar{1}$, $2/m$, mmm, $4/m$, $4/mmm$, $\bar{3}$, $\bar{3}m1$ or $\bar{3}1m$, $6/m$, $6/mmm$, $m3$, $m3m$.

TABLE 3.7.1. **Point-group Projection Symmetry**

System	Point group	{100}	{010}	{001}	{0*kl*}	{*h*0*l*}	{*hk*0}	{*hkl*}
Triclinic	1	1	1	1	1	1	1	1
	$\bar{1}$	2	2	2	2	2	2	2
Monoclinic *z*-axis unique	2	*m*	*m*	2	1	1	*m*	1
	m	*m*	*m*	1	1	1	*m*	1
	$2/m$	2*mm*	2*mm*	2	2	2	2*mm*	2
y-axis unique	2	*m*	2	*m*	1	*m*	1	1
	m	*m*	1	*m*	1	*m*	1	1
	$2/m$	2*mm*	2	2*mm*	2	2*mm*	2	2
Orthorhombic	222	2*mm*	2*mm*	2*mm*	*m*	*m*	*m*	1
	*mm*2	*m*	*m*	2*mm*	*m*	*m*	*m*	1
	*m*2*m*	*m*	2*mm*	*m*	*m*	*m*	*m*	1
	2*mm*	2*mm*	*m*	*m*	*m*	*m*	*m*	1
	mmm	2*mm*	2*mm*	2*mm*	2*mm*	2*mm*	2*mm*	2

TABLE 3.7.1. **Point-group Projection Symmetry** (*continued*)

System	Point group	{001}	{100}	{110}	{*hk*0}	{*h*0*l*}	{*hhl*}	{*hkl*}
Tetragonal	4	4	*m*	*m*	*m*	1	1	1
	$\bar{4}$	4	*m*	*m*	*m*	1	1	1
	4/*m*	4	2*mm*	2*mm*	2*mm*	2	2	2
	422	4*mm*	2*mm*	2*mm*	*m*	*m*	*m*	1
	4*mm*	4*mm*	*m*	*m*	*m*	*m*	*m*	1
	[$\bar{4}2m$	4*mm*	2*mm*	*m*	*m*	*m*	*m*	1
	[$\bar{4}m2$	4*mm*	*m*	2*mm*	*m*	*m*	*m*	1
	4/*mmm*	4*mm*	2*mm*	2*mm*	2*mm*	2*mm*	2*mm*	2

System	Point group	{0001}	{10$\bar{1}$0}	{11$\bar{2}$0}	{*hki*0}	{*h*0$\bar{h}$*l*}	{*hh*2$\bar{h}$*l*}	{*hkil*}
Trigonal	3	3	1	1	1	1	1	1
	$\bar{3}$	6	2	2	2	2	2	2
	[321	31*m*	*m*	2	1	*m*	1	1
	[312	3*m*1	2	*m*	1	1	*m*	1
	[3*m*1	3*m*1	*m*	1	1	*m*	1	1
	[31*m*	31*m*	1	*m*	1	1	*m*	1
	[$\bar{3}m1$	6*mm*	2*mm*	2	2	2*mm*	2	2
	[$\bar{3}1m$	6*mm*	2	2*mm*	2	2	2*mm*	2
Hexagonal	6	6	*m*	*m*	*m*	1	1	1
	$\bar{6}$	3	*m*	*m*	*m*	1	1	1
	6/*m*	6	2*mm*	2*mm*	2*mm*	2	2	2
	622	6*mm*	2*mm*	2*mm*	*m*	*m*	*m*	1
	6*mm*	6*mm*	*m*	*m*	*m*	*m*	*m*	1
	[$\bar{6}m2$	3*m*1	2*mm*	*m*	*m*	*m*	*m*	1
	[$\bar{6}2m$	31*m*	*m*	2*mm*	*m*	*m*	*m*	1
	6/*mmm*	6*mm*	2*mm*	2*mm*	2*mm*	2*mm*	2*mm*	2

System	Point group	{100}	{111}	{110}	{*hk*0}	{*hhl*}		{*hkl*}
						h > *l*	*h* < *l*	
Cubic	23	2*mm*	3	*m*	*m*	1	1	1
	*m*3	2*mm*	6	2*mm*	2*mm*	2	2	2
	432	4*mm*	3*m*	2*mm*	*m*	*m*	*m*	1
	$\bar{4}3m$	4*mm*	3*m*	*m*	*m*	*m*	*m*	1
	*m*3*m*	4*mm*	6*mm*	2*mm*	2*mm*	2*mm*	2*mm*	2

NOTES FOR TABLES 3.7.1 AND 3.7.2

1. For the arrangement in seven columns see section 3.5.
2. The indices *h*, *k*, *l* are not zero unless this is explicitly stated. These indices may be equal except where this is provided for in another column of the same system.
3. Short symbols are given for the three-dimensional point groups except where orientation is important, but full symbols are given for the two-dimensional projection point groups.
4. The trigonal space groups are here described only on hexagonal axes. The symmetry on rhombohedral axes is identical, but the indices of the projection planes must be transformed by means of the matrix given on p. 21.
5. All three orientations are given for the orthorhombic polar point group and both orientations for the five other point groups in which these are distinguishable from each other. Different orientations of the same point group are linked by a square bracket.

TABLE 3.7.2. **Etch-figure Symmetry** (including **Laue-projection Symmetry,** but see p. 38)

System	Point group	{100}	{010}	{001}	{0*kl*}	{*h*0*l*}	{*hk*0}	{*hkl*}
Triclinic	1	1	1	1	1	1	1	1
	$\bar{1}$	1	1	1	1	1	1	1
Monoclinic *z*-axis unique	2	1	1	2	1	1	1	1
	m	*m*	*m*	1	1	1	*m*	1
	2/*m*	*m*	*m*	2	1	1	*m*	1
y-axis unique	2	1	2	1	1	1	1	1
	m	*m*	1	*m*	1	*m*	1	1
	2/*m*	*m*	2	*m*	1	*m*	1	1
Orthorhombic	222	2	2	2	1	1	1	1
	*mm*2	*m*	*m*	2*mm*	*m*	*m*	1	1
	*m*2*m*	*m*	2*mm*	*m*	*m*	1	*m*	1
	2*mm*	2*mm*	*m*	*m*	1	*m*	*m*	1
	mmm	2*mm*	2*mm*	2*mm*	*m*	*m*	*m*	1

System	Point group	{001}	{100}	{110}	{*hk*0}	{*h*0*l*}	{*hhl*}	{*hkl*}
Tetragonal	4	4	1	1	1	1	1	1
	$\bar{4}$	2	1	1	1	1	1	1
	4/*m*	4	*m*	*m*	*m*	1	1	1
	422	4	2	2	1	1	1	1
	4*mm*	4*mm*	*m*	*m*	1	*m*	*m*	1
	$\bar{4}2m$	2*mm*	2	*m*	1	1	*m*	1
	$\bar{4}m2$	2*mm*	*m*	2	1	*m*	1	1
	4/*mmm*	4*mm*	2*mm*	2*mm*	*m*	*m*	*m*	1

System	Point group	{0001}	{10$\bar{1}$0}	{11$\bar{2}$0}	{*hki*0}	{*h*0$\bar{h}$*l*}	{*hh*2$\bar{h}$*l*}	{*hkil*}
Trigonal	3	3	1	1	1	1	1	1
	$\bar{3}$	3	1	1	1	1	1	1
	321	3	1	2	1	1	1	1
	312	3	2	1	1	1	1	1
	3*m*1	3*m*1	*m*	1	1	*m*	1	1
	31*m*	31*m*	1	*m*	1	1	*m*	1
	$\bar{3}m1$	3*m*1	*m*	2	1	*m*	1	1
	$\bar{3}1m$	31*m*	2	*m*	1	1	*m*	1
Hexagonal	6	6	1	1	1	1	1	1
	$\bar{6}$	3	*m*	*m*	*m*	1	1	1
	6/*m*	6	*m*	*m*	*m*	1	1	1
	622	6	2	2	1	1	1	1
	6*mm*	6*mm*	*m*	*m*	1	*m*	*m*	1
	$\bar{6}m2$	3*m*1	2*mm*	*m*	*m*	*m*	1	1
	$\bar{6}2m$	31*m*	*m*	2*mm*	*m*	1	*m*	1
	6/*mmm*	6*mm*	2*mm*	2*mm*	*m*	*m*	*m*	1

System	Point group	{100}	{111}	{110}	{*hk*0}	{*hhl*}		{*hkl*}
						(*h*>*l*)	(*h*<*l*)	
Cubic	23	2	3	1	1	1	1	1
	*m*3	2*mm*	3	*m*	*m*	1	1	1
	432	4	3	2	1	1	1	1
	$\bar{4}3m$	2*mm*	3*m*	*m*	1	*m*	*m*	1
	*m*3*m*	4*mm*	3*m*	2*mm*	*m*	*m*	*m*	1

3.8. Point-group Symmetry and the Physical Properties of Crystals

In this section we consider what information about symmetry can be obtained by the use of techniques auxiliary to X-ray methods. The term "physical properties" is used to include crystal morphology and also the nature of etch figures produced by a reagent the effect of which varies with direction in the crystal. The use of any one of these auxiliary techniques may not give the complete determination of symmetry, but when used in conjunction much information is often obtained. It is important to realise that the evidence of these techniques is often negative and that in general the symmetry conclusions drawn from such evidence must be considered only as provisional.

1. Morphology

If the crystal shows good faces, measurement by means of the optical goniometer gives information about the symmetry. In theory each of the 32 crystal classes can be distinguished if the appropriate forms or combinations of forms are developed. In practice the amount of symmetry information which can be obtained depends on the development of the particular specimen.

2. Etch Figures

Where the development of faces on a crystal is inadequate, etch figures can often be used to give additional information. A non-optically active reagent must be used, and in favourable cases this will act at different speeds in different crystal directions. The resulting etch figures will have the symmetry of one of the 10 two-dimensional point groups, as given in Table 3.7.2, page 40. Often, however, the etch reaction proceeds at the same speed along crystallographically different directions, and the resulting etch figure has a higher apparent symmetry than that of the face in question. Consequently all deductions from etch figures must be considered only as the maximum possible symmetry which the face can possess.

3. Optics

The study of transparent crystals by means of transmitted light readily gives information about the symmetry. On the basis of optical refraction (and all other second-order properties such as dia- or paramagnetic susceptibility) crystals can be divided into 5 groups as shown below. It must be remembered, however, that strain can lower the apparent symmetry owing to the great sensitivity of the optical behaviour.

Isotropic		(1) Cubic system
Anisotropic	Uniaxial	(2) Trigonal, tetragonal, hexagonal systems
	Biaxial	(3) Orthorhombic system
		(4) Monoclinic system
		(5) Triclinic system

4. Optical Activity

The symmetry information given by optical activity is quite different from that given by optical refraction in general. Optical activity is, of course, confined to the non-centrosymmetrical classes, but it occurs in only 15 out of the 21. In the 11 enantiomorphous classes a given crystal is either right- or left-handed. In the four non-enantiomorphous classes, m, $mm2$, $\bar{4}$ and $\bar{4}2m$, optical activity may also occur; when it does occur, directions of both right- and left-handed rotation of the plane of polarisation must exist in the same crystal. These classes are shown in Tables 3.8.1 and 3.8.2.

5. Pyroelectricity

True pyroelectricity (i.e. where the electric moment is produced solely by the change of temperature) can, theoretically, exist only where there is a unique polar axis in the point group of the crystal. But in experimental practice it is not possible to obviate the strains set up by differential heating or cooling throughout the crystal, and this gives rise to a piezoelectric effect mixed with the pyroelectric effect. Consequently, when the pyroelectric effect is observed, the only safe deduction is that the specimen must lack a centre of symmetry. Failure to detect the effect may be due to the extreme smallness of this effect, although modern methods are very sensitive. The deduction from lack of observed pyroelectric effect that the crystal possesses a centre of symmetry must be regarded as only provisional.

TABLE 3.8.1

The 32 Crystal Classes grouped according to Centrosymmetry, Laue Symmetry and Enantiomorphism

System	Enantio-morphous	Non-enantiomorphous		Enantio-morphous	Non-enantiomorphous	
Triclinic	1		$\bar{1}$			
Monoclinic	2	$m=\bar{2}$	$2/m$			
Orthorhombic				222	$mm2$	mmm
Tetragonal	4	$\bar{4}$	$4/m$	422	$4mm$ $\bar{4}2m$	$4/mmm$
Trigonal	3		$\bar{3}$	32	$3m$	$\bar{3}m$
Hexagonal	6	$\bar{6}$	$6/m$	622	$6mm$ $\bar{6}m2$	$6/mmm$
Cubic	23		$m3$	432	$\bar{4}3m$	$m3m$
	non-centro-symmetrical		centro-symmetrical	non-centro-symmetrical		centro-symmetrical

NOTE
The classes enclosed within any one rectangle have the same Laue symmetry.

TABLE 3.8.2

The 21 Non-centrosymmetrical Classes grouped according to Optical Activity and Piezoelectricity

	Triclinic	Monoclinic	Ortho-rhombic	Tetragonal	Trigonal	Hexagonal	Cubic	Types of piezoelectric moduli
Optically active					32			Compression and torsion
	1	2 m	$mm2$	4	3	6		Hydrostatic, compression and torsion
Non-optically active				$4mm$	$3m$	$6mm$		
						$\bar{6}$ $\bar{6}m2$		Compression and torsion
							$\bar{4}3m$	Torsion
Optically active			222	$\bar{4}$ 422 $\bar{4}2m$		622	23	
							432	Non-piezoelectric

TABLE 3.8.3

Polar and Non-polar Directions in the 21 Non-centrosymmetrical Classes

(All directions, other than those in the non-polar column, are polar.)

System	Class	Symmetry axes and crystallographic axes which are polar	Non-polar directions	
Triclinic	1	x-, y- and z-axes	None.	
Monoclinic 1st setting	2	z (diad)	All directions normal to z-axis.	
	m	x and y[1]	z-axis only.	
Monoclinic 2nd setting	2	y (diad)	All directions normal to y-axis.	
	m	x and z[1]	y-axis only.	
Orthorhombic	222	None	All directions normal to x-, y- or z-axis.	
	$mm2$	z (diad)	All directions normal to z-axis.	
Tetragonal	4	z (tetrad)	All directions normal to z-axis.	
	$\bar{4}$	None	z-axis and all directions normal to it.	
	422	None	All directions normal to x-, y- or z-axis or to [110] or [1$\bar{1}$0].	
	$4mm$	z (tetrad)	All directions normal to z-axis.	
	$\bar{4}2m$	None	All directions normal to x-, y- or z-axis.	
Trigonal	3	x, y, u[2] and z (triad)	None.	
	32	x, y, u (diads)	All directions normal to x-, y- or u-axis.	
	$3m$	z (triad)	x-, y- and u-axes only.	
Hexagonal	6	z (hexad)	All directions normal to z-axis.	
	$\bar{6}$	x, y, u[2]	z-axis only.	
	622	None	All directions normal to z-axis, or to the x-, y- or u-axes, or to any of the diads which lie between these axes.	
	$6mm$	z (hexad)	All directions normal to z-axis.	
	$\bar{6}m2$	3 diads	x-, y- and u-axes and all other directions normal to any of the diads which lie between these axes.	
Cubic	23	4 triads	All directions normal to any of the x-, y- or z-axes; i.e. directions with only one zero in the zone symbol.	
	432	None		In 432 only, add all directions normal to any of the six diads ⟨110⟩; i.e with two figures equal in the zone symbol.
	$\bar{4}3m$	4 triads		

(1) All zone axes in the symmetry plane are polar and no special importance in this connection is attached to those chosen as x and y (1st setting) or x and z (2nd setting).
(2) All zone axes normal to the z-axis are polar and no special importance in this connection is attached to the zone axes chosen as x-, y- and u-.

6. Piezoelectricity

The piezoelectric effect can, of course, be observed only in non-centrosymmetrical classes, but in one of these, 432, the moduli are all zero owing to the high symmetry. The 20 classes remaining can be divided up according to the types of moduli which they show. When compression (positive or negative) along a direction causes an electric moment along the same direction, the type of modulus is called "compression"; this can occur only along a polar direction in the crystal. When a torque is applied to the crystal in order to produce electric moment along a given axis, the type of modulus is called "torsion"; this occurs with both polar and non-polar axes, but is the only way of producing electric moment along a non-polar direction. When electric moment is produced by hydrostatic pressure, the type of modulus is called "hydrostatic"; this will produce electric moment only along a unique polar axis. The division of the 20 classes on the basis of type of piezoelectric moment is shown in Table 3.8.2, and in Table 3.8.3 are given the polar and non-polar directions for the 21 non-centrosymmetrical classes.

3.9. Names and Symbols of the Crystal Classes

Additional Note

Three of the various sets of names for the 32 crystal classes are given in Table 3.9.1. In the Friedel names for the trigonal classes the following amendment should be made.

Friedel based his seven systems on the symmetry of the lattice. Since a trigonal point group can have either a rhombohedral or a hexagonal lattice, each trigonal point group has two names. Correct the table below as follows, under "Friedel (1926)": If the lattice is rhombohedral, replace 'trigonal' by 'rhombohedral' in front of the adjectives that describe the merohedries. If the lattice is hexagonal, use the word 'hexagonal' in front of the following adjectives: ogdohedral, paratetartohedral, tetartohedral-holoaxial, antitetartohedral, parahemihedral.

TABLE 3.9.1. **Names and Symbols of the 32 Crystal Classes**

Point groups: International symbol		Schoenflies symbol	Class names			System used in this volume
Short	Full		Groth (1921)	Friedel (1926)	Rogers (1937)	
1	1	C_1	Pedial	Triclinic hemihedral	Asymmetric	Triclinic
$\bar{1}$	$\bar{1}$	$C_i(S_2)$	Pinakoidal	Triclinic holohedral	Pinakoidal	
2	2	C_2	Sphenoidal	Monoclinic hemihedral-holoaxial	Sphenoidal	Monoclinic
m	m	$C_s(C_{1h})$	Domatic	Monoclinic antihemihedral	Domatic	
$2/m$	$\frac{2}{m}$	C_{2h}	Prismatic	Monoclinic holohedral	Prismatic	
222	222	$D_2(V)$	Disphenoidal	Orthorhombic hemihedral-holoaxial	Rhombic-disphenoidal	Orthorhombic
$mm2$	$mm2$	C_{2v}	Pyramidal	Orthorhombic antihemihedral	Rhombic-pyramidal	
mmm	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$D_{2h}(V_h)$	Dipyramidal	Orthorhombic holohedral	Rhombic-dipyramidal	
4	4	C_4	Pyramidal	Tetragonal tetartohedral	Tetragonal-pyramidal	Tetragonal
$\bar{4}$	$\bar{4}$	S_4	Disphenoidal	Tetragonal sphenohedral-tetartohedral	Tetragonal-disphenoidal	
$4/m$	$\frac{4}{m}$	C_{4h}	Dipyramidal	Tetragonal parahemihedral	Tetragonal-dipyramidal	
422	422	D_4	Trapezohedral	Tetragonal hemihedral-holoaxial	Tetragonal-trapezohedral	
$4mm$	$4mm$	C_{4v}	Ditetragonal-pyramidal	Tetragonal antihemihedral	Ditetragonal-pyramidal	
$\bar{4}2m$	$\bar{4}2m$	$D_{2d}(V_d)$	Scalenohedral	Tetragonal sphenohedral-antihemihedral	Tetragonal-scalenohedral	
$4/mmm$	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	D_{4h}	Ditetragonal-dipyramidal	Tetragonal holohedral	Ditetragonal-dipyramidal	
3	3	C_3	Pyramidal	Trigonal tetartohedral	Trigonal-pyramidal	Trigonal
$\bar{3}$	$\bar{3}$	$C_{3i}(S_6)$	Rhombohedral	Trigonal parahemihedral	Rhombohedral	
32	32	D_3	Trapezohedral	Trigonal hemihedral-holoaxial	Trigonal-trapezohedral	
$3m$	$3m$	C_{3v}	Ditrigonal-pyramidal	Trigonal antihemihedral	Ditrigonal-pyramidal	
$\bar{3}m$	$\bar{3}\frac{2}{m}$	D_{3d}	Ditrigonal-scalenohedral	Trigonal holohedral	Hexagonal-scalenohedral	
6	6	C_6	Pyramidal	Hexagonal tetartohedral	Hexagonal-pyramidal	Hexagonal
$\bar{6}$	$\bar{6}$	C_{3h}	Trigonal-dipyramidal	Trigonohedral antitetartohedral	Trigonal-dipyramidal	
$6/m$	$\frac{6}{m}$	C_{6h}	Dipyramidal	Hexagonal parahemihedral	Hexagonal-dipyramidal	
622	622	D_6	Trapezohedral	Hexagonal hemihedral-holoaxial	Hexagonal-trapezohedral	
$6mm$	$6mm$	C_{6v}	Dihexagonal-pyramidal	Hexagonal antihemihedral	Dihexagonal-pyramidal	
$\bar{6}m2$	$\bar{6}m2$	D_{3h}	Ditrigonal-dipyramidal	Trigonohedral antihemihedral	Ditrigonal-dipyramidal	
$6/mmm$	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	D_{6h}	Dihexagonal-dipyramidal	Hexagonal holohedral	Dihexagonal-dipyramidal	
23	23	T	Tetrahedral-pentagonal-dodecahedral	Cubic tetartohedral	Tetartoidal	Cubic
$m3$	$\frac{2}{m}\bar{3}$	T_h	Dyakis-dodecahedral	Cubic parahemihedral	Diploidal	
432	432	O	Pentagonal-icositetrahedral	Cubic hemihedral-holoaxial	Gyroidal	
$\bar{4}3m$	$\bar{4}3m$	T_d	Hexakis-tetrahedral	Cubic antihemihedral	Hextetrahedral	
$m3m$	$\frac{4}{m}\bar{3}\frac{2}{m}$	O_h	Hexakis-octahedral	Cubic holohedral	Hexoctahedral	

4. SPACE-GROUP SYMMETRY

4.1. Introduction to Space-group Symmetry and Possible Reflections

The different Bravais lattices and their symbols are described in sections 2.1 to 2.3, while the point groups and their symbols are described in sections 3.1 to 3.3. In the present section tables of lattices and point-group symmetry are repeated, with the addition of the symmetry elements and symbols required in the analysis of space-group symmetry. Space groups are obtained by the application of point-group symmetry to infinite lattices, the possibility of translation symmetry being taken into account. The one- and two-dimensional groups are discussed first, and a full explanation is given of the tables of the latter (given in section 4.2). An analysis of the relations of the 17 two-dimensional space groups and of their determination is also given here. The corresponding discussion for the three-dimensional groups follows, but the systematic determination of these is given in a later section (4.4).

One- and Two-dimensional Space Groups

As was noted in section 2.1, there is only 1 one-dimensional lattice consisting of a row of equally spaced points. There are only two point groups, as the point can be one of no reflection or one of reflection, giving the groups 1 and *m*. Since the lattice simply repeats the point group along a line, no new combinations arise, and so there are only two one-dimensional space groups, the symbols of which may be taken as $p\,1$ and $p\,m$, using the script p to distinguish the one-dimensional lattice type (Fig. 4.1.1). One-dimensional groups will not be referred to again in these tables.

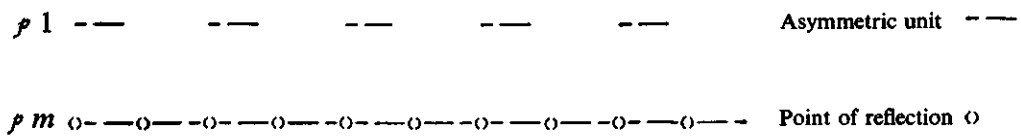


Fig. 4.1.1. The two one-dimensional space groups

There are four systems of axes in two dimensions (see section 2.1), but since the rectangular lattice can be centred as well as primitive, the total number of different lattices is 5. In the symbol of a two-dimensional space group the lattice type is always printed with a small letter (*p*, primitive; *c*, centred) in order to distinguish the group symbol from that of a three-dimensional one. The positions of the following symbols correspond to the directions given in Table 3.2.1.

The symbols which occur in two-dimensional groups are given in Table 4.1.1. The only operator involving translation is the glide line of symmetry denoted by *g*. The symbol *g* is peculiar to two-dimensional groups because in these the direction of glide is fixed by the orientation of the glide line, and hence there is no need to make the symbol specify the direction of glide, as in three-dimensional groups, where there is always a choice of direction in the glide plane.

TABLE 4.1.1. **Symbols of Two-dimensional Symmetry Operators**

Point symmetry (1st position)			Line symmetry (2nd and 3rd positions)		
Printed symbol	Graphical symbol	Operator	Printed symbol	Graphical symbol	Operator
2	⬮	2-fold (180°) point	*m*	———	Mirror-reflection line of symmetry
3	▲	3-fold (120°) point			
4	◆	4-fold (90°) point	*g*	- - - - - -	Glide-reflection line with translation of one half the repeat distance along the line
6	⬢	6-fold (60°) point			

NOTE. The symbol 1 denotes the identity operation and hence the absence of any other (point or line) symmetry.

In Table 4.1.2 are shown the relations between the two-dimensional lattices, point groups and space groups. The grouping of the point groups according to the kind of lattice with which they can combine to form space groups is analogous to the grouping of three-dimensional point groups into "systems." The space-group numbers given in the last column have been allocated to facilitate reference, as in the case of the three-dimensional groups.

TABLE 4.1.2. **Two-dimensional Lattices, Point Groups and Space Groups**

System and lattice symbol	Point group	Space-group symbols		Space-group number
		Full	Short	
Oblique *p* (primitive)	1	*p*1	*p*1	1
	2	*p*211	*p*2	2
Rectangular *p* and *c* (centred)	*m*	*p*1*m*1 *p*1*g*1 *c*1*m*1	*pm* *pg* *cm*	3 4 5
	2*mm*	*p*2*mm* *p*2*mg* *p*2*gg* *c*2*mm*	*pmm* *pmg* *pgg* *cmm*	6 7 8 9
Square *p*	4	*p*4	*p*4	10
	4*mm*	*p*4*mm* *p*4*gm*	*p*4*m* *p*4*g*	11 12
Hexagonal *p*	3	*p*3	*p*3	13
	3*m*	*p*3*m*1 *p*31*m*	*p*3*m*1 *p*31*m*	14 15
	6	*p*6	*p*6	16
	6*mm*	*p*6*mm*	*p*6*m*	17

NOTE. The two distinct space groups *p*3*m*1 and *p*31*m* correspond to different orientations of the point group relative to the lattice. This does not lead to distinct groups in any other case.

In the systematic tables of the two-dimensional space groups the page headings are:

Space group (short symbol)	Space-group number	Space group (full symbol)	Point group (short symbol)	System

(This is for a left-hand page and is reversed for a right-hand page.)

The left-hand diagram is that of the equivalent general positions of the space group, i.e. the complete set of positions produced by the operation of the symmetry elements of the space group upon one initial position chosen at random. The total number of general positions per unit cell is the number enclosed by the outline of the cell, but surrounding positions belonging to adjacent cells are always inserted as well in order to show the relations more clearly. The right-hand diagram is that of the space group proper, i.e. the group of spatially distributed symmetry operators. As in three-dimensional groups, any two-fold symmetry element at a distance t along any direction necessarily involves the

repetition of this element at a distance $(\frac{1}{2}+t)$ along the same direction. Also, the presence of a centred lattice involves the "interleaving" of mirror- and glide-reflection lines of symmetry; this can be seen in the *c*-lattice of the rectangular type. But it occurs also in diagonal directions of the square lattice because, if we take these directions as the axes of the unit cell, the lattice is centred. Similarly, it occurs with the plane hexagonal lattice in which rectangular axes can be chosen so as to give a centred lattice. Two mutually perpendicular lines of symmetry necessarily involve the presence of 2-fold symmetry about the point of their intersection. In all diagrams the *y*-axis is taken *across* the page pointing in a positive direction to the *right*; the positive direction of the *x*-axis is *down* the page.

Below the diagrams are tabulated the co-ordinates of the equivalent positions, the general positions being given first. The italic *x*, *y* stand here for general co-ordinates, expressed as fractions of the cell-edge lengths, along the corresponding *x*- and *y*-axes of the unit cell. To the left is given the number of the equivalent positions per unit cell in each set, then a letter to distinguish the set, this being analogous to the Wyckoff symbol in the three-dimensional space groups; then comes the symbol of the point symmetry existing at each of the equivalent positions of the set. When the initial position is taken on a mirror-reflection line of symmetry (not on a glide-reflection line) a set of special equivalent positions results in which one of the two co-ordinates is fixed. When the initial position is taken on a point about which there is rotational symmetry, a set of special equivalent positions results in which both of the co-ordinates are fixed. *The total number of equivalent positions per unit cell is always less in special sets than in the general set.*

The remaining information given for each two-dimensional space group consists of the possible reflections which may occur. The systematic absence of certain types of reflection can be regarded as a restriction imposed by the space group on the possible reflections (Table 4.1.3).

TABLE 4.1.3

Deduction of Two-dimensional Lattice Type and Symmetry Elements from Possible Reflections

Type of reflection	Restriction	Type of lattice or of symmetry element
hk	None	Primitive lattice *p*
	$(h+k)$ even only	Centred lattice *c*
*h*0	*h* even only	Glide line normal to *y*-axis
0*k*	*k* even only	Glide line normal to *x*-axis

Three-dimensional Space Groups

Symbols

The space-group symbol shows first the lattice type (Table 2.2.1), then the nature of the axes (rotation, inversion, screw) corresponding to the three sets of directions given in Table 3.3.2. Diad inversion axes may now correspond either to mirror planes or to glide planes (Table 4.1.6). The other types of rotation, inversion and screw axes are listed in Table 4.1.7.

Headings

The page headings are analogous to those of the two-dimensional space groups given on page 46. Again attention is drawn to the allocation of numbers (for convenience of reference only) to the space groups. Within each point group the space groups are arranged in the Schoenflies sequence. But the order in which the point groups are taken is different from that of Schoenflies. For some purposes the Schoenflies order within a given point group is unsuitable and a more convenient order is given in section 4.4. Table 4.1.4 shows the order adopted in sections 4.3 and 4.7.

TABLE 4.1.4. **Order adopted in Space-group Tables**

System	Point group	Space-group numbers
Triclinic	1	1
	$\bar{1}$	2
Monoclinic	2	3–5
	m	6–9
	$2/m$	10–15
Orthorhombic	222	16–24
	$mm2$	25–46
	mmm	47–74
Tetragonal	4	75–80
	$\bar{4}$	81–82
	$4/m$	83–88
	422	89–98
	$4mm$	99–110
	$\bar{4}2m$	111–122
	$4/mmm$	123–142
Trigonal	3	143–146
	$\bar{3}$	147–148
	32	149–155
	$3m$	156–161
	$\bar{3}m$	162–167
Hexagonal	6	168–173
	$\bar{6}$	174
	$6/m$	175–176
	622	177–182
	$6mm$	183–186
	$\bar{6}m2$	187–190
	$6/mmm$	191–194
Cubic	23	195–199
	$m3$	200–206
	432	207–214
	$\bar{4}3m$	215–220
	$m3m$	221–230

Diagrams of Equivalent General Positions

In the diagrams of equivalent general positions the conventional symbols and orientations adopted are as follows. Suppose the page to be lying horizontally on a table.

The heights of positions indicated on the projection are the co-ordinates along the z-axis.

The symbol + means a distance z in an upward direction from the level indicated, while the symbol − means the same distance in a downward direction. Where these symbols stand alone they are really shorthand for "a distance z upwards from the zero level of the unit cell" and "a distance z downward from the zero level of the unit cell" respectively. Where they are preceded by a fraction, e.g. $\frac{1}{4}$, $\frac{1}{2}$, $\frac{1}{3}$, this fraction indicates the level upwards of the unit cell from which z is added or subtracted.

If we consider the symbol ○ to indicate a position which could be occupied by a right-handed molecule, for example, then the symbol ⊙ indicates a position which could be occupied only by a left-handed molecule. The two positions denoted by ○ and ⊙, although symmetrically equivalent, are enantiomorphous, that is, related to each other by a symmetry operation involving a change of hand.

Where a mirror plane of symmetry exists parallel to the plane of projection, the positions superposed in the projection are indicated by the use of a ring divided vertically down the middle. The information given on the right and left sides respectively refer to one and the other of the two positions related by the mirror plane parallel to the plane of projection, as in − ⦶ +.

NOTE. It can be seen in the triclinic and in the second setting of the monoclinic system of axes that these diagrams are clinographic projections. The equivalent positions and the symmetry operators not lying in the plane of projection are projected on to it along the z-axis, which is inclined to this plane. In the first setting of the monoclinic, and in the orthorhombic, tetragonal, cubic and hexagonal systems, the diagrams are orthographic projections because the z-axis is normal to the plane of projection. In the drawings of the rhombohedral space groups the projection of the corresponding triple hexagonal unit cell is given as well as that of the (smallest) rhombohedral unit cell. But for convenience *the heights given are those along the z-axis (triad) of the hexagonal set of axes* (which is the body-diagonal direction of the rhombohedral cell), and so these diagrams are also orthographic projections.

Orientations of Axes in the Diagrams

In the diagrams of all systems of axes, except the rhombohedral, the projection is made on the plane of the x- and y-axes with the origin at the upper left corner. The positive direction of the x-axis points downwards and that of the y-axis to the right *in* the page, the angle γ between the two axes being related to the symmetry. The positive direction of the z-axis points upwards *from* the page, its angular relations to the other two axes being related to the symmetry.

TABLE 4.1.5. **Arrangements of Axes in Space-group Tables**

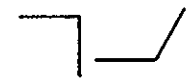
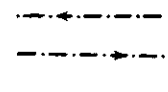
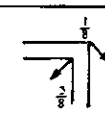
System of axes	Angle γ between $+x$ and $+y$	Relation of z-axis to plane of projection
Triclinic	General	General
Monoclinic 1st setting (z-axis unique) 2nd setting (y-axis unique)	 General 90°	 Perpendicular Normal to y-axis but not to x-axis
Orthorhombic .. .. Tetragonal .. .. Cubic	90°	Perpendicular
Hexagonal	120°	Perpendicular
Rhombohedral	All three axes x-, y-, z-, are equally inclined to the plane of projection; the origin is at height zero in the centre of the diagram. The diagram shows the appearance of the cell seen along [111] towards the origin, the three *lower* edges (the x-, y-, z-axes) being omitted.	

Symmetry Symbols

In the diagrams of space groups, heights are indicated in the manner described above for equivalent general positions. Any two-fold symmetry operator at any primitive translation t along an axis always implies one also at $(\frac{1}{2}+t)$ along the same axis. It should be noted that a similar rule does *not* apply to equivalent positions.

The graphical symbols used in the drawings are given in Tables 4.1.6 and 4.1.7, which also give the nature of the translations corresponding to the various symbols.

TABLE 4.1.6. **Symbols of Symmetry Planes**

Symbol	Symmetry plane	Graphical symbol: Normal to plane of projection	Graphical symbol: Parallel to plane of projection	Nature of glide translation
m	Reflection plane (mirror)			None (NOTE. If the plane is at $z=\frac{1}{4}$ this is shown by printing $\frac{1}{4}$ beside the symbol.)
a, b	Axial glide plane			$a/2$ along [100] or $b/2$ along [010]; or along ⟨100⟩.
c		.....	None	$c/2$ along z-axis; or $(a+b+c)/2$ along [111] on rhombohedral axes.
n	Diagonal glide plane (net)			$(a+b)/2$ or $(b+c)/2$ or $(c+a)/2$; or $(a+b+c)/2$ (tetragonal and cubic).
d	"Diamond" glide plane			$(a\pm b)/4$ or $(b\pm c)/4$ or $(c\pm a)/4$; or $(a\pm b\pm c)/4$ (tetragonal and cubic). See note below.

NOTE. In the "diamond" glide plane the glide translation is half of the resultant of the two possible axial glide translations. The arrows in the first diagram show the direction of the horizontal component of the translation when the z-component is positive. In the second diagram the arrow shows the actual direction of the glide translation; there is always another diamond-glide reflection plane parallel to the first with a height difference of $\frac{1}{4}$ and with the arrow pointing along the other diagonal of the cell face.

TABLE 4.1.7

Symbols of Symmetry Axes

Symbol	Symmetry axis	Graphical symbol	Nature of right-handed screw translation along the axis	Symbol	Symmetry axis	Graphical symbol (normal to plane of paper)	Nature of right-handed screw translation along the axis
1	Rotation monad	None	None	4	Rotation tetrad		None
$\bar{1}$	Inversion monad		None	4_1	Screw tetrads		$c/4$
2	Rotation diad	(normal to paper)	None	4_2			$2c/4$
				4_3			$3c/4$
		(parallel to paper)		$\bar{4}$	Inversion tetrad		None
2_1	Screw diad	(normal to paper)	$c/2$	6	Rotation hexad		None
		(parallel to paper)	Either $a/2$ or $b/2$	6_1	Screw hexads		$c/6$
		Normal to paper		6_2			$2c/6$
3	Rotation triad		None	6_3			$3c/6$
				6_4			$4c/6$
3_1	Screw triads		$c/3$	6_5			$5c/6$
3_2			$2c/3$				
$\bar{3}$	Inversion triad		None	$\bar{6}$	Inversion hexad		None

In any space-group symbol the order in which the various parts of the symbol are written is, in general, the same as in the corresponding point groups (see Table 3.3.2).

The nomenclature described is sufficient to cover all but four of the 230 space groups. A convention is necessary to distinguish between the members of the pairs $I222$, $I2_12_12_1$ and $I23$, $I2_13$. This arises because in all four of these groups both 2-fold rotation and screw axes are present in each of the three mutually perpendicular directions denoted, the arrangement in space of these axes being different in the different members of each pair. Thus we have to use a conventional symbol to distinguish between the members of each pair. The symbol 2 is used in the groups in which all three 2-fold rotation axes intersect in a point (the three screw axes intersecting in another point), as in the groups $I222$ and $I23$. On the other hand, the symbol 2_1 is used where this intersection of all three axes of the same kind does not occur, as in the groups $I2_12_12_1$ and $I2_13$.

Changes in Space-group Symbols here used in Systematic Description as compared with the Old International Tables (1935)

Triclinic system
No change.

Monoclinic system
Addition of alternative setting with z- as the unique axis.

Orthorhombic system
In the class $mm2$, the symbol for the unique axis parallel to the z-axis is given for all space-group symbols. This is just the full Hermann-Mauguin symbol given in vol. 1, page 35, of the old *International Tables* (1935).

Tetragonal system
In class 422 the full symbol is used. In classes $4mm$ and $4/mmm$ the symbols have been altered for 16 space groups. In these the subscripts have been added to show the nature of the tetrad axis. The old symbols were quite correct because, given the rest of the symbol, it is sufficient to know that the system is tetragonal in order to identify the space group uniquely. But the new symbols give the nature of the tetrad axis directly.

Class							
$4mm$	Old Symbols	$P4cm$	$P4nm$	$P4mc$	$P4bc$	$I4md$	$I4cd$
	New	$P4_2cm$	$P4_2nm$	$P4_2mc$	$P4_2bc$	$I4_1md$	$I4_1cd$

Class						
$4/mmm$	Old Symbols	$P4/mmc$	$P4/mcm$	$P4/nbc$	$P4/nnm$	$P4/mbc$
	New	$P4_2/mmc$	$P4_2/mcm$	$P4_2/nbc$	$P4_2/nnm$	$P4_2/mbc$

Class						
$4/mmm$	Old Symbols	$P4/mnm$	$P4/nmc$	$P4/ncm$	$I4/amd$	$I4/acd$
	New	$P4_2/mnm$	$P4_2/nmc$	$P4_2/ncm$	$I4_1/amd$	$I4_1/acd$

Trigonal and hexagonal systems
The old symbol H denoting the alternative orientation of the hexagonal lattice is not used. The old symbol C is replaced by the symbol P because the conventional choice of unit cell is a primitive one. The rhombohedral lattice (R_{obv} or R_{hex}) is always denoted by the symbol R in order to distinguish it from the hexagonal lattice denoted by P. In class 622 the full symbol is used. In classes $6mm$ and $6/mmm$ the symbols have been altered for 4 space groups, for the reason explained above under the tetragonal system.

Class				Class			
$6mm$	Old Symbols	$C6cm$	$C6mc$	$6/mmm$	Old Symbols	$C6/mcm$	$C6/mmc$
	New	$P6_3cm$	$P6_3mc$		New	$P6_3/mcm$	$P6_3/mmc$

Cubic system
In class 432 the full symbol is used.

Equivalent Positions and Point Symmetry

The first column in section 4.3 gives the number of equivalent positions in the set, each set being denoted by a letter in the second column. This letter is the same as that given by Wyckoff (1930)[1] but the order has been reversed so that the general set is given first, followed by the special sets in order of increasing point symmetry of the special positions. In the third column is given the symbol of the point symmetry of the positions of each set. Next are given the co-ordinates of all the equivalent positions in each set, the symbols in italic type x, y, z being used for the general co-ordinates, expressed as fractions of the unit-cell edge lengths, along the three corresponding x-, y- and z-axes. In the description based on rhombohedral axes the letters used for these co-ordinates are in ordinary roman type (not italic) x, y, z to avoid confusion with the alternative description on hexagonal axes for which the *actual values* of the co-ordinates will be different. When the lattice is face- or body-centred, the co-ordinates of the centring points are given at the top; to obtain all the positions of any set, these point co-ordinates must be added in turn to all those given in the lines below. No official importance is attached to the particular setting of the space group adopted as standard in this section (see section 6.2).

Determination of Diffraction Symbol from Possible Reflections

From observations of "extinctions" (sets of reflections which are systematically absent), the existence of certain restrictions, imposed by the space group, on possible reflections is deduced. From these possible reflections an "extinction symbol" of the particular crystal can be derived (see section 4.4).

This extinction symbol is that part of the space-group symbol that is observable by direct X-ray methods. This includes first the lattice type and then any screw axes or glide planes (not the result of the lattice type) with their appropriate translations. The parts of the space-group symbol not directly observable (rotation axes, mirror planes: the apparent presence of which may be due only to the Friedel condition) are left unfilled except by a dot (Table 4.4.3). One method of procedure is as follows:

The first step is the determination, from *hkl* reflections, of the lattice type corresponding to the unit cell selected (Table 4.1.8). From the shape of the unit cell the system will be provisionally known, although it is the symmetry of the lattice which finally decides this, as the shape may be conditioned by parameters which have, accidentally, special values. In practice, in order to avoid confusion, it is important to observe the conventional rules of setting appropriate to the system (see section 2.3.1.). If the lattice type turns out to be centred, examination should be made to see whether the smallest unit cell has been selected, within the conventional rules appropriate to the system, since the tables for space-group determination are based on such a selection of the unit cell. All possibilities of centring in a more symmetrical lattice should be eliminated before the conclusion is reached that the lattice type is primitive (see also section 5.1). The Laue group is next determined. Given single crystals, this is always uniquely possible (sections 3.4, 3.7 and 3.8). This confirms the system also. Lastly, the nature of the symbols in the primary, secondary and tertiary point-group positions (see Table 3.3.2), which indicate the existence of translation elements of symmetry (that is, of glide-reflection planes and screw axes) must be found.

The complete diffraction symbol (as first defined by M. J. Buerger, *Z. Kristallogr.* (1935), **91**, 287) gives the Laue symbol followed by the extinction symbol. It should be noted that the formulation of the diffraction symbol does not require a knowledge of the shape of the unit cell (lengths of sides and values of angles) and another method of procedure is to leave the determination of these until after the determination of Laue symmetry and the lattice and translation extinctions. In other words, the complete diffraction symbol may be determined first by the use, say, of moving-film methods; and the actual dimensions of the unit cell may be determined independently.

Note

Reference may be made to section 4.4 which has been completely revised for the present reprint.

[1] Wyckoff, R. W. G., 1930. *The Analytical Expression of the Results of the Theory of Space Groups*, 2nd ed. (Washington).

TABLE 4.1.8. **Determination of Lattice Type from General Reflections, *hkl***

Condition for possible reflection[1]	Lattice type	Symbol
$h+k=2n$	Centred on the C-face (001)	C
$k+l=2n$	Centred on the A-face (100)	A
$l+h=2n$	Centred on the B-face (010)	B
h, k, l all odd or all even	Centred on all faces	F
$h+k+l=2n$	Body centred	I
$-h+k+l=3n$[2]	Obverse position } rhombohedral	R
$+h-k+l=3n$[2]	Reverse position } lattice[3]	
$h-k=3n$	Hexagonal. Triple unit cell as in Fig. 2.5.2(a)	H[4]
No restriction	Primitive	P[5]

(1) The symbol n stands here for any integer.
(2) These conditions refer to indexing on hexagonal axes which are always used both for hexagonal crystals and, in the first instance, for trigonal crystals, although some of the latter may turn out to be more simply described on rhombohedral axes.
(3) For definition of "obverse" and "reverse" see section 2.5, Fig. 2.5.3.
(4) The symbol H is dropped in the present volume for systematic description (see, however, section 2.5).
(5) The symbol P is applied in the present work also to the primitive hexagonal lattice which was designated by the symbol C in the former *International Tables* (1935). See Note 7, Table 2.2.1.

In Table 4.1.9 are given the restrictions imposed on certain special reflections by the presence of certain translation elements of symmetry in the space group. (Here the term "special reflections" means those with one or two indices zero, and should not be confused with "reflections corresponding to special positions" in the space group.) In this table are given only data which are required for space-group determination, and these are given only in the form in which subsequent use is made of them. In the last column of the table are given the systems of co-ordinate axes with which particular types of symmetry elements are associated. In this table it should be noticed that in some cases the symbol represents a *form* of planes or axes, as is shown by the use of the appropriate brackets. Table 4.1.9 also shows what each symbol represents, and gives, for each system, a list of the reflections to be considered in connection with the determination of translation elements of symmetry.

The deduction of the presence of a translation element of symmetry should be made only when the corresponding condition for possible reflections is independent of any more general condition. The deduction should always proceed from the more general to the more special, i.e. from lattice type to glide planes to screw axes. Any special condition which is a sub-condition of a more general one should be disregarded, since the translation element of symmetry which is apparently indicated in this way may, or may not, be present in the space group. For example, in the space group $C1c1$ (page 89) the conditions of possible reflection for the general positions are:

$$\begin{aligned} hkl&: h+k=2n \text{ and} \\ h0l&: h=2n,\ l=2n \text{ and} \\ 0k0&: k=2n \end{aligned}$$

But the h in the second line and the k in the third line are even only because of the lattice condition. In the actual space group there is a glide component along the x-axis in a plane normal to the y-axis, but this is a diagonal glide plane which interleaves the c-glide planes because of the action of the C-face-centred lattice; there is no a-glide plane present. The space group could be called $C1n1$ as an alternative to $C1c1$, but it cannot be called $C1a1$, which is a different space group. Although reflections of the type $0k0$ occur only when k is even, this is not an independent condition, and there is, in fact, no screw diad axis in this space group.

When all possible information has been gathered from the conditions for possible reflections, this is put in a standard order, according to the Laue class (Table 4.4.3), in the diffraction symbol. Use is then made of the tables in section 4.4 in order to track down the space group, as far as is possible in this way. Use may also be made of Table 6.2.1 (see p. 549) if necessary.

TABLE 4.1.9. **Determination of Translation Elements of Symmetry from Special Reflections**

Type of reflection	Condition for possible reflection[1]	Glide plane or screw axis: Orientation	Component	Symbol[1]	Systems of co-ordinate axes involved	
$0kl$	$k=2n$	(100)	$b/2$	b	Orthorhombic, tetragonal, cubic	
	$l=2n$		$c/2$	c		
	$k+l=2n$		$b/2+c/2$	n		
	$k+l=4n$ $(k,l=2n)$		$b/4\pm c/4$	d		
$h0l$	$l=2n$	(010)	$c/2$	c	Monoclinic (2nd setting)	Orthorhombic
	$h=2n$		$a/2$	a		
	$l+h=2n$		$c/2+a/2$	n		
	$l+h=4n$ $(l,h=2n)$		$c/4\pm a/4$	d		
$hk0$	$h=2n$	(001)	$a/2$	a	Monoclinic (1st setting), tetragonal	Orthorhombic
	$k=2n$		$b/2$	b		
	$h+k=2n$		$a/2+b/2$	n		
	$h+k=4n$ $(h,k=2n)$		$a/4\pm b/4$	d		
$h\bar{h}0l$	$l=2n$	$(11\bar{2}0)$	$c/2$	c	Hexagonal	
$hh2\bar{h}l$	$l=2n$	$(1\bar{1}00)$	$c/2$	c		
hhl	$(2h+)l=2n$	$(1\bar{1}0)$	$(a/2+b/2+)c/2$	$(n)\ c$	Rhombohedral[2]	Tetragonal, cubic[3]
	$2h+l=4n$		$a/4+b/4+c/4$	d		
$h00$	$h=2n$	[100]	$a/2$	2_1	Orthorhombic, tetragonal	Cubic
				4_2		
	$h=4n$		$a/4$	4_1, 4_3		
$0k0$	$k=2n$	[010]	$b/2$	2_1	Monoclinic (2nd setting), orthorhombic	
$00l$	$l=2n$	[001]	$c/2$	2_1	Monoclinic (1st setting), orthorhombic	
				4_2	Tetragonal	
	$l=4n$		$c/4$	4_1, 4_3		
$000l$	$l=2n$	[0001]	$c/2$	6_3	Hexagonal	
	$l=3n$		$c/3$	3_1, 3_2, 6_2, 6_4		
	$l=6n$		$c/6$	6_1, 6_5		

(1) The symbol n stands for an integer in column 2 and for a diagonal glide plane in column 5.
(2) For hhl (rhombohedral axes) the condition $2h+l=2n$ (that is, $l=2n$) implies interleaving n and c glide-planes $(1\bar{1}0)$ The form of reflections does not include $h\bar{h}l$.
(3) For hhl (tetragonal and cubic systems, where the form includes $h\bar{h}l$, etc.) the only independent systematic conditions for possible reflection are $2h+l=2n$ (that is, $l=2n$) and $2h+l=4n$. The former implies interleaving n and c glide-planes $(1\bar{1}0)$ and is found not only in P tetragonal space groups, but also in P and F cubic space groups. See p. 554 for comments on tetragonal and cubic symbols.

Conditions for Possible Reflections

In section 4.3 the different kinds of reflections which can occur for the 230 space groups are given for each space group and for each set of equivalent positions. For sets of special positions, the general conditions must always be added to those given opposite each special set. It should be remembered that the special conditions only apply when the special positions are assumed to be occupied by spherical groups. In the determination of the actual space group it is the reflections (general and special) for the general equivalent positions which are considered, not those for special positions.

Certain shorthand methods of presenting these data should be noted.

1. The symbol n is used to represent any integer. For example, $h0l$: $h=2n$ means that reflections of the type $h0l$ occur only when h is even. (There is no reference here to an n-glide.)
2. In special reflections the printing of parentheses indicates that the condition enclosed is imposed by a more general condition; the conditions in parentheses should be disregarded. In section 4.3, the example of the space group $Clcl$, discussed on p. 53, is printed in the following way:

$$\begin{array}{l} hkl\colon\ h+k=2n \\ h0l\colon\ l=2n;\quad (h=2n) \\ 0k0\colon\ (k=2n) \end{array}$$

The following types of special reflection are used in the determination of translation elements of symmetry and hence of space groups:

Monoclinic	1st setting: $hk0$, $00l$. 2nd setting: $h0l$, $0k0$.	Tetragonal	hhl, $0kl$ ($h0l$), $hk0$, $h00$ ($0k0$), $00l$.
Orthorhombic	$0kl$, $h0l$, $hk0$. $h00$, $0k0$, $00l$.	Cubic	hhl ↻, $0kl$ ↻ $h00$ ↻.
Trigonal and Hexagonal	$hh2\bar{h}l$, $h\bar{h}0l$, $000l$ (hhl rhombohedral)		

Other Data

1. In the monoclinic system all the data are given for the two alternative conventional settings.
   1st setting: with the unique axis as the z-axis and the centred lattice as B.
   2nd setting: with the unique axis as the y-axis and the centred lattice as C.

   NOTE. By a decision of the International Union of Crystallography (Stockholm 1951) the 2nd setting is accepted as standard for morphological and structural crystallographic studies.
2. In the present tables only those symbols are used in the monoclinic and orthorhombic systems which conform to the rules of precedence of symmetry operators—

   (highest) m, a, b, c, n, d (lowest)

   planes being taken before axes and rotation axes before screw axes. No. 73, which should be $Ibaa$ on the above rule, is an exception, as there is a certain advantage here in retaining the cyclic order, $Ibca$.
3. For the space groups of the triclinic, monoclinic and orthorhombic systems the symmetries of the projections on to the planes (001), (100) and (010) are given in terms of the symbols of the two-dimensional groups. The sides of the unit cell of the projection are denoted by the symbols a', b', c', and their magnitudes, relative to those of the sides a, b, c of the original three-dimensional unit cell, are given. The symbol for the projection symmetry contains either two or three separate symbols. The first always shows the lattice type. If there is no reflection symmetry the second shows the rotational symmetry about the point (origin). If there is reflection symmetry the rotation symmetry symbol can be omitted. The three projections on (001), (100) and (010) then give, in the second and third places of the symbol, the symmetries about lines normal to x- and y-, y- and z-, z- and x- respectively. The result of keeping to the cyclic order is that some of the two-dimensional symbols used are alternatives to the conventional ones listed in section 4.2.

Note on Line Groups in Two and Three Dimensions and on Plane Groups in Three Dimensions

It must be noted that the two one-dimensional space groups given above are line groups (rows) in one dimension only. It is possible (Speiser, 1927, pp. 82–3) to deduce 7 line groups (borders) in two dimensions, that is, if symmetry in the plane is permitted, and 75 line groups in three dimensions if all crystallographic symmetries, but no other, are permitted. This number includes both members of eight enantiomorphous pairs. It should be noted that in the line groups in three dimensions the distinction between secondary and tertiary axes is lost. These line groups can be formally obtained by substituting $x=0$ or $y=0$ in the two-dimensional space-group co-ordinates, or by substituting $y=z=0$ or $z=x=0$ or $x=y=0$ in the three-dimensional space-group co-ordinates, and selecting those which then reduce to non-zero co-ordinates in one direction (x, y or z) only. They are in general not strictly one-dimensional space groups although they include the latter.

Speiser (1927, pp. 84–6) has deduced 31 possible two-dimensional strips or ribbons by permitting symmetry operations above and below the plane, but regarded as line groups in three dimensions these are not all distinct, although they are distinct for certain mathematical purposes.

If the symmetry is not limited to the crystallographic axes (1, 2, 3, 4, 6; $\bar{1}$, $\bar{2}$, $\bar{3}$, $\bar{4}$, $\bar{6}$ and combinations of these) there are an infinite number of distinct line groups in three dimensions corresponding to an unlimited choice of symmetry axes.

Similarly 80 plane groups (nets), which include the 17 strictly two-dimensional space groups, can be deduced if the two sides of the plane are regarded as distinct (inversion, or mirror- or glide-reflection across the plane permitted). These are formally obtained by substituting $x=0$ or $y=0$ or $z=0$ in the three-dimensional space-group co-ordinates and selecting those which then reduce to non-zero co-ordinates in two directions only. In all cases the symmetry relationships of the points must be taken into account. Thus x,y; $\bar{x},y$; $x,\bar{y}$; $\bar{x},\bar{y}$ could correspond to points related by mm, or by 22, or by $2\bar{2}$ ($2/m$) symmetry, and these would be three different plane groups in three dimensions, although only the first is a strictly two-dimensional group.

Such line groups and plane groups are useful in the consideration of some projection properties and in the study of random or semi-crystalline structures of various kinds. They are not further discussed in this Volume, but reference may be made to the papers given below, for their systematic description.

References

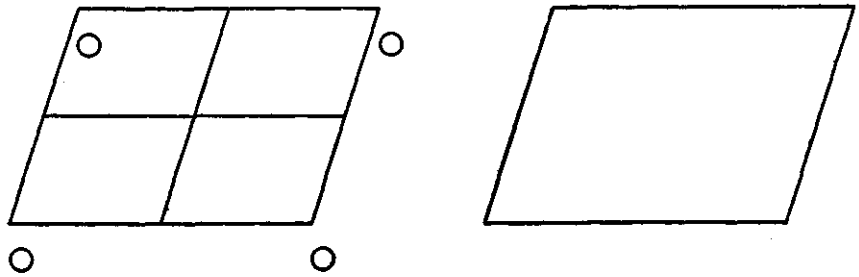
Alexander, E., and Herrmann, K. *Zeit. f. Krist.*, **69**, 285 (1928); **70**, 328, 460 (1929).
Alexander, E. *Ibid.*, **70**, 367 (1929); **89**, 606 (1934).
Speiser, A. *Die Theorie der Gruppen von endlicher Ordnung*, 2te, Aufl. Berlin, Springer (1927).
Weber, L. *Zeit. f. Krist.*, **70**, 309 (1929).

4.2. THE 17 TWO-DIMENSIONAL SPACE GROUPS:

Equivalent Positions, Symmetry and Possible Reflections

p 1

No. 1 *p* 1 1 Oblique

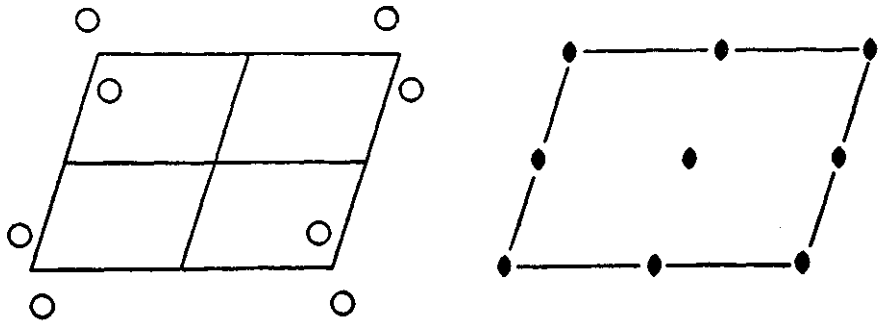


Origin on 1

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
1	*a*	1	$x,y.$	No conditions

p 2

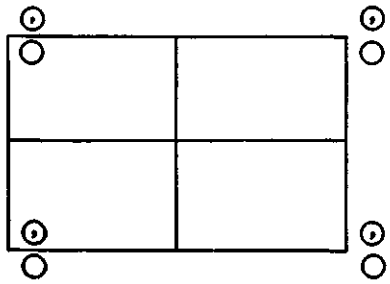
No. 2 *p* 2 1 1 2 Oblique

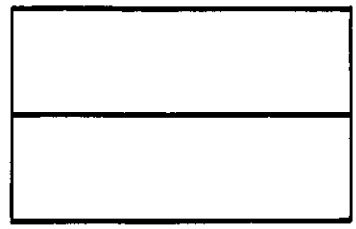


Origin at 2

				General:
2	*e*	1	$x,y;\ \bar{x},\bar{y}.$	No conditions
				Special:
1	*d*	2	$\frac{1}{2},\frac{1}{2}.$	No conditions
1	*c*	2	$\frac{1}{2},0.$	
1	*b*	2	$0,\frac{1}{2}.$	
1	*a*	2	$0,0.$	

Rectangular m — $p\,1\,m\,1$ — No. 3 — pm

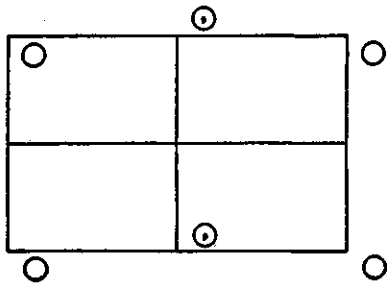


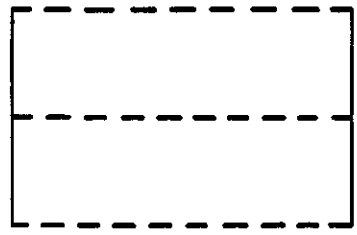


Origin on m

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
2	c	1	$x,y;\ \bar{x},y.$	No conditions
				Special:
1	b	m	$\frac{1}{2},y.$	No conditions
1	a	m	$0,y.$	

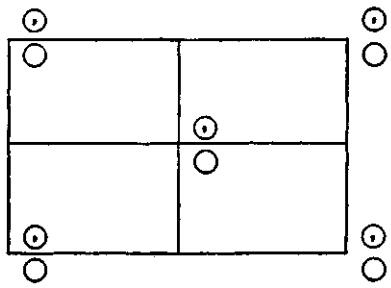
Rectangular m — $p\,1\,g\,1$ — No. 4 — pg

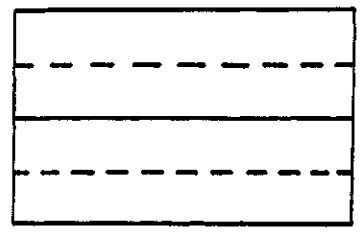




Origin on g

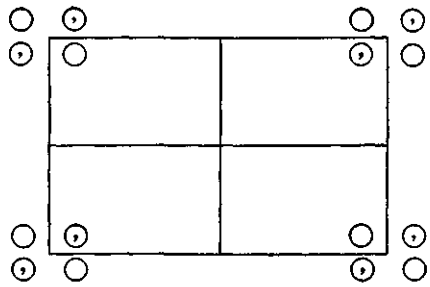
				General:
2	a	1	$x,y;\ \bar{x},\frac{1}{2}+y.$	hk: No conditions $0k$: $k=2n$

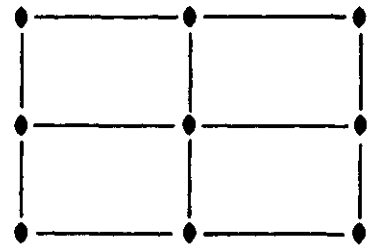




Origin on *m*

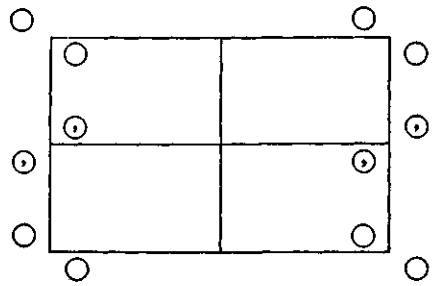
Number of positions, Wyckoff notation, and point symmetry	Co-ordinates of equivalent positions	Conditions limiting possible reflections
	$(0,0;\ \frac{1}{2},\frac{1}{2})+$	
		General:
4 *b* 1	$x,y;\ \bar{x},y.$	hk: $h+k=2n$
		Special: as above only
2 *a* *m*	$0,y.$	

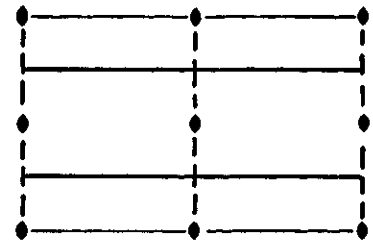




Origin at 2*mm*

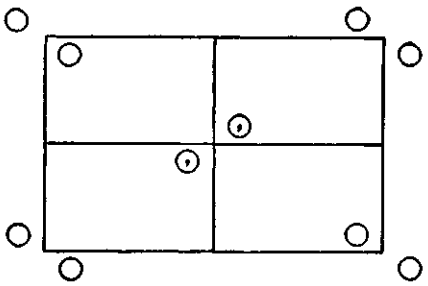
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	*i*	1	$x,y;\ \bar{x},y;\ \bar{x},\bar{y};\ x,\bar{y}.$	No conditions
				Special:
2	*h*	*m*	$\frac{1}{2},y;\ \frac{1}{2},\bar{y}.$	No conditions
2	*g*	*m*	$0,y;\ 0,\bar{y}.$	
2	*f*	*m*	$x,\frac{1}{2};\ \bar{x},\frac{1}{2}.$	
2	*e*	*m*	$x,0;\ \bar{x},0.$	
1	*d*	*mm*	$\frac{1}{2},\frac{1}{2}.$	
1	*c*	*mm*	$\frac{1}{2},0.$	
1	*b*	*mm*	$0,\frac{1}{2}.$	
1	*a*	*mm*	$0,0.$	

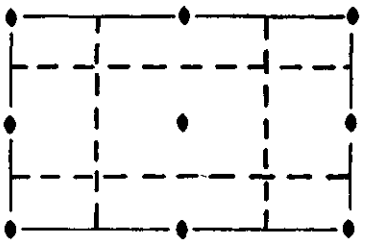




Origin at 2

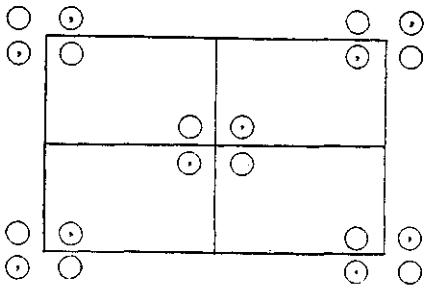
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	*d*	1	$x,y;\ \bar{x},\bar{y};\ \frac{1}{2}+x,\bar{y};\ \frac{1}{2}-x,y.$	*hk*: No conditions *h*0: $h=2n$
				Special: as above, plus
2	*c*	*m*	$\frac{1}{4},y;\ \frac{3}{4},\bar{y}.$	no extra conditions
2	*b*	2	$0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2}.$	*hk*: $h=2n$
2	*a*	2	$0,0;\ \frac{1}{2},0.$	

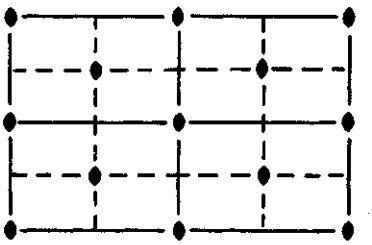




Origin at 2

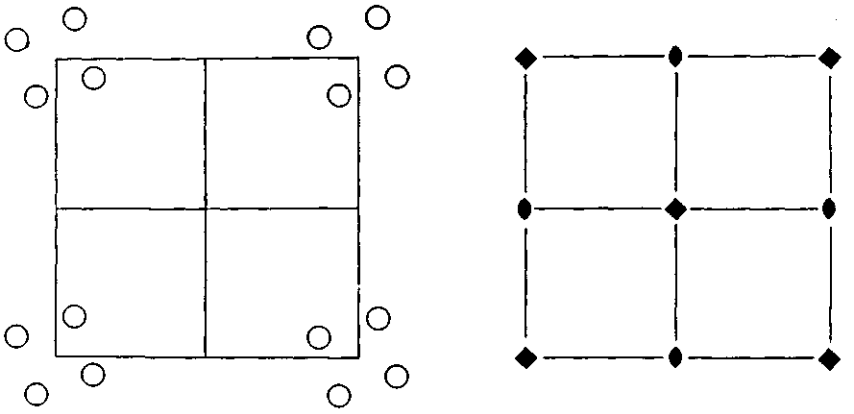
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	*c*	1	$x,y;\ \bar{x},\bar{y};\ \frac{1}{2}+x,\frac{1}{2}-y;\ \frac{1}{2}-x,\frac{1}{2}+y.$	hk: No conditions $h0$: $h=2n$ $0k$: $k=2n$
				Special: as above, plus
2	*b*	2	$\frac{1}{2},0;\ 0,\frac{1}{2}.$	hk: $h+k=2n$
2	*a*	2	$0,0;\ \frac{1}{2},\frac{1}{2}.$	





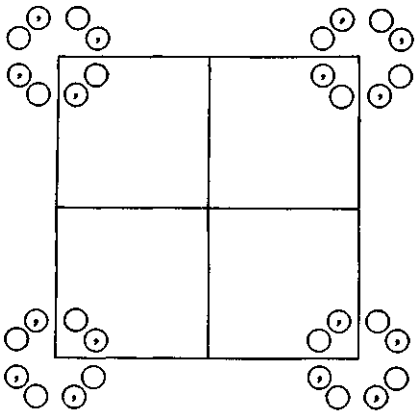
Origin at $2mm$

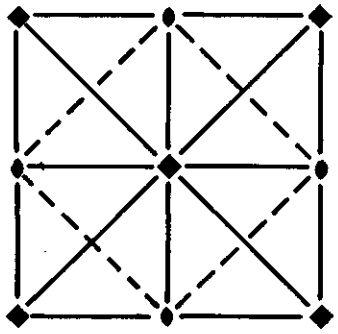
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0;\ \frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
8	f	1	$x,y;\ \bar{x},y;\ \bar{x},\bar{y};\ x,\bar{y}.$	hk: $h+k=2n$
				Special: as above, plus
4	e	m	$0,y;\ 0,\bar{y}.$	no extra conditions
4	d	m	$x,0;\ \bar{x},0.$	
4	c	2	$\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4}.$	hk: $h=2n$; $(k=2n)$
2	b	mm	$0,\frac{1}{2}.$	no extra conditions
2	a	mm	$0,0.$	



Origin at 4

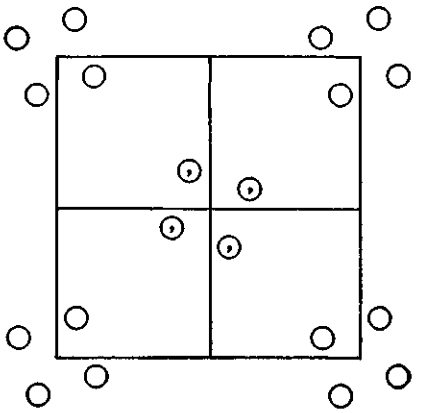
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	d	1	$x,y;\ \bar{x},\bar{y};\ y,\bar{x};\ \bar{y},x.$	No conditions
				Special:
2	c	2	$\frac{1}{2},0;\ 0,\frac{1}{2}.$	hk: $h+k=2n$
1	b	4	$\frac{1}{2},\frac{1}{2}.$	No conditions
1	a	4	$0,0.$	No conditions

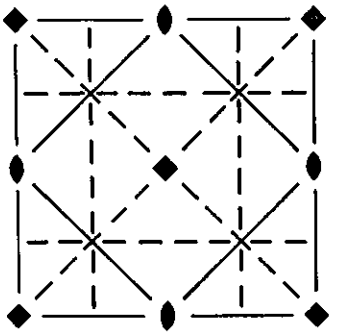




Origin at $4mm$

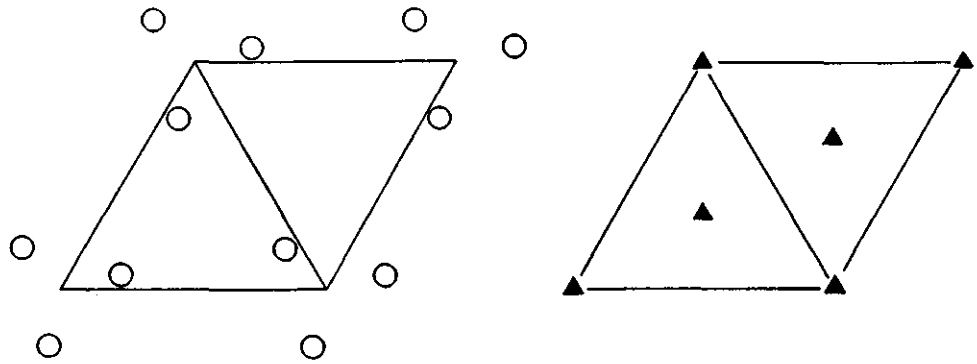
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	g	1	$x,y;\ \bar{x},\bar{y};\ y,\bar{x};\ \bar{y},x;\ \bar{x},y;\ x,\bar{y};\ \bar{y},\bar{x};\ y,x.$	No conditions
				Special:
4	f	m	$x,x;\ \bar{x},\bar{x};\ \bar{x},x;\ x,\bar{x}.$	No conditions
4	e	m	$x,\frac{1}{2};\ \bar{x},\frac{1}{2};\ \frac{1}{2},x;\ \frac{1}{2},\bar{x}.$	No conditions
4	d	m	$x,0;\ \bar{x},0;\ 0,x;\ 0,\bar{x}.$	No conditions
2	c	mm	$\frac{1}{2},0;\ 0,\frac{1}{2}.$	hk: $h+k=2n$
1	b	$4mm$	$\frac{1}{2},\frac{1}{2}.$	No conditions
1	a	$4mm$	$0,0.$	No conditions





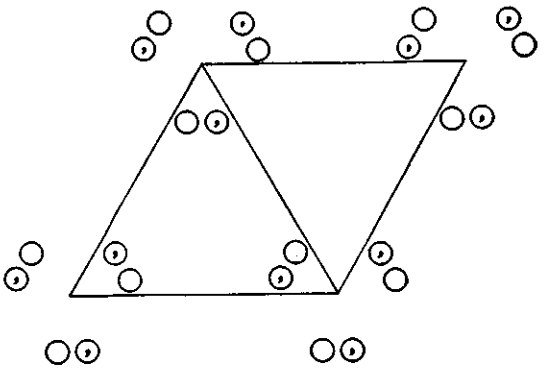
Origin at 4

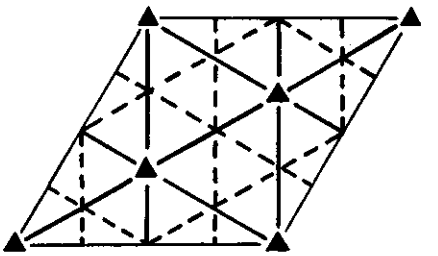
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	d	1	$x,y;\ y,\bar{x};\ \frac{1}{2}-x,\frac{1}{2}+y;\ \frac{1}{2}-y,\frac{1}{2}-x;$ $\bar{x},\bar{y};\ \bar{y},x;\ \frac{1}{2}+x,\frac{1}{2}-y;\ \frac{1}{2}+y,\frac{1}{2}+x.$	hk: No conditions $h0$: $h=2n$ ($0k$: $k=2n$) hh: No conditions
				Special: as above, plus
4	c	m	$x,\frac{1}{2}+x;\ \bar{x},\frac{1}{2}-x;\ \frac{1}{2}+x,\bar{x};\ \frac{1}{2}-x,x.$	no extra conditions
2	b	mm	$\frac{1}{2},0;\ 0,\frac{1}{2}.$	hk: $h+k=2n$
2	a	4	$0,0;\ \frac{1}{2},\frac{1}{2}.$	



Origin at 3

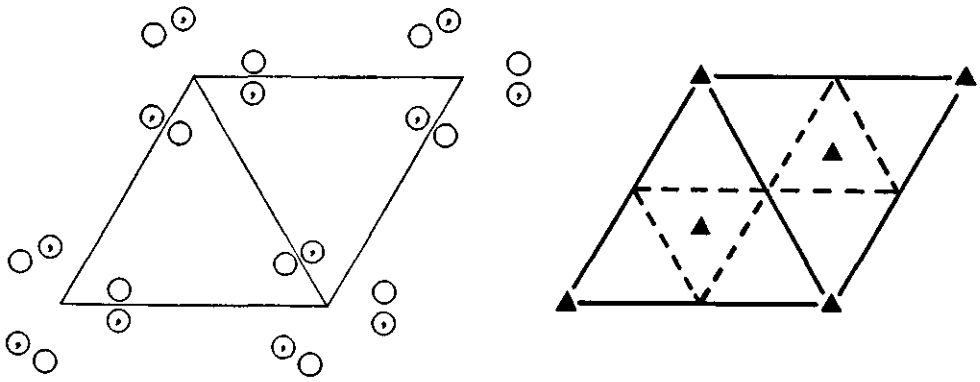
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
3	*d*	1	$x,y;\ \bar{y},x-y;\ y-x,\bar{x}.$	No conditions
				Special:
1	*c*	3	$\frac{2}{3},\frac{1}{3}.$	No conditions
1	*b*	3	$\frac{1}{3},\frac{2}{3}.$	
1	*a*	3	0,0.	





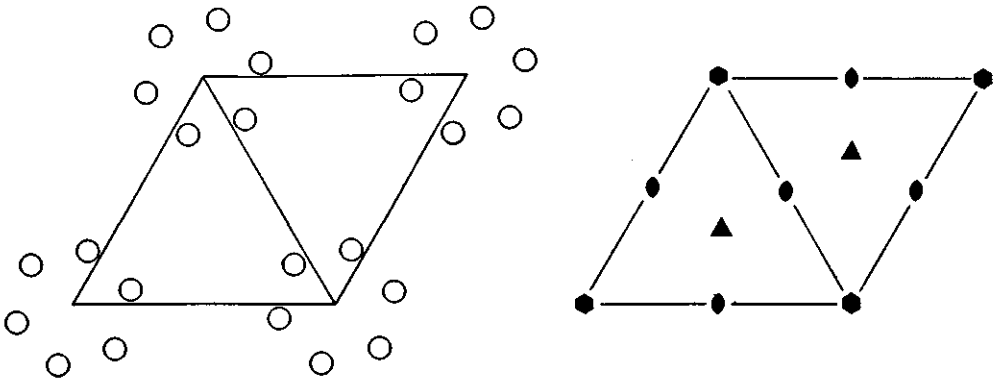
Origin at 3*m*1

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	*e*	1	$x,y;\ \bar{y},x-y;\ y-x,\bar{x};$ $\bar{y},\bar{x};\ x,x-y;\ y-x,y.$	No conditions
				Special:
3	*d*	*m*	$x,\bar{x};\ x,2x;\ 2\bar{x},\bar{x}.$	No conditions
1	*c*	3*m*	$\frac{2}{3},\frac{1}{3}.$	
1	*b*	3*m*	$\frac{1}{3},\frac{2}{3}.$	
1	*a*	3*m*	0,0.	



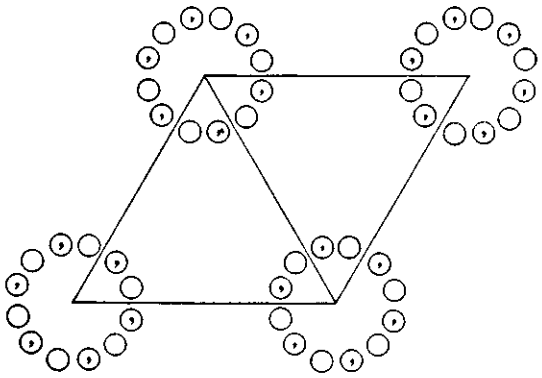
Origin at $31m$

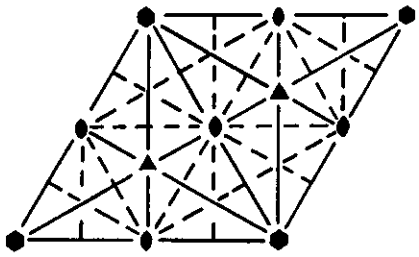
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	d	1	$x,y;\ \bar{y},x-y;\ y-x,\bar{x};$ $y,x;\ \bar{x},y-x;\ x-y,\bar{y}.$	No conditions
				Special:
3	c	m	$x,0;\ 0,x;\ \bar{x},\bar{x}.$	No conditions
2	b	3	$\frac{1}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3}.$	
1	a	$3m$	$0,0.$	



Origin at 6

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	*d*	1	$x,y;\ \bar{y},x-y;\ y-x,\bar{x};$ $\bar{x},\bar{y};\ y,y-x;\ x-y,x.$	No conditions
				Special:
3	*c*	2	$\frac{1}{2},0;\ 0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2}.$	No conditions
2	*b*	3	$\frac{1}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3}.$	
1	*a*	6	$0,0.$	





Origin at 6*mm*

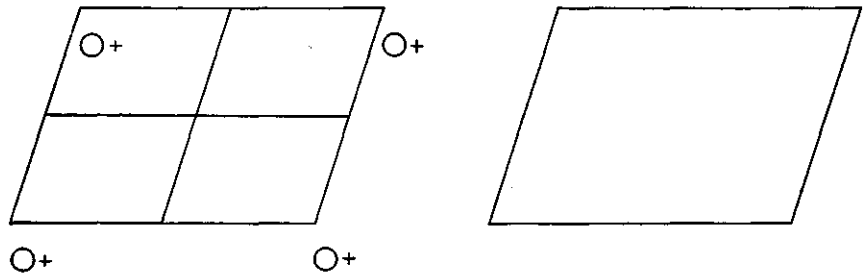
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	*f*	1	x,y; $\bar{y},x-y$; $y-x,\bar{x}$; y,x; $\bar{x},y-x$; $x-y,\bar{y}$; $\bar{x},\bar{y}$; $y,y-x$; $x-y,x$; $\bar{y},\bar{x}$; $x,x-y$; $y-x,y$.	No conditions
				Special:
6	*e*	*m*	$x,\bar{x}$; $x,2x$; $2\bar{x},\bar{x}$; $\bar{x},x$; $\bar{x},2\bar{x}$; $2x,x$.	No conditions
6	*d*	*m*	$x,0$; $0,x$; $\bar{x},\bar{x}$; $\bar{x},0$; $0,\bar{x}$; x,x.	
3	*c*	*mm*	$\frac{1}{2},0$; $0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}$.	
2	*b*	3*m*	$\frac{1}{3},\frac{2}{3}$; $\frac{2}{3},\frac{1}{3}$.	
1	*a*	6*mm*	0,0.	

4.3. THE 230 THREE-DIMENSIONAL SPACE GROUPS:

Equivalent Positions, Symmetry and Possible Reflections

G

No. 1 $P1$ 1 Triclinic

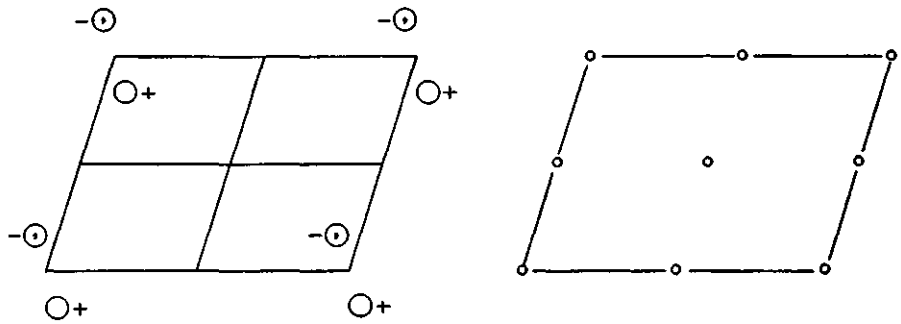


Origin on 1

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
1	a	1	$x,y,z.$	No conditions

Symmetry of special projections

All $p1$

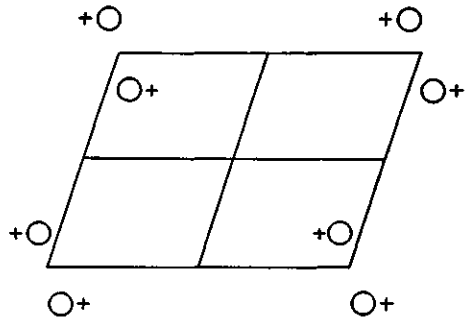


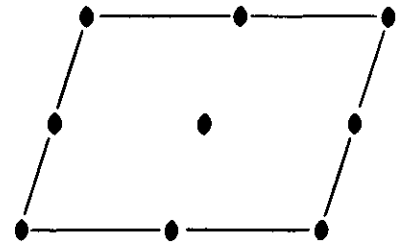
Origin at $\bar{1}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
2	i	1	x,y,z; $\bar{x},\bar{y},\bar{z}$.	No conditions
				Special:
1	h	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	No conditions
1	g	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$.	
1	f	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$.	
1	e	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$.	
1	d	$\bar{1}$	$\frac{1}{2},0,0$.	
1	c	$\bar{1}$	$0,\frac{1}{2},0$.	
1	b	$\bar{1}$	$0,0,\frac{1}{2}$.	
1	a	$\bar{1}$	$0,0,0$.	

Symmetry of special projections

All $p2$





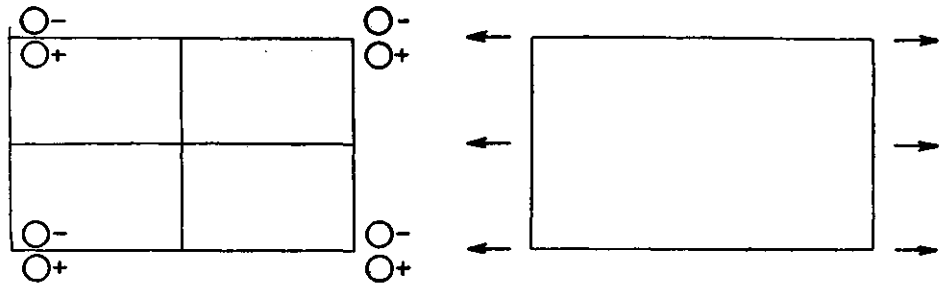
1ST SETTING

Origin on 2; unique axis c

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
2	e	1	x,y,z; $\bar{x},\bar{y},z$.	hkl: No conditions $hk0$: No conditions $00l$: No conditions
				Special:
1	d	2	$\frac{1}{2},\frac{1}{2},z$.	No conditions
1	c	2	$\frac{1}{2},0,z$.	
1	b	2	$0,\frac{1}{2},z$.	
1	a	2	$0,0,z$.	

Symmetry of special projections

(001) $p2$; $a'=a, b'=b$ (100) $pm1$; $b'=b, c'=c$ (010) $p1m$; $c'=c, a'=a$

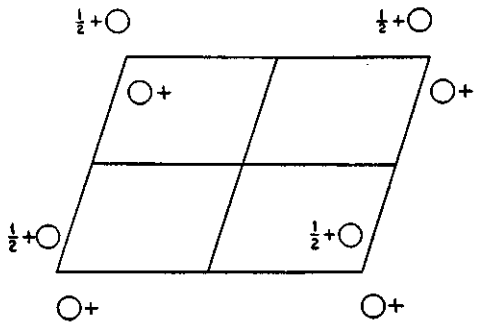


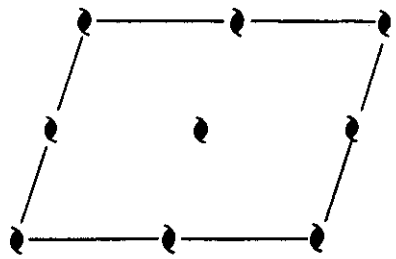
Origin on 2; unique axis *b* 2ND SETTING

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
2	*e*	1	x,y,z; $\bar{x},y,\bar{z}$.	*hkl*: *h0l*: *0k0*: No conditions
				Special:
1	*d*	2	$\frac{1}{2},y,\frac{1}{2}$.	No conditions
1	*c*	2	$\frac{1}{2},y,0$.	
1	*b*	2	$0,y,\frac{1}{2}$.	
1	*a*	2	$0,y,0$.	

Symmetry of special projections

(001) $pm1$; $a'=a$, $b'=b$ (100) $p1m$; $b'=b$, $c'=c$ (010) $p2$; $c'=c$, $a'=a$





1ST SETTING

Origin on 2_1; unique axis c

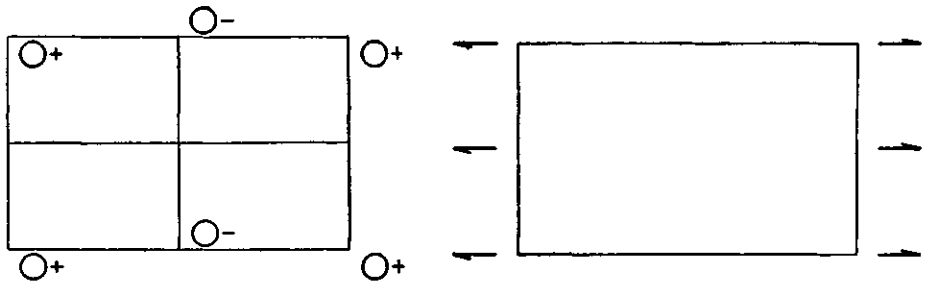
Number of positions, Wyckoff notation and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
2	a	1	x,y,z; $\bar{x},\bar{y},\frac{1}{2}+z$.	hkl: No conditions $hk0$: No conditions $00l$: $l=2n$

Symmetry of special projections

(001) $p2$; $a'=a$, $b'=b$

(100) $pg1$; $b'=b$, $c'=c$

(010) $p1g$; $c'=c$, $a'=a$



Origin on 2_1; unique axis b

2ND SETTING

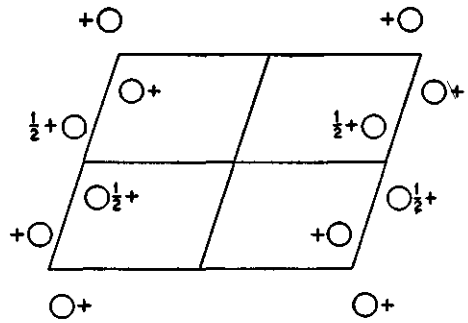
Number of positions, Wyckoff notation, and point symmetry	Co-ordinates of equivalent positions	Conditions limiting possible reflections
2 a 1	x,y,z; $\bar{x},\frac{1}{2}+y,\bar{z}$.	hkl: No conditions $h0l$: No conditions $0k0$: $k=2n$

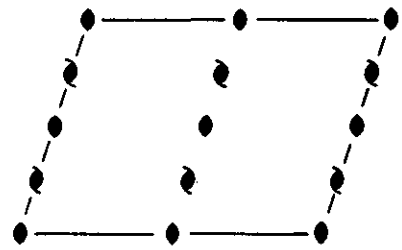
Symmetry of special projections

(001) $pg1$; $a'=a$, $b'=b$

(100) $p1g$; $b'=b$, $c'=c$

(010) $p2$; $c'=c$, $a'=a$





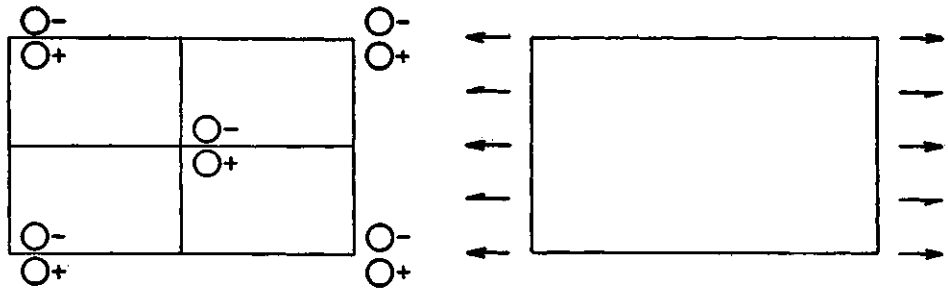
1ST SETTING

Origin on 2; unique axis c

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},0,\frac{1}{2})+$	
				General:
4	c	1	$x,y,z;\ \bar{x},\bar{y},z.$	hkl: $h+l=2n$ $hk0$: $(h=2n)$ $00l$: $(l=2n)$
2	b	2	$0,\frac{1}{2},z.$	Special: as above only
2	a	2	$0,0,z.$	

Symmetry of special projections

(001) $p2$; $a'=a/2$, $b'=b$ (100) $pm1$; $b'=b$, $c'=c/2$ (010) $c1m$; $c'=c$, $a'=a$



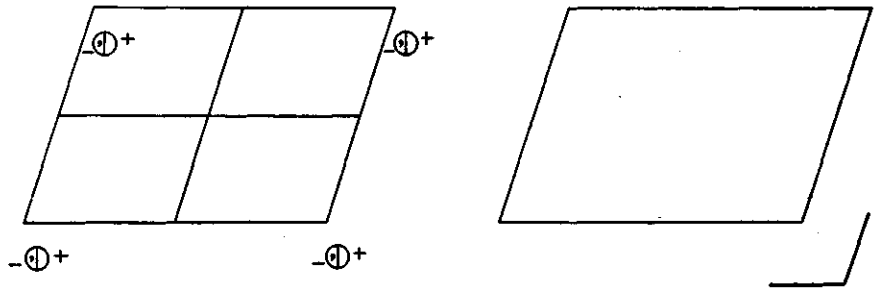
Origin on 2; unique axis b

2ND SETTING

Number of positions, Wyckoff notation, and point symmetry	Co-ordinates of equivalent positions	Conditions limiting possible reflections
	$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	
		General:
4 c 1	$x,y,z;\ \bar{x},y,\bar{z}.$	hkl: $h+k=2n$ $h0l$: $(h=2n)$ $0k0$: $(k=2n)$
2 b 2	$0,y,\frac{1}{2}.$	Special: as above only
2 a 2	$0,y,0.$	

Symmetry of special projections

(001) $cm1$; $a'=a$, $b'=b$ (100) $p1m$; $b'=b/2$, $c'=c$ (010) $p2$; $c'=c$, $a'=a/2$

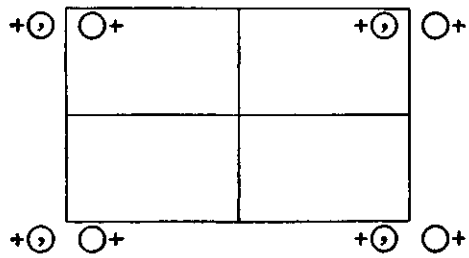


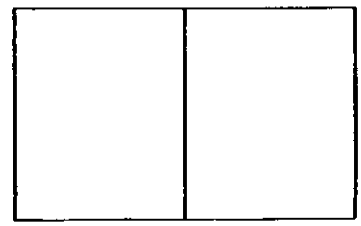
1ST SETTING Origin on plane m; unique axis c

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
2	c	1	x,y,z; $x,y,\bar{z}$.	hkl: $hk0$: $00l$: No conditions
				Special:
1	b	m	$x,y,\frac{1}{2}$.	No conditions
1	a	m	$x,y,0$.	

Symmetry of special projections

(001) $p1$; $a'=a$, $b'=b$ (100) $p1m$; $b'=b$, $c'=c$ (010) $pm1$; $c'=c$, $a'=a$





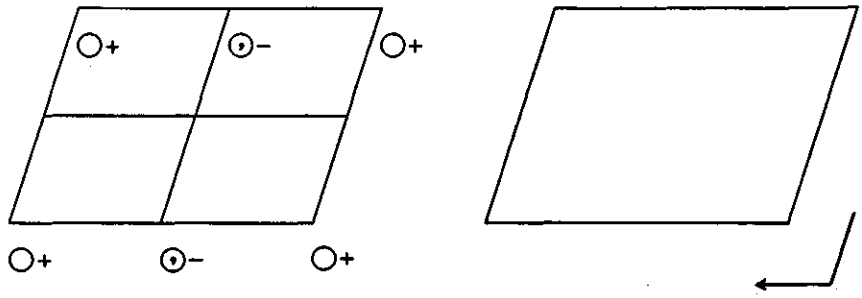
Origin on plane *m*; unique axis *b* 2ND SETTING

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
2	*c*	1	x,y,z; $x,\bar{y},z$.	hkl: $h0l$: $0k0$: No conditions
				Special:
1	*b*	*m*	$x,\frac{1}{2},z$.	No conditions
1	*a*	*m*	$x,0,z$.	

Symmetry of special projections

(001) $p1m$; $a'=a$, $b'=b$ (100) $pm1$; $b'=b$, $c'=c$ (010) $p1$; $c'=c$, $a'=a$

No. 7 $P\,1\,1\,b$ m Monoclinic



1ST SETTING

Origin on glide-plane b; unique axis c

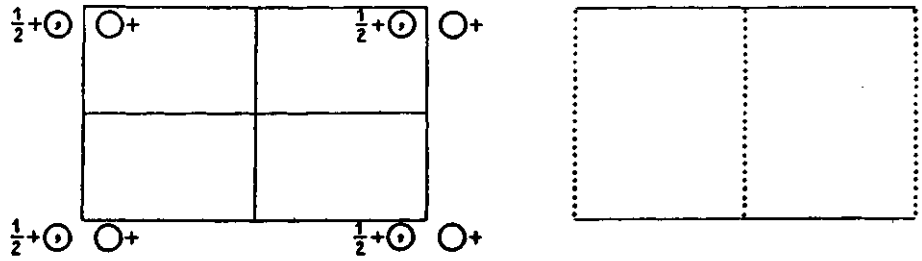
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
2	a	1	x,y,z; $x,\frac{1}{2}+y,\bar{z}$.	hkl: No conditions $hk0$: $k=2n$ $00l$: No conditions

Symmetry of special projections

(001) $p1$; $a'=a$, $b'=b/2$

(100) $p1g$; $b'=b$, $c'=c$

(010) $pm1$; $c'=c$, $a'=a$

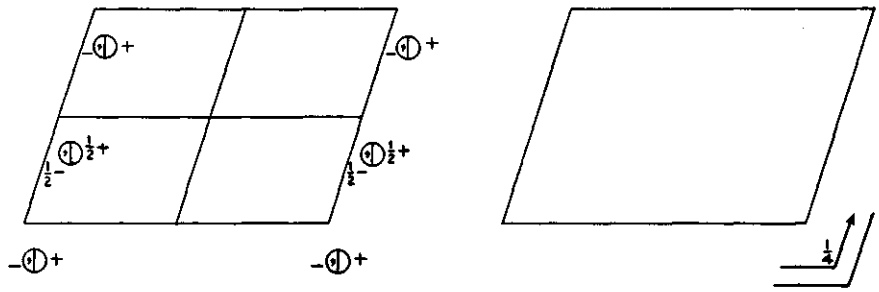


Origin on glide-plane *c*; unique axis *b* 2ND SETTING

Number of positions, Wyckoff notation, and point symmetry	Co-ordinates of equivalent positions	Conditions limiting possible reflections
2 *a* 1	x,y,z; $x,\bar{y},\frac{1}{2}+z$.	*hkl*: No conditions *h*0*l*: $l=2n$ 0*k*0: No conditions

Symmetry of special projections

(001) $p1m$; $a'=a$, $b'=b$ (100) $pg1$; $b'=b$, $c'=c$ (010) $p1$; $c'=c/2$, $a'=a$



1ST SETTING Origin on plane m; unique axis c

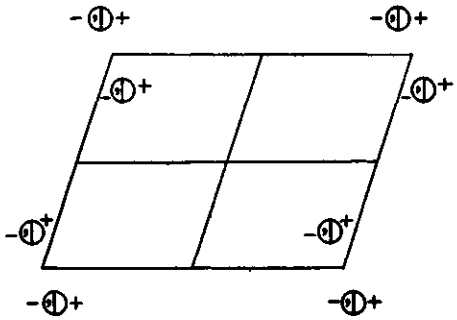
Number of positions, Wyckoff notation, and point symmetry	Co-ordinates of equivalent positions	Conditions limiting possible reflections
	$(0,0,0;\ \frac{1}{2},0,\frac{1}{2})+$	
		General:
4 b 1	$x,y,z;\ x,y,\bar{z}.$	hkl: $h+l=2n$ $hk0$: $(h=2n)$ $00l$: $(l=2n)$
2 a m	$x,y,0.$	Special: as above only

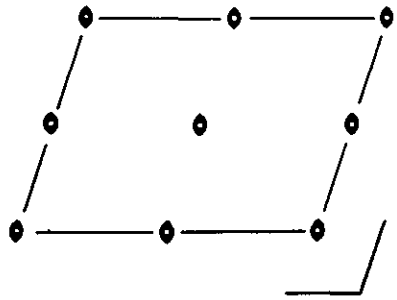
Symmetry of special projections

(001) $p1$; $a'=a/2$, $b'=b$	(100) $p1m$; $b'=b$, $c'=c/2$	(010) $cm1$; $c'=c$, $a'=a$

$P2/m$ C_{2h}^{1}

No. 10 $P\,1\,1\,2/m$ $2/m$ Monoclinic





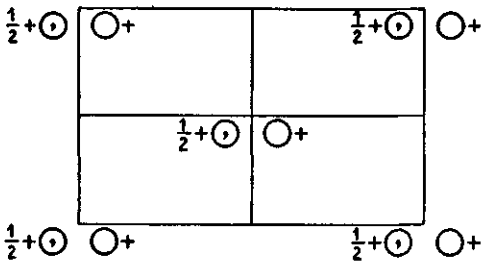
1ST SETTING

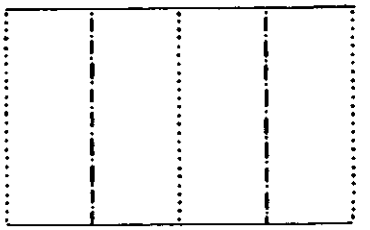
Origin at centre ($2/m$); unique axis c

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	o	1	x,y,z; $x,y,\bar{z}$; $\bar{x},\bar{y},z$; $\bar{x},\bar{y},\bar{z}$.	No conditions
				Special:
2	n	m	$x,y,\frac{1}{2}$; $\bar{x},\bar{y},\frac{1}{2}$.	No conditions
2	m	m	$x,y,0$; $\bar{x},\bar{y},0$.	
2	l	2	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	
2	k	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$.	
2	j	2	$\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$.	
2	i	2	$0,0,z$; $0,0,\bar{z}$.	
1	h	$2/m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
1	g	$2/m$	$\frac{1}{2},\frac{1}{2},0$.	
1	f	$2/m$	$0,\frac{1}{2},\frac{1}{2}$.	
1	e	$2/m$	$\frac{1}{2},0,\frac{1}{2}$.	
1	d	$2/m$	$\frac{1}{2},0,0$.	
1	c	$2/m$	$0,\frac{1}{2},0$.	
1	b	$2/m$	$0,0,\frac{1}{2}$.	
1	a	$2/m$	$0,0,0$.	

Symmetry of special projections

(001) $p2$; $a'=a$, $b'=b$ (100) pmm; $b'=b$, $c'=c$ (010) pmm; $c'=c$, $a'=a$



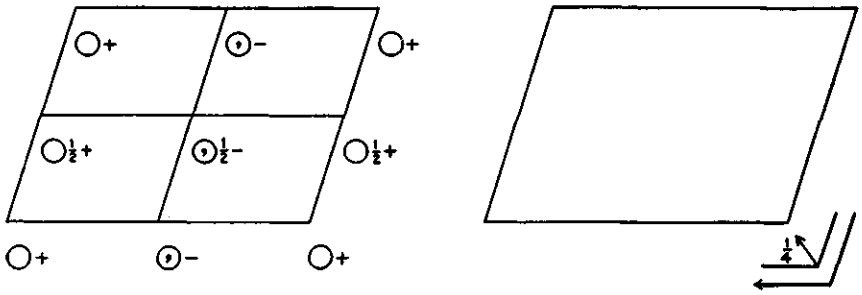


Origin on glide-plane *c*; unique axis *b* 2ND SETTING

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},0)+$	
4	*a*	1	$x,y,z;\ x,\bar{y},\tfrac{1}{2}+z.$	hkl: $h+k=2n$ $h0l$: $l=2n$; $(h=2n)$ $0k0$: $(k=2n)$

Symmetry of special projections

(001) $c1m$; $a'=a$, $b'=b$ (100) $pg1$; $b'=b/2$, $c'=c$ (010) $p1$; $c'=c/2$, $a'=a/2$



1ST SETTING

Origin on glide-plane b; unique axis c

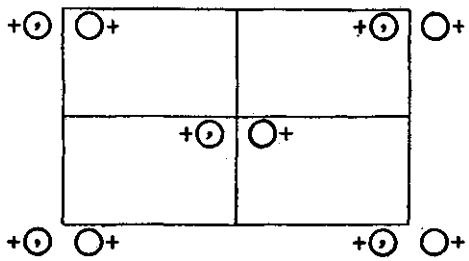
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},0,\frac{1}{2})+$	
4	a	1	$x,y,z;\ x,\frac{1}{2}+y,\bar{z}.$	hkl: $h+l=2n$ $hk0$: $k=2n$; $(h=2n)$ $00l$: $(l=2n)$

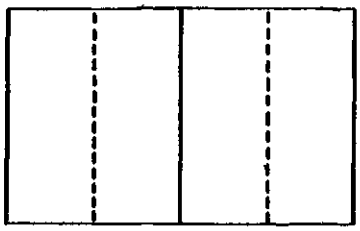
Symmetry of special projections

(001) $p1$; $a'=a/2$, $b'=b/2$

(100) $p1g$; $b'=b$, $c'=c/2$

(010) $cm1$; $c'=c$, $a'=a$





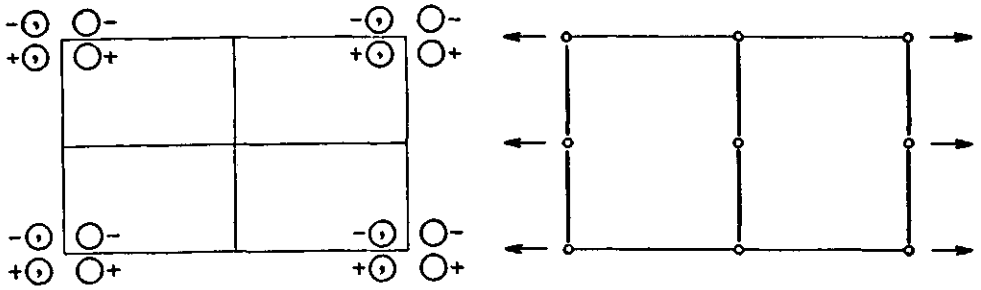
Origin on plane m; unique axis b

2ND SETTING

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
4	b	1	$x,y,z;\ x,\bar{y},z.$	hkl: $h+k=2n$ $h0l$: $(h=2n)$ $0k0$: $(k=2n)$
2	a	m	$x,0,z.$	Special: as above only

Symmetry of special projections

(001) $c1m$; $a'=a$, $b'=b$ (100) $pm1$; $b'=b/2$, $c'=c$ (010) $p1$; $c'=c$, $a'=a/2$



Origin at centre (2/m); unique axis b — 2ND SETTING

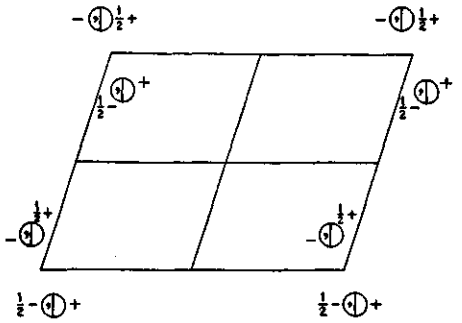
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	o	1	x,y,z; $x,\bar{y},z$; $\bar{x},y,\bar{z}$; $\bar{x},\bar{y},\bar{z}$.	No conditions
				Special:
2	n	m	$x,\frac{1}{2},z$; $\bar{x},\frac{1}{2},\bar{z}$.	No conditions
2	m	m	$x,0,z$; $\bar{x},0,\bar{z}$.	
2	l	2	$\frac{1}{2},y,\frac{1}{2}$; $\frac{1}{2},\bar{y},\frac{1}{2}$.	
2	k	2	$0,y,\frac{1}{2}$; $0,\bar{y},\frac{1}{2}$.	
2	j	2	$\frac{1}{2},y,0$; $\frac{1}{2},\bar{y},0$.	
2	i	2	$0,y,0$; $0,\bar{y},0$.	
1	h	2/m	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
1	g	2/m	$\frac{1}{2},0,\frac{1}{2}$.	
1	f	2/m	$0,\frac{1}{2},\frac{1}{2}$.	
1	e	2/m	$\frac{1}{2},\frac{1}{2},0$.	
1	d	2/m	$\frac{1}{2},0,0$.	
1	c	2/m	$0,0,\frac{1}{2}$.	
1	b	2/m	$0,\frac{1}{2},0$.	
1	a	2/m	$0,0,0$.	

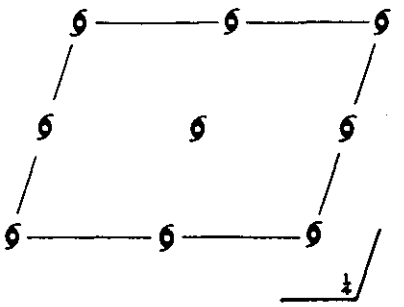
Symmetry of special projections

(001) pmm; $a'=a$, $b'=b$ (100) pmm; $b'=b$, $c'=c$ (010) $p2$; $c'=c$, $a'=a$

$P2_1/m$ C_{2h}^2

No. 11 $P\,1\,1\,2_1/m$ $2/m$ Monoclinic





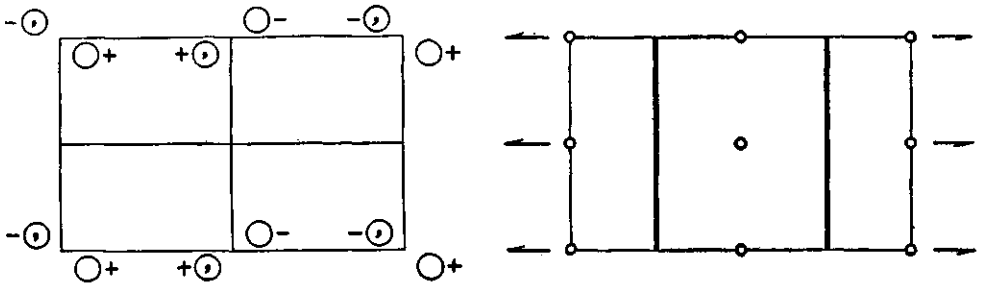
1ST SETTING

Origin at $\bar{1}$; unique axis c

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	f	1	x,y,z; $\bar{x},\bar{y},\bar{z}$; $\bar{x},\bar{y},\frac{1}{2}+z$; $x,y,\frac{1}{2}-z$.	hkl: No conditions $hk0$: No conditions $00l$: $l=2n$
				Special: as above, plus
2	e	m	$x,y,\frac{1}{4}$; $\bar{x},\bar{y},\frac{3}{4}$.	no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $l=2n$
2	c	$\bar{1}$	$0,\frac{1}{2},0$; $0,\frac{1}{2},\frac{1}{2}$.	
2	b	$\bar{1}$	$\frac{1}{2},0,0$; $\frac{1}{2},0,\frac{1}{2}$.	
2	a	$\bar{1}$	$0,0,0$; $0,0,\frac{1}{2}$.	

Symmetry of special projections

(001) $p2$; $a'=a$, $b'=b$ (100) pgm; $b'=b$, $c'=c$ (010) pmg; $c'=c$, $a'=a$



Origin at $\bar{1}$; unique axis b 2ND SETTING

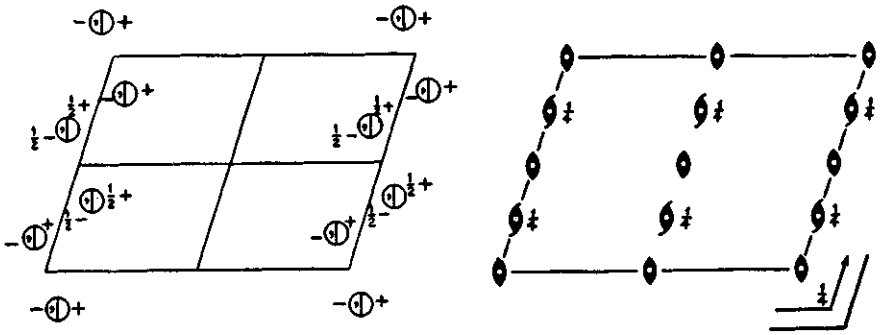
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	f	1	$x,y,z;\ \bar{x},\bar{y},\bar{z};\ \bar{x},\frac{1}{2}+y,\bar{z};\ x,\frac{1}{2}-y,z.$	hkl: No conditions $h0l$: No conditions $0k0$: $k=2n$
				Special: as above, plus
2	e	m	$x,\frac{1}{4},z;\ \bar{x},\frac{3}{4},\bar{z}.$	no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	hkl: $k=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2}.$	
2	b	$\bar{1}$	$\frac{1}{2},0,0;\ \frac{1}{2},\frac{1}{2},0.$	
2	a	$\bar{1}$	$0,0,0;\ 0,\frac{1}{2},0.$	

Symmetry of special projections

(001) pgm; $a'=a$, $b'=b$ (100) pmg; $b'=b$, $c'=c$ (010) $p2$; $c'=c$, $a'=a$

$B2/m$ C_{2h}^{3}

No. 12 $B\,1\,1\,2/m$ $2/m$ Monoclinic

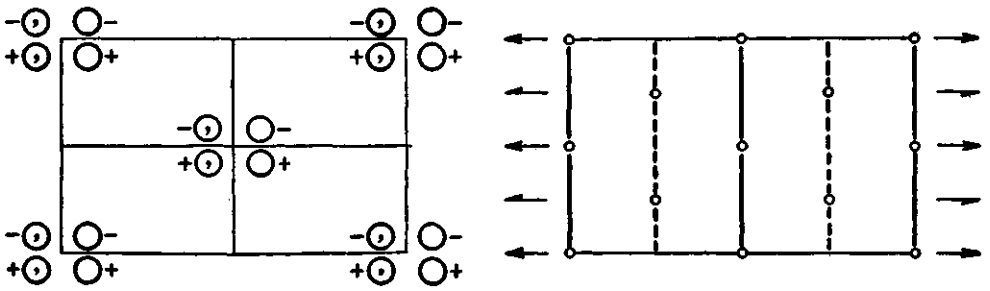


1ST SETTING Origin at centre ($2/m$); unique axis c

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},0,\frac{1}{2})+$	
				General:
8	j	1	$x,y,z;\ x,y,\bar{z};\ \bar{x},\bar{y},z;\ \bar{x},\bar{y},\bar{z}.$	hkl: $h+l=2n$ $hk0$: $(h=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	i	m	$x,y,0;\ \bar{x},\bar{y},0.$	no extra conditions
4	h	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\bar{z}.$	
4	g	2	$0,0,z;\ 0,0,\bar{z}.$	
4	f	$\bar{1}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4};\ \frac{1}{4},\frac{1}{2},\frac{3}{4}.$	hkl: $h=2n$; $(l=2n)$
4	e	$\bar{1}$	$\frac{1}{4},0,\frac{1}{4};\ \frac{1}{4},0,\frac{3}{4}.$	
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}.$	no extra conditions
2	c	$2/m$	$0,\frac{1}{2},0.$	
2	b	$2/m$	$0,0,\frac{1}{2}.$	
2	a	$2/m$	$0,0,0.$	

Symmetry of special projections

(001) $p2$; $a'=a/2$, $b'=b$ (100) pmm; $b'=b$, $c'=c/2$ (010) cmm; $c'=c$, $a'=a$



Origin at centre ($2/m$); unique axis b 2ND SETTING

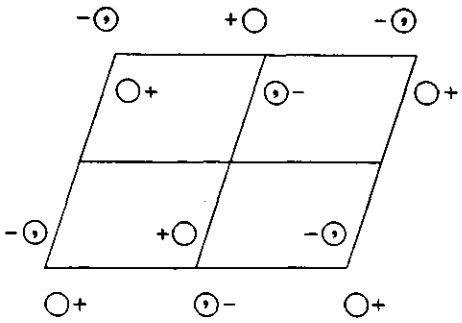
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
8	j	1	$x,y,z;\ \ x,\bar{y},z;\ \ \bar{x},y,\bar{z};\ \ \bar{x},\bar{y},\bar{z}.$	hkl: $h+k=2n$ $h0l$: $(h=2n)$ $0k0$: $(k=2n)$
				Special: as above, plus
4	i	m	$x,0,z;\ \ \bar{x},0,\bar{z}.$	no extra conditions
4	h	2	$0,y,\frac{1}{2};\ \ 0,\bar{y},\frac{1}{2}.$	
4	g	2	$0,y,0;\ \ 0,\bar{y},0.$	
4	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2};\ \ \frac{1}{4},\frac{3}{4},\frac{1}{2}.$	hkl: $h=2n$; $(k=2n)$
4	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0;\ \ \frac{1}{4},\frac{3}{4},0.$	
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}.$	no extra conditions
2	c	$2/m$	$0,0,\frac{1}{2}.$	
2	b	$2/m$	$0,\frac{1}{2},0.$	
2	a	$2/m$	$0,0,0.$	

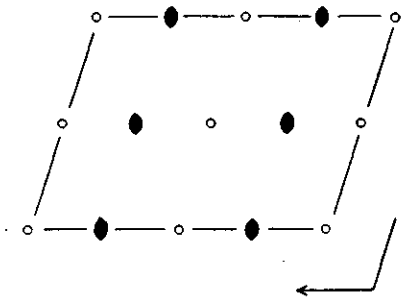
Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) pmm; $b'=b/2$, $c'=c$ (010) $p2$; $c'=c$, $a'=a/2$

$P2/b$ C_{2h}^{4}

No. 13 $P\,1\,1\,2/b$ $2/m$ Monoclinic





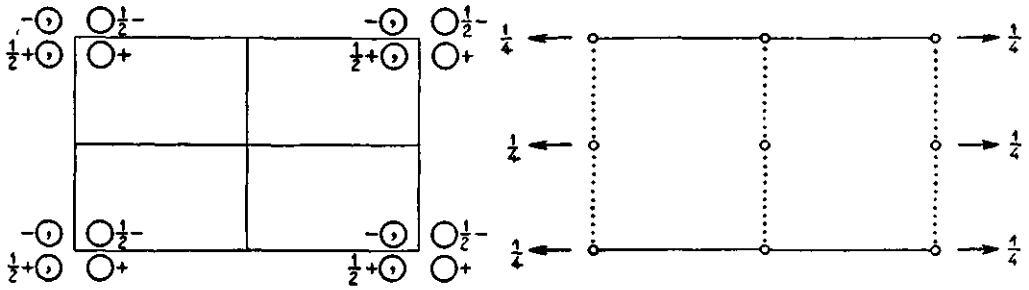
1ST SETTING

Origin at $\bar{1}$; unique axis c

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	g	1	$x,y,z;\ \bar{x},\bar{y},\bar{z};\ \bar{x},\frac{1}{2}-y,z;\ x,\frac{1}{2}+y,\bar{z}.$	hkl: No conditions $hk0$: $k=2n$ $00l$: No conditions
				Special: as above, plus
2	f	2	$\frac{1}{2},\frac{1}{4},z;\ \frac{1}{2},\frac{3}{4},\bar{z}.$	no extra conditions
2	e	2	$0,\frac{1}{4},z;\ 0,\frac{3}{4},\bar{z}.$	
2	d	$\bar{1}$	$\frac{1}{2},0,0;\ \frac{1}{2},\frac{1}{2},0.$	hkl: $k=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2}.$	
2	b	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	
2	a	$\bar{1}$	$0,0,0;\ 0,\frac{1}{2},0.$	

Symmetry of special projections

(001) $p2$; $a'=a$, $b'=b/2$ (100) pmg; $b'=b$, $c'=c$ (010) pmm; $c'=c$, $a'=a$



Origin at $\bar{1}$; unique axis b 2ND SETTING

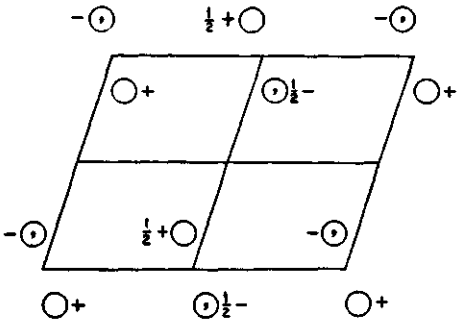
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	g	1	$x,y,z;\ \bar{x},\bar{y},\bar{z};\ \bar{x},y,\frac{1}{2}-z;\ x,\bar{y},\frac{1}{2}+z.$	hkl: No conditions $h0l$: $l=2n$ $0k0$: No conditions
				Special: as above, plus
2	f	2	$\frac{1}{2},y,\frac{1}{4};\ \frac{1}{2},\bar{y},\frac{3}{4}.$	no extra conditions
2	e	2	$0,y,\frac{1}{4};\ 0,\bar{y},\frac{3}{4}.$	
2	d	$\bar{1}$	$\frac{1}{2},0,0;\ \frac{1}{2},0,\frac{1}{2}.$	hkl: $l=2n$
2	c	$\bar{1}$	$0,\frac{1}{2},0;\ 0,\frac{1}{2},\frac{1}{2}.$	
2	b	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	
2	a	$\bar{1}$	$0,0,0;\ 0,0,\frac{1}{2}.$	

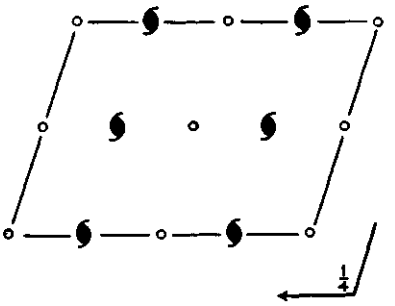
Symmetry of special projections

(001) pmm; $a'=a$, $b'=b$ (100) pgm; $b'=b$, $c'=c$ (010) $p2$; $c'=c/2$, $a'=a$

$P2_1/b$ C_{2h}^5

No. 14 $P\,1\,1\,2_1/b$ $2/m$ Monoclinic





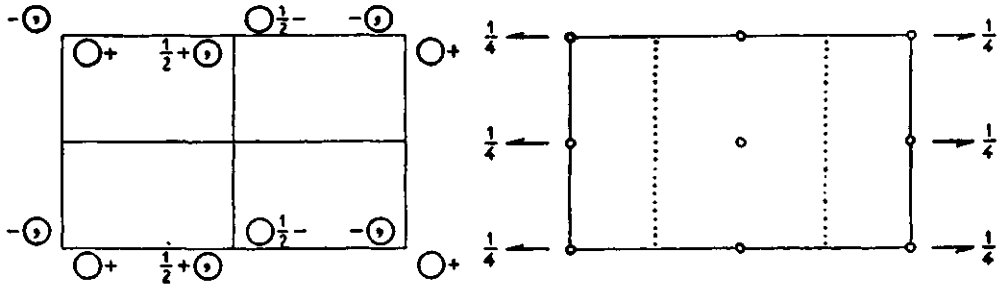
1ST SETTING

Origin at $\bar{1}$; unique axis c

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	e	1	x,y,z; $\bar{x},\bar{y},\bar{z}$; $\bar{x},\frac{1}{2}-y,\frac{1}{2}+z$; $x,\frac{1}{2}+y,\frac{1}{2}-z$.	hkl: No conditions $hk0$: $k=2n$ $00l$: $l=2n$
				Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$.	hkl: $k+l=2n$
2	c	$\bar{1}$	$0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	
2	b	$\bar{1}$	$\frac{1}{2},0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
2	a	$\bar{1}$	$0,0,0$; $0,\frac{1}{2},\frac{1}{2}$.	

Symmetry of special projections

(001) $p2$; $a'=a$, $b'=b/2$ (100) pgg; $b'=b$, $c'=c$ (010) pmg; $c'=c$, $a'=a$

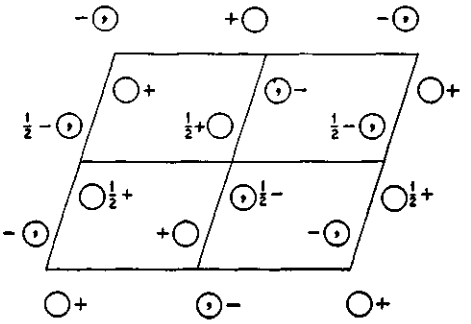


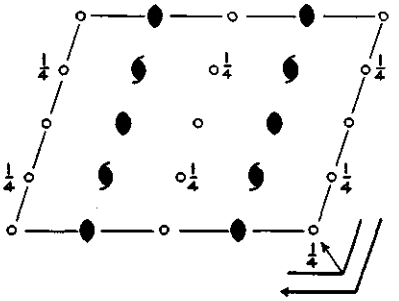
Origin at $\bar{1}$; unique axis b 2ND SETTING

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	e	1	x,y,z; $\bar{x},\bar{y},\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$; $x,\frac{1}{2}-y,\frac{1}{2}+z$.	hkl: No conditions $h0l$: $l=2n$ $0k0$: $k=2n$
				Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	hkl: $k+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$; $0,\frac{1}{2},0$.	
2	b	$\bar{1}$	$\frac{1}{2},0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
2	a	$\bar{1}$	$0,0,0$; $0,\frac{1}{2},\frac{1}{2}$.	

Symmetry of special projections

(001) pgm; $a'=a$, $b'=b$ (100) pgg; $b'=b$, $c'=c$ (010) $p2$; $c'=c/2$, $a'=a$



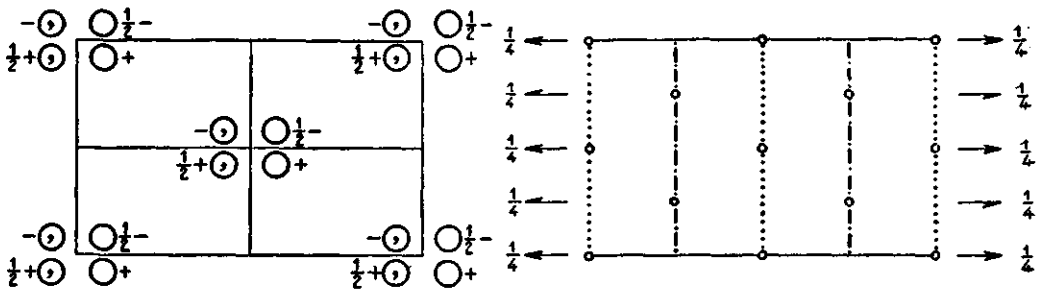


1ST SETTING Origin at $\bar{1}$ on glide-plane b; unique axis c

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},0,\frac{1}{2})+$	
				General:
8	f	1	$x,y,z;\ \bar{x},\bar{y},\bar{z};\ \bar{x},\frac{1}{2}-y,z;\ x,\frac{1}{2}+y,\bar{z}.$	hkl: $h+l=2n$ $hk0$: $k=2n$; $(h=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	e	2	$0,\frac{1}{4},z;\ 0,\frac{3}{4},\bar{z}.$	no extra conditions
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4};\ \frac{3}{4},0,\frac{1}{4}.$	hkl: $k+l=2n$; $(h+k=2n)$
4	c	$\bar{1}$	$\frac{1}{4},0,\frac{1}{4};\ \frac{3}{4},\frac{1}{2},\frac{1}{4}.$	
4	b	$\bar{1}$	$0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2}.$	hkl: $k=2n$
4	a	$\bar{1}$	$0,0,0;\ 0,\frac{1}{2},0.$	

Symmetry of special projections

(001) $p2$; $a'=a/2$, $b'=b/2$ (100) pmg; $b'=b$, $c'=c/2$ (010) cmm; $c'=c$, $a'=a$

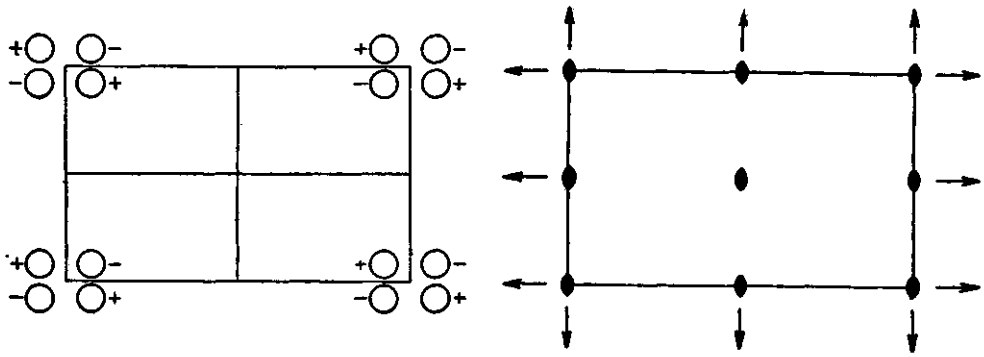


Origin at $\bar{1}$ on glide-plane c; unique axis b 2ND SETTING

Number of positions, Wyckoff notation and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	
8	f	1	$x,y,z;\ \bar{x},\bar{y},\bar{z};\ \bar{x},y,\frac{1}{2}-z;\ x,\bar{y},\frac{1}{2}+z.$	General: hkl: $h+k=2n$ $h0l$: $l=2n$; $(h=2n)$ $0k0$: $(k=2n)$
				Special: as above, plus
4	e	2	$0,y,\frac{1}{4};\ 0,\bar{y},\frac{3}{4}.$	no extra conditions
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2};\ \frac{3}{4},\frac{1}{4},0.$	hkl: $k+l=2n$; $(l+h=2n)$
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0;\ \frac{3}{4},\frac{1}{4},\frac{1}{2}.$	
4	b	$\bar{1}$	$0,\frac{1}{2},0;\ 0,\frac{1}{2},\frac{1}{2}.$	hkl: $l=2n$
4	a	$\bar{1}$	$0,0,0;\ 0,0,\frac{1}{2}.$	

Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) pgm; $b'=b/2$, $c'=c$ (010) $p2$; $c'=c/2$, $a'=a/2$

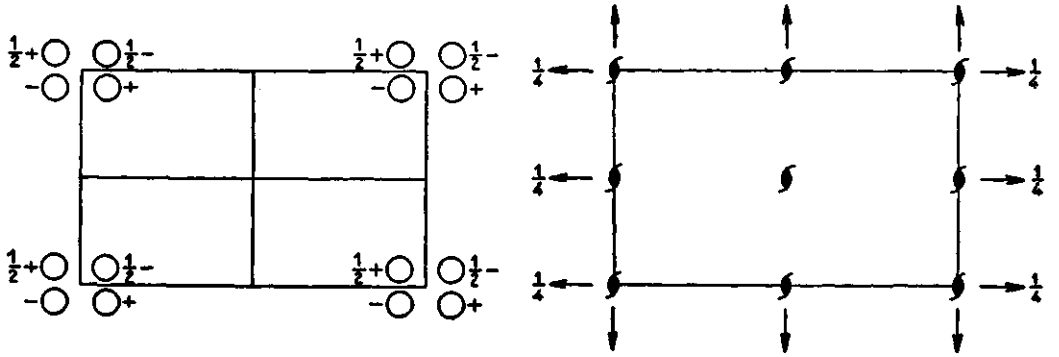


Origin at 222

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions								Conditions limiting possible reflections
											General:
4	u	1	x,y,z;	$\bar{x},\bar{y},z$;	$x,\bar{y},\bar{z}$;	$\bar{x},y,\bar{z}$.					No conditions
											Special:
2	t	2	$\frac{1}{2},\frac{1}{2},z$;	$\frac{1}{2},\frac{1}{2},\bar{z}$.							No conditions
2	s	2	$0,\frac{1}{2},z$;	$0,\frac{1}{2},\bar{z}$.							
2	r	2	$\frac{1}{2},0,z$;	$\frac{1}{2},0,\bar{z}$.							
2	q	2	$0,0,z$;	$0,0,\bar{z}$.							
2	p	2	$\frac{1}{2},y,\frac{1}{2}$;	$\frac{1}{2},\bar{y},\frac{1}{2}$.		2	l	2	$x,\frac{1}{2},\frac{1}{2}$;	$\bar{x},\frac{1}{2},\frac{1}{2}$.	
2	o	2	$\frac{1}{2},y,0$;	$\frac{1}{2},\bar{y},0$.		2	k	2	$x,\frac{1}{2},0$;	$\bar{x},\frac{1}{2},0$.	
2	n	2	$0,y,\frac{1}{2}$;	$0,\bar{y},\frac{1}{2}$.		2	j	2	$x,0,\frac{1}{2}$;	$\bar{x},0,\frac{1}{2}$.	
2	m	2	$0,y,0$;	$0,\bar{y},0$.		2	i	2	$x,0,0$;	$\bar{x},0,0$.	
1	h	222	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.			1	d	222	$0,0,\frac{1}{2}$.		
1	g	222	$0,\frac{1}{2},\frac{1}{2}$.			1	c	222	$0,\frac{1}{2},0$.		
1	f	222	$\frac{1}{2},0,\frac{1}{2}$.			1	b	222	$\frac{1}{2},0,0$.		
1	e	222	$\frac{1}{2},\frac{1}{2},0$.			1	a	222	$0,0,0$.		

Symmetry of special projections

(001) pmm; $a'=a$, $b'=b$ (100) pmm; $b'=b$, $c'=c$ (010) pmm; $c'=c$, $a'=a$



Origin at 212_1

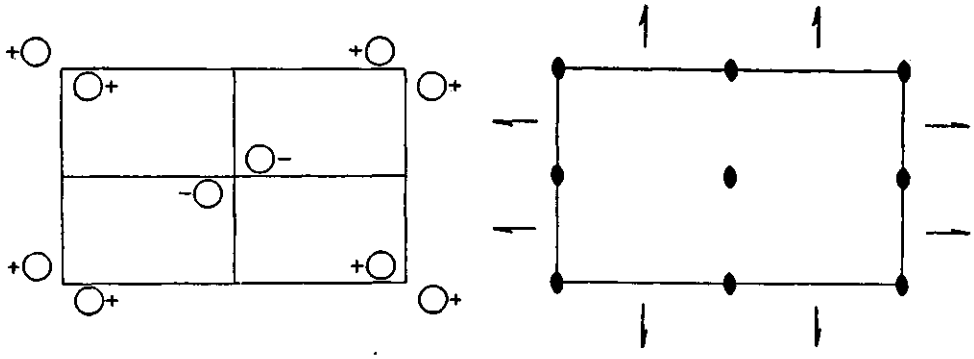
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	e	1	x,y,z; $x,\bar{y},\bar{z}$; $\bar{x},\bar{y},\frac{1}{2}+z$; $\bar{x},y,\frac{1}{2}-z$.	hkl: No conditions; $0kl$: No conditions; $h0l$: No conditions; $hk0$: No conditions; $h00$: No conditions; $0k0$: No conditions; $00l$: $l=2n$
				Special: as above, plus
2	d	2	$\frac{1}{2},y,\frac{1}{4}$; $\frac{1}{2},\bar{y},\frac{3}{4}$.	$h0l$: $l=2n$
2	c	2	$0,y,\frac{1}{4}$; $0,\bar{y},\frac{3}{4}$.	$h0l$: $l=2n$
2	b	2	$x,\frac{1}{2},0$; $\bar{x},\frac{1}{2},\frac{1}{2}$.	$0kl$: $l=2n$
2	a	2	$x,0,0$; $\bar{x},0,\frac{1}{2}$.	$0kl$: $l=2n$

Symmetry of special projections

(001) pmm; $a'=a$, $b'=b$

(100) pgm; $b'=b$, $c'=c$

(010) pmg; $c'=c$, $a'=a$

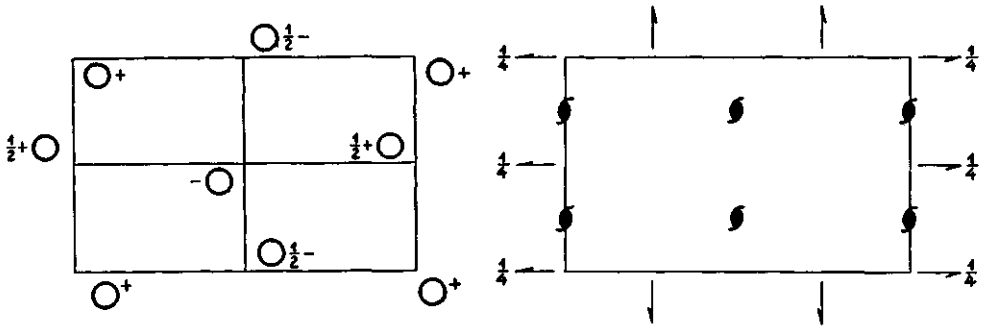


Origin at 112 in plane of 2_12_1

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	c	1	$x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}+x,\frac{1}{2}-y,\bar{z};\ \frac{1}{2}-x,\frac{1}{2}+y,\bar{z}.$	hkl: No conditions $0kl$: No conditions $h0l$: No conditions $hk0$: No conditions $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: No conditions
				Special: as above, plus
2	b	2	$0,\frac{1}{2},z;\ \frac{1}{2},0,\bar{z}.$	$hk0$: $h+k=2n$
2	a	2	$0,0,z;\ \frac{1}{2},\frac{1}{2},\bar{z}.$	$hk0$: $h+k=2n$

Symmetry of special projections

(001) pgg; $a'=a$, $b'=b$ (100) pmg; $b'=b$, $c'=c$ (010) pgm; $c'=c$, $a'=a$



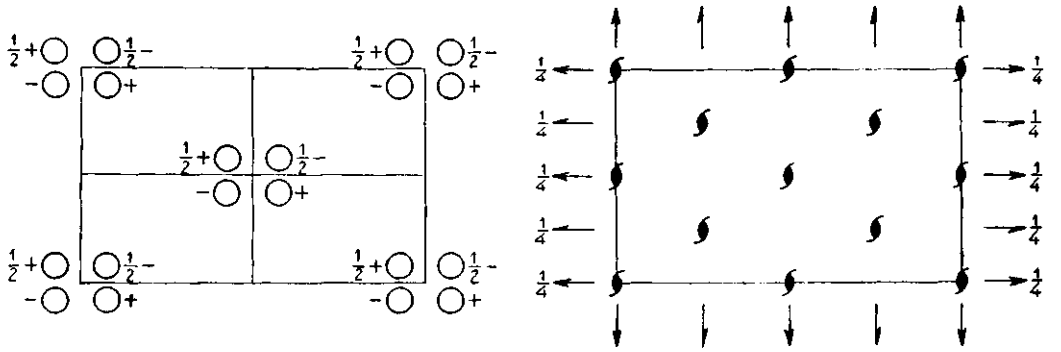
Origin halfway between three pairs of non-intersecting screw axes

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
4	a	1	x,y,z; $\frac{1}{2}-x,\bar{y},\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$.	hkl: $0kl$: $h0l$: $hk0$: No conditions $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$

Symmetry of special projections

(001) pgg; $a'=a$, $b'=b$ (100) pgg; $b'=b$, $c'=c$ (010) pgg; $c'=c$, $a'=a$

1

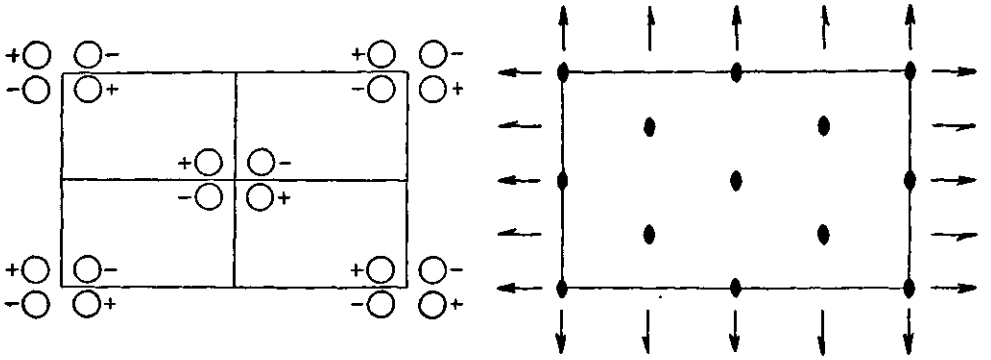


Origin at 212_1

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
8	c	1	$x,y,z;\ \ x,\bar{y},\bar{z};\ \ \bar{x},\bar{y},\frac{1}{2}+z;\ \ \bar{x},y,\frac{1}{2}-z.$	hkl: $h+k=2n$ $0kl$: $(k=2n)$ $h0l$: $(h=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $l=2n$
				Special: as above, plus
4	b	2	$0,y,\frac{1}{4};\ \ 0,\bar{y},\frac{3}{4}.$	$h0l$: $l=2n$; $(h=2n)$
4	a	2	$x,0,0;\ \ \bar{x},0,\frac{1}{2}.$	$0kl$: $l=2n$; $(k=2n)$

Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) pgm; $b'=b/2$, $c'=c$ (010) pmg; $c'=c$, $a'=a/2$

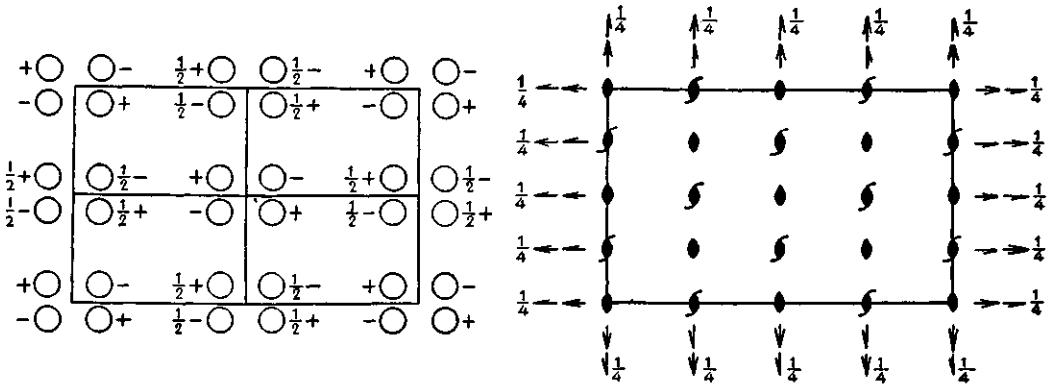


Origin at 222

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions							Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$							
										General:
8	l	1	$x,y,z;$	$\bar{x},\bar{y},z;$	$x,\bar{y},\bar{z};$	$\bar{x},y,\bar{z}.$				hkl: $h+k=2n$ $0kl$: $(k=2n)$ $h0l$: $(h=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: No conditions
										Special: as above, plus
4	k	2	$\frac{1}{4},\frac{1}{4},z;$	$\frac{1}{4},\frac{3}{4},\bar{z}.$						$hk0$: $h=2n;\ (k=2n)$
4	j	2	$0,\frac{1}{2},z;$	$0,\frac{1}{2},\bar{z}.$						
4	i	2	$0,0,z;$	$0,0,\bar{z}.$						
4	h	2	$0,y,\frac{1}{2};$	$0,\bar{y},\frac{1}{2}.$	2	d	222	$0,0,\frac{1}{2}.$		(a) to (j) inclusive no extra conditions
4	g	2	$0,y,0;$	$0,\bar{y},0.$	2	c	222	$\frac{1}{2},0,\frac{1}{2}.$		
4	f	2	$x,0,\frac{1}{2};$	$\bar{x},0,\frac{1}{2}.$	2	b	222	$0,\frac{1}{2},0.$		
4	e	2	$x,0,0;$	$\bar{x},0,0.$	2	a	222	$0,0,0.$		

Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) pmm; $b'=b/2$, $c'=c$ (010) pmm; $c'=c$, $a'=a/2$

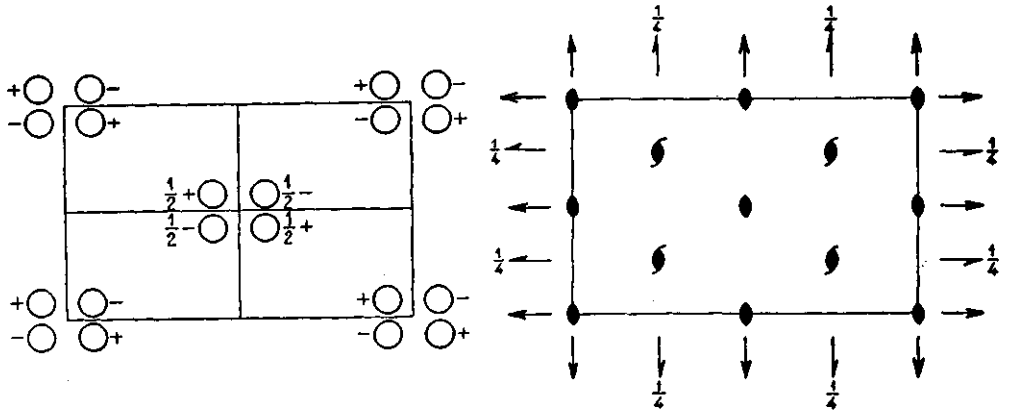


Origin at 222

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	Conditions limiting possible reflections
				General:
16	k	1	$x,y,z;\ \bar{x},\bar{y},z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z}.$	hkl: $h+k, k+l, (l+h)=2n$ $0kl$: $(k,l=2n)$ $h0l$: $(l,h=2n)$ $hk0$: $(h,k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above only
8	j	2	$x,\frac{1}{4},\frac{1}{4};\ \frac{1}{2}-x,\frac{1}{4},\frac{1}{4}.$	
8	i	2	$\frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{2}-y,\frac{1}{4}.$	
8	h	2	$\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{2}-z.$	
8	g	2	$0,0,z;\ 0,0,\bar{z}.$	
8	f	2	$0,y,0;\ 0,\bar{y},0.$	
8	e	2	$x,0,0;\ \bar{x},0,0.$	
4	d	222	$\frac{1}{4},\frac{1}{4},\frac{3}{4}.$	
4	c	222	$\frac{1}{4},\frac{1}{4},\frac{1}{4}.$	
4	b	222	$0,0,\frac{1}{2}.$	
4	a	222	$0,0,0.$	

Symmetry of special projections

(001) pmm; $a'=a/2$, $b'=b/2$ (100) pmm; $b'=b/2$, $c'=c/2$ (010) pmm; $c'=c/2$, $a'=a/2$

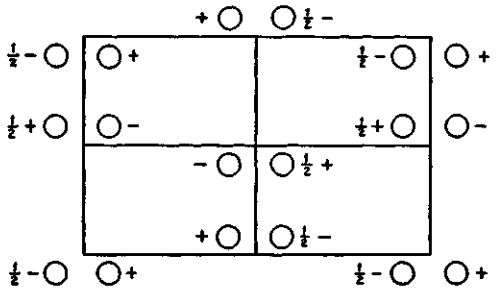


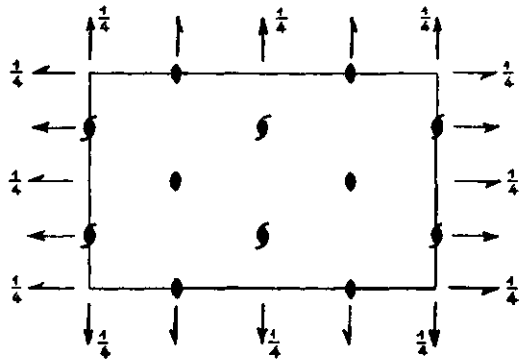
Origin at 222

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
8	*k*	1	$x,y,z;\ \bar{x},\bar{y},z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z}.$	General: hkl: $h+k+l=2n$ $0kl$: $(k+l=2n)$ $h0l$: $(l+h=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
4	*j*	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\bar{z}.$	Special: as above only
4	*i*	2	$0,0,z;\ 0,0,\bar{z}.$	
4	*h*	2	$\frac{1}{2},y,0;\ \frac{1}{2},\bar{y},0.$	
4	*g*	2	$0,y,0;\ 0,\bar{y},0.$	
4	*f*	2	$x,0,\frac{1}{2};\ \bar{x},0,\frac{1}{2}.$	
4	*e*	2	$x,0,0;\ \bar{x},0,0.$	
2	*d*	222	$0,\frac{1}{2},0.$	
2	*c*	222	$0,0,\frac{1}{2}.$	
2	*b*	222	$\frac{1}{2},0,0.$	
2	*a*	222	$0,0,0.$	

Symmetry of special projections

(001) *cmm*; $a'=a$, $b'=b$ (100) *cmm*; $b'=b$, $c'=c$ (010) *cmm*; $c'=c$, $a'=a$



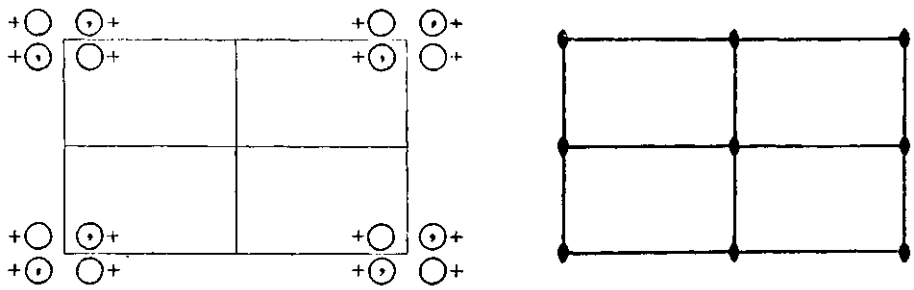


Origin halfway between three pairs of non-intersecting diad axes

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
				General:
8	d	1	$x,y,z;\ \frac{1}{2}-x,\bar{y},\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}-y,\bar{z};\ \bar{x},\frac{1}{2}+y,\frac{1}{2}-z.$	hkl: $h+k+l=2n$ $0kl$: $(k+l=2n)$ $h0l$: $(l+h=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	c	2	$0,\frac{1}{4},z;\ \frac{1}{2},\frac{1}{4},\bar{z}.$	$hk0$: $h=2n$; $(k=2n)$
4	b	2	$\frac{1}{4},y,0;\ \frac{1}{4},\bar{y},\frac{1}{2}.$	$h0l$: $l=2n$; $(h=2n)$
4	a	2	$x,0,\frac{1}{4};\ \bar{x},\frac{1}{2},\frac{1}{4}.$	$0kl$: $k=2n$; $(l=2n)$

Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) cmm; $b'=b$, $c'=c$ (010) cmm; $c'=c$, $a'=a$



Origin on $mm2$

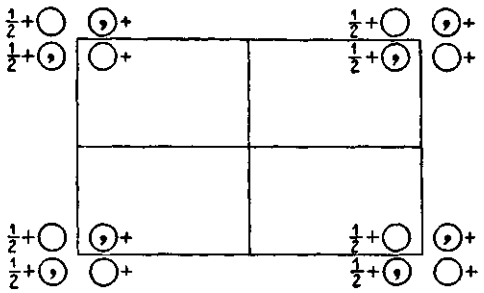
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	i	1	x,y,z; $\bar{x},\bar{y},z$; $x,\bar{y},z$; $\bar{x},y,z$.	No conditions
				Special:
2	h	m	$\frac{1}{2},y,z$; $\frac{1}{2},\bar{y},z$.	No conditions
2	g	m	$0,y,z$; $0,\bar{y},z$.	
2	f	m	$x,\frac{1}{2},z$; $\bar{x},\frac{1}{2},z$.	
2	e	m	$x,0,z$; $\bar{x},0,z$.	
1	d	mm	$\frac{1}{2},\frac{1}{2},z$.	
1	c	mm	$\frac{1}{2},0,z$.	
1	b	mm	$0,\frac{1}{2},z$.	
1	a	mm	$0,0,z$.	

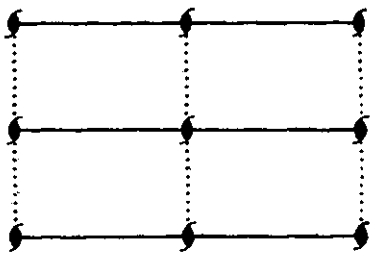
Symmetry of special projections

(001) pmm; $a'=a$, $b'=b$ (100) $pm1$; $b'=b$, $c'=c$ (010) $p1m$; $c'=c$, $a'=a$

$Pmc2_1$ C_{2v}^2

No. 26 $P\,m\,c\,2_1$ $m\,m\,2$ Orthorhombic



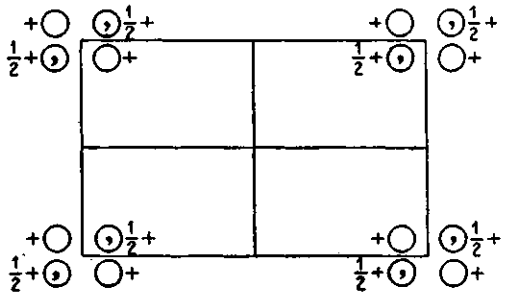


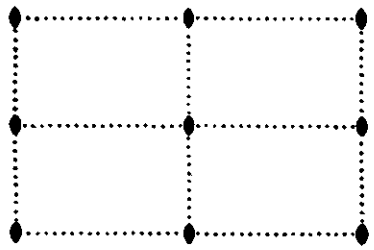
Origin on 2_1

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	c	1	$x,y,z;\ \bar{x},y,z;\ \bar{x},\bar{y},\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z.$	hkl: No conditions $0kl$: No conditions $h0l$: $l=2n$ $hk0$: $h00$: $0k0$: No conditions $00l$: $(l=2n)$
				Special: as above only
2	b	m	$\frac{1}{2},y,z;\ \frac{1}{2},\bar{y},\frac{1}{2}+z.$	
2	a	m	$0,y,z;\ 0,\bar{y},\frac{1}{2}+z.$	

Symmetry of special projections

(001) pmm; $a'=a$, $b'=b$ (100) $pg1$; $b'=b$, $c'=c$ (010) $p1m$; $c'=c/2$, $a'=a$





Origin on 2

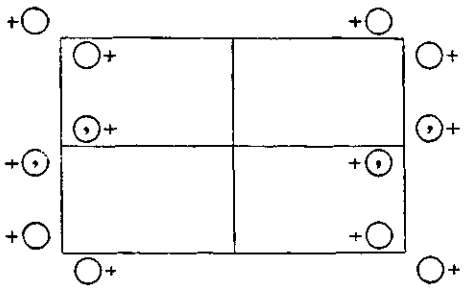
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	e	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\frac{1}{2}+z$; $x,\bar{y},\frac{1}{2}+z$.	hkl: No conditions $0kl$: $l=2n$ $h0l$: $l=2n$ $hk0$: } No conditions $h00$: } $0k0$: } $00l$: $(l=2n)$
				Special: as above, plus
2	d	2	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$.	} hkl: $l=2n$
2	c	2	$\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{2}+z$.	} hkl: $l=2n$
2	b	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{2}+z$.	} hkl: $l=2n$
2	a	2	$0,0,z$; $0,0,\frac{1}{2}+z$.	} hkl: $l=2n$

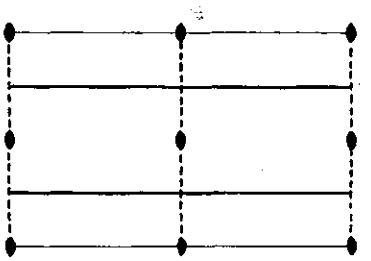
Symmetry of special projections

(001) pmm; $a'=a$, $b'=b$ (100) $pm1$; $b'=b$, $c'=c/2$ (010) $p1m$; $c'=c/2$, $a'=a$

$Pma2$ C_{2v}^{4}

No. 28 $P\,m\,a\,2$ $m\,m\,2$ Orthorhombic



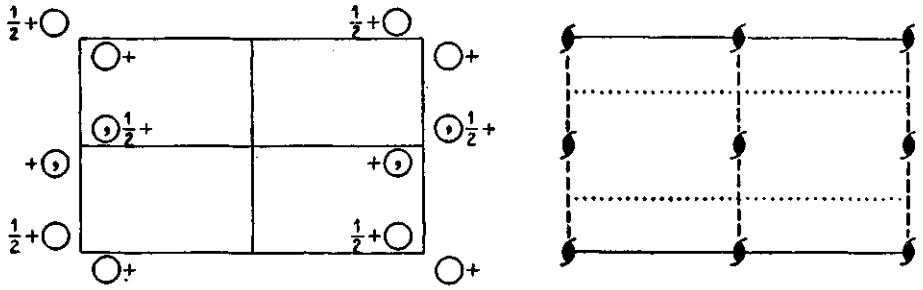


Origin on 2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	d	1	$x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,y,z;\ \frac{1}{2}+x,\bar{y},z.$	hkl: No conditions $0kl$: No conditions $h0l$: $h=2n$ $hk0$: No conditions $h00$: $(h=2n)$ $0k0$: No conditions $00l$: No conditions
				Special: as above, plus
2	c	m	$\frac{1}{4},y,z;\ \frac{3}{4},\bar{y},z.$	no extra conditions
2	b	2	$0,\frac{1}{2},z;\ \frac{1}{2},\frac{1}{2},z.$	hkl: $h=2n$
2	a	2	$0,0,z;\ \frac{1}{2},0,z.$	

Symmetry of special projections

(001) pmg; $a'=a$, $b'=b$ (100) $pm1$; $b'=b$, $c'=c$ (010) $p1m$; $c'=c$, $a'=a/2$



Origin on 2_1

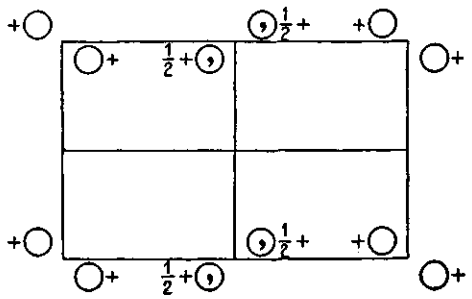
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
4	a	1	x,y,z; $\bar{x},\bar{y},\frac{1}{2}+z$; $\frac{1}{2}-x,y,\frac{1}{2}+z$; $\frac{1}{2}+x,\bar{y},z$.	hkl: No conditions $0kl$: $l=2n$ $h0l$: $h=2n$ $hk0$: No conditions $h00$: $(h=2n)$ $0k0$: No conditions $00l$: $(l=2n)$

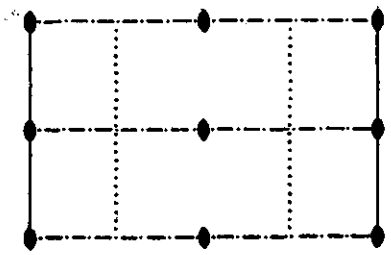
Symmetry of special projections

(001) pmg; $a'=a$, $b'=b$ (100) $pm1$; $b'=b$, $c'=c/2$ (010) $p1g$; $c'=c$, $a'=a/2$

$Pnc2$ C_{2v}^{6}

No. 30 $P\,n\,c\,2$ $m\,m\,2$ Orthorhombic



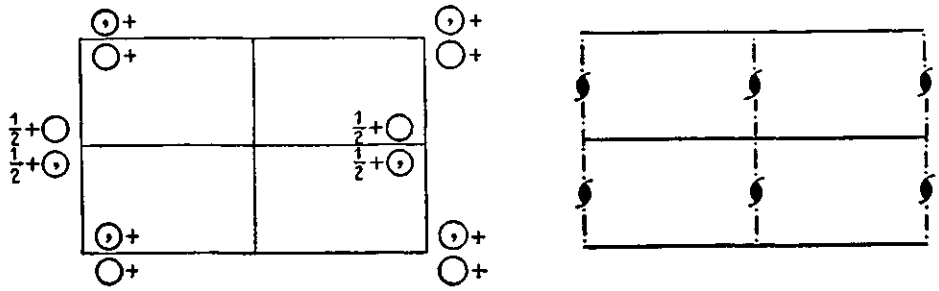


Origin on 2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	c	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},\frac{1}{2}+y,\frac{1}{2}+z;\ x,\frac{1}{2}-y,\frac{1}{2}+z.$	hkl: No conditions $0kl$: $k+l=2n$ $h0l$: $l=2n$ $hk0$: No conditions $h00$: No conditions $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
2	b	2	$\frac{1}{2},0,z;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}+z.$	hkl: $k+l=2n$
2	a	2	$0,0,z;\ 0,\frac{1}{2},\frac{1}{2}+z.$	

Symmetry of special projections

(001) pgm; $a'=a$, $b'=b$ (100) $cm1$; $b'=b$, $c'=c$ (010) $p1m$; $c'=c/2$, $a'=a$



Origin on mn

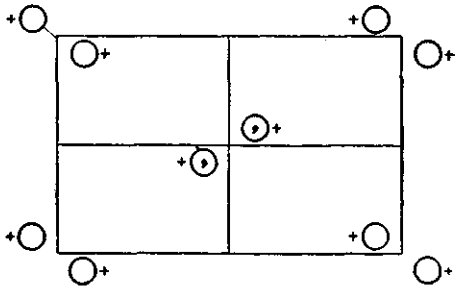
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	b	1	$x,y,z;\ \bar{x},y,z;\ \frac{1}{2}-x,\bar{y},\frac{1}{2}+z;\ \frac{1}{2}+x,\bar{y},\frac{1}{2}+z.$	hkl: No conditions $0kl$: No conditions $h0l$: $l+h=2n$ $hk0$: No conditions $h00$: $(h=2n)$ $0k0$: No conditions $00l$: $(l=2n)$
				Special: as above only
2	a	m	$0,y,z;\ \frac{1}{2},\bar{y},\frac{1}{2}+z.$	

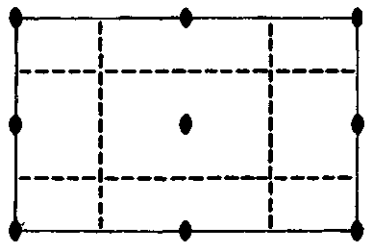
Symmetry of special projections

(001) pmg; $a'=a$, $b'=b$ (100) $pg1$; $b'=b$, $c'=c$ (010) $c1m$; $c'=c$, $a'=a$

$Pba2$ C_{2v}^{8}

No. 32 $P\,b\,a\,2$ $m\,m\,2$ Orthorhombic



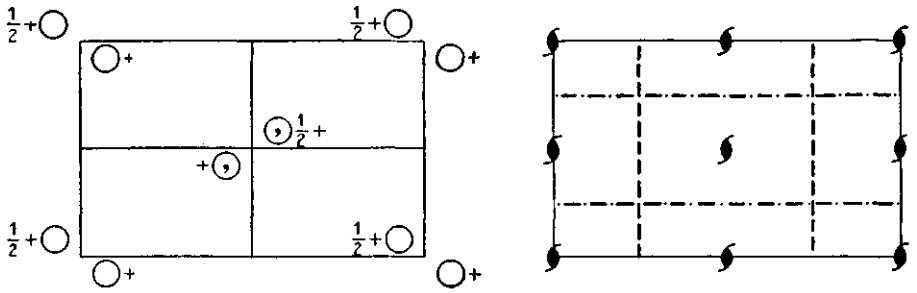


Origin on 2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	c	1	$x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}+y,z;\ \frac{1}{2}+x,\frac{1}{2}-y,z.$	hkl: No conditions $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: No conditions $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: No conditions
				Special: as above, plus
2	b	2	$0,\frac{1}{2},z;\ \frac{1}{2},0,z.$	hkl: $h+k=2n$
2	a	2	$0,0,z;\ \frac{1}{2},\frac{1}{2},z.$	

Symmetry of special projections

(001) pgg; $a'=a$, $b'=b$ (100) $pm1$; $b'=b/2$, $c'=c$ (010) $p1m$; $c'=c$, $a'=a/2$



Origin on 2_1

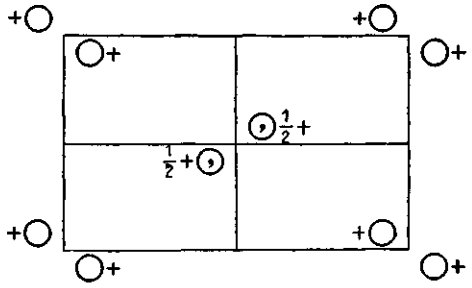
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
4	a	1	$x,y,z;\ \bar{x},\bar{y},\frac{1}{2}+z;\ \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}-y,z.$	hkl: No conditions $0kl$: $k+l=2n$ $h0l$: $h=2n$ $hk0$: No conditions $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$

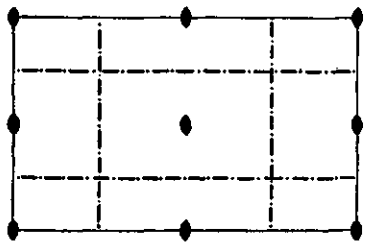
Symmetry of special projections

(001) pgg; $a'=a$, $b'=b$ (100) $cm1$; $b'=b$, $c'=c$ (010) $p1g$; $c'=c$, $a'=a/2$

$Pnn2$ C_{2v}^{10}

No. 34 $P\,n\,n\,2$ $m\,m\,2$ Orthorhombic



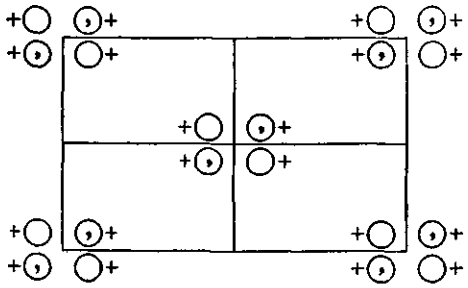


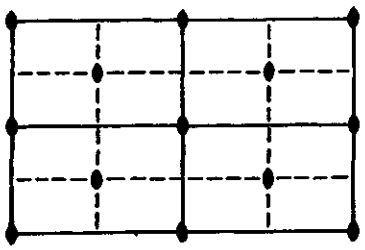
Origin on 2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	c	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$.	hkl: No conditions $0kl$: $k+l=2n$ $h0l$: $l+h=2n$ $hk0$: No conditions $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
2	b	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,\frac{1}{2}+z$.	hkl: $h+k+l=2n$
2	a	2	$0,0,z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$.	

Symmetry of special projections

(001) pgg; $a'=a$, $b'=b$ (100) $cm1$; $b'=b$, $c'=c$ (010) $c1m$; $c'=c$, $a'=a$



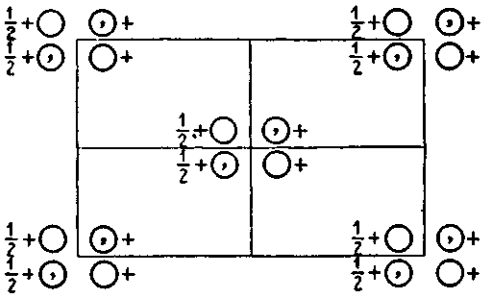


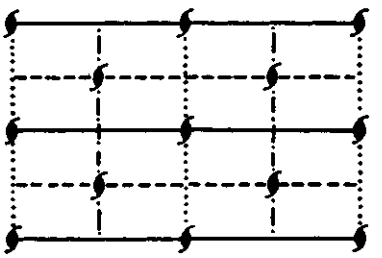
Origin on $mm2$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
8	f	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z.$	hkl: $h+k=2n$ $0kl$: $(k=2n)$ $h0l$: $(h=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: No conditions
				Special: as above, plus
4	e	m	$0,y,z;\ 0,\bar{y},z.$	no extra conditions
4	d	m	$x,0,z;\ \bar{x},0,z.$	
4	c	2	$\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{3}{4},z.$	hkl: $h=2n$; $(k=2n)$
2	b	mm	$0,\frac{1}{2},z.$	no extra conditions
2	a	mm	$0,0,z.$	

Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) $pm1$; $b'=b/2$, $c'=c$ (010) $p1m$; $c'=c$, $a'=a/2$



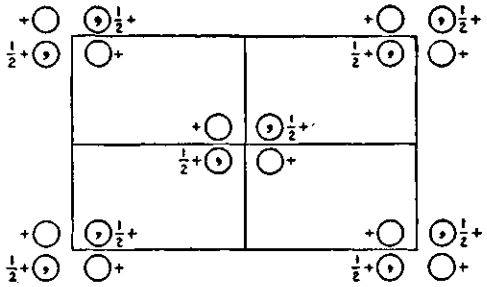


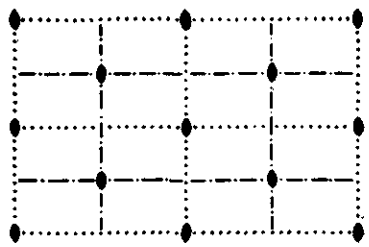
Origin on $mc2_1$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
8	b	1	$x,y,z;\ \bar{x},y,z;\ \bar{x},\bar{y},\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z.$	hkl: $h+k=2n$ $0kl$: $(k=2n)$ $h0l$: $l=2n$; $(h=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above only
4	a	m	$0,y,z;\ 0,\bar{y},\frac{1}{2}+z.$	

Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) $pg1$; $b'=b/2$, $c'=c$ (010) $p1m$; $c'=c/2$, $a'=a/2$





Origin on $cc2$

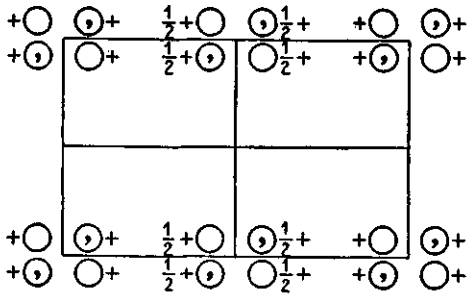
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
8	d	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z.$	hkl: $h+k=2n$ $0kl$: $l=2n$; $(k=2n)$ $h0l$: $l=2n$; $(h=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above plus
4	c	2	$\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{3}{4},\frac{1}{2}+z.$	hkl: $k+l=2n$; $(l+h=2n)$
4	b	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\frac{1}{2}+z.$	hkl: $l=2n$
4	a	2	$0,0,z;\ 0,0,\frac{1}{2}+z.$	hkl: $l=2n$

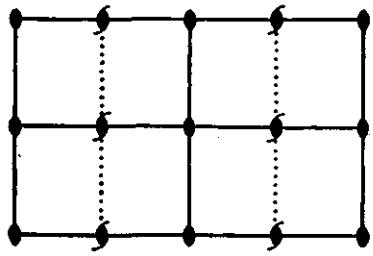
Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) $pm1$; $b'=b/2$, $c'=c/2$ (010) $p1m$; $c'=c/2$, $a'=a/2$

$Amm2$ C_{2v}^{14}

No. 38 $A\,m\,m\,2$ $m\,m\,2$ Orthorhombic



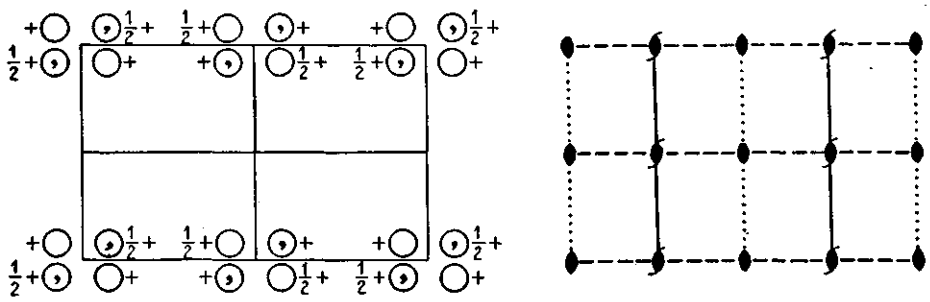


Origin on $mm2$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2})+$	
				General:
8	f	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z.$	hkl: $k+l=2n$ $0kl$: $(k+l=2n)$ $h0l$: $(l=2n)$ $hk0$: $(k=2n)$ $h00$: No conditions $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above only
4	e	m	$\frac{1}{2},y,z;\ \frac{1}{2},\bar{y},z.$	
4	d	m	$0,y,z;\ 0,\bar{y},z.$	
4	c	m	$x,0,z;\ \bar{x},0,z.$	
2	b	mm	$\frac{1}{2},0,z.$	
2	a	mm	$0,0,z.$	

Symmetry of special projections

(001) pmm; $a'=a$, $b'=b/2$ (100) $cm1$; $b'=b$, $c'=c$ (010) $p1m$; $c'=c/2$, $a'=a$



Origin on 2

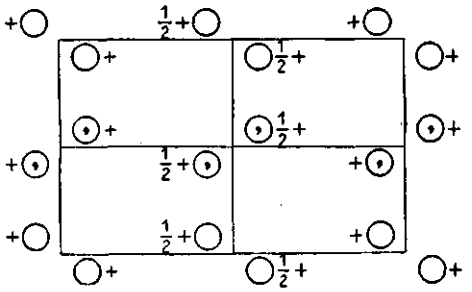
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2})+$	
				General:
8	d	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},\frac{1}{2}+y,z;\ x,\frac{1}{2}-y,z.$	hkl: $k+l=2n$ $0kl$: $k=2n$; $(l=2n)$ $h0l$: $(l=2n)$ $hk0$: $(k=2n)$ $h00$: No conditions $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	c	m	$x,\frac{1}{4},z;\ \bar{x},\frac{3}{4},z.$	no extra conditions
4	b	2	$\frac{1}{2},0,z;\ \frac{1}{2},\frac{1}{2},z.$	hkl: $k=2n$; $(l=2n)$
4	a	2	$0,0,z;\ 0,\frac{1}{2},z.$	

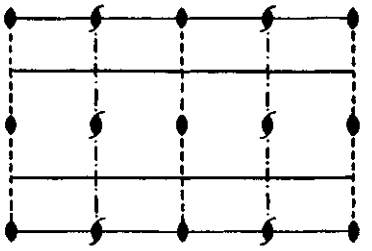
Symmetry of special projections

(001) pmm; $a'=a$, $b'=b/2$ (100) $pm1$; $b'=b/2$, $c'=c/2$ (010) $p1m$; $c'=c/2$, $a'=a$

$Ama2$ C_{2v}^{16}

No. 40 $A\,m\,a\,2$ $m\,m\,2$ Orthorhombic



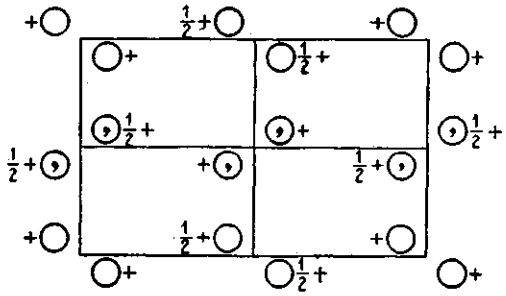


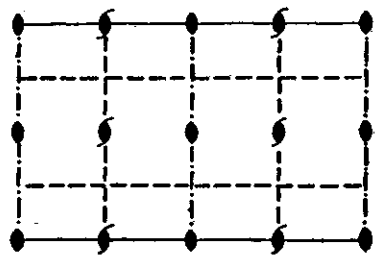
Origin on 2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2})+$	
				General:
8	c	1	$x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,y,z;\ \frac{1}{2}+x,\bar{y},z.$	hkl: $k+l=2n$ $0kl$: $(k+l=2n)$ $h0l$: $h=2n$; $(l=2n)$ $hk0$: $(k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	b	m	$\frac{1}{4},y,z;\ \frac{3}{4},\bar{y},z.$	no extra conditions
4	a	2	$0,0,z;\ \frac{1}{2},0,z.$	hkl: $h=2n$

Symmetry of special projections

(001) pmg; $a'=a$, $b'=b/2$ (100) $cm1$; $b'=b$, $c'=c$ (010) $p1m$; $c'=c/2$, $a'=a/2$





Origin on 2

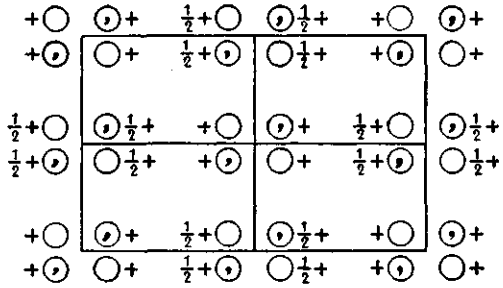
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2})+$	
8	b	1	$x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}+y,z;\ \frac{1}{2}+x,\frac{1}{2}-y,z.$	General: hkl: $k+l=2n$ $0kl$: $k=2n$; $(l=2n)$ $h0l$: $h=2n$; $(l=2n)$ $hk0$: $(k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
4	a	2	$0,0,z;\ \frac{1}{2},\frac{1}{2},z.$	Special: as above, plus hkl: $h+k=2n$; $(l+h=2n)$

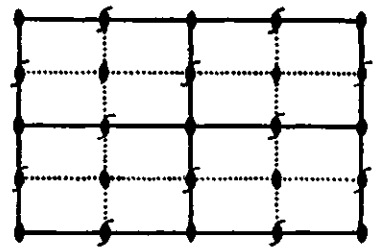
Symmetry of special projections

(001) pmg; $a'=a$, $b'=b/2$ (100) $pm1$; $b'=b/2$, $c'=c/2$ (010) $p1m$; $c'=c/2$, $a'=a/2$

$Fmm2$ C_{2v}^{18}

No. 42 $F\,m\,m\,2$ $m\,m\,2$ Orthorhombic



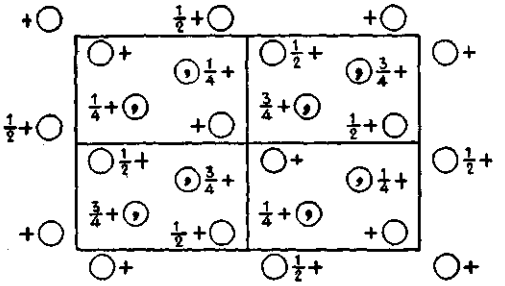


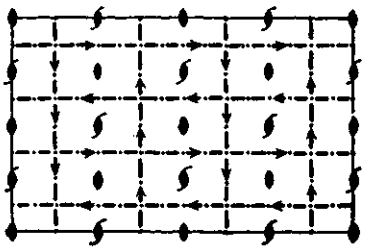
Origin on $mm2$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
16	e	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z.$	hkl: $h+k, k+l, (l+h)=2n$ $0kl$: $(k,l=2n)$ $h0l$: $(l,h=2n)$ $hk0$: $(h,k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
8	d	m	$x,0,z;\ \bar{x},0,z.$	no extra conditions
8	c	m	$0,y,z;\ 0,\bar{y},z.$	no extra conditions
8	b	2	$\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{3}{4},z.$	hkl: $h=2n;\ (k,l=2n)$
4	a	mm	$0,0,z.$	no extra conditions

Symmetry of special projections

(001) pmm; $a'=a/2,\ b'=b/2$ (100) $pm1$; $b'=b/2,\ c'=c/2$ (010) $p1m$; $c'=c/2,\ a'=a/2$





Origin on 2

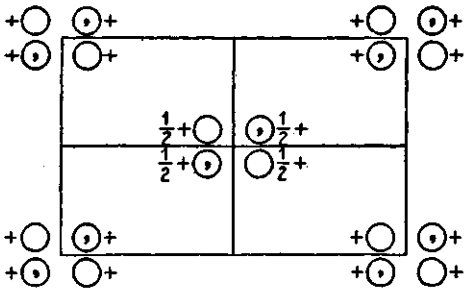
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	
16	h	1	$x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{4}-x,\frac{1}{4}+y,\frac{1}{4}+z;\ \frac{1}{4}+x,\frac{1}{4}-y,\frac{1}{4}+z.$	General: hkl: $h+k, k+l, (l+h)=2n$ $0kl$: $k+l=4n$; $(k,l=2n)$ $h0l$: $l+h=4n$; $(l,h=2n)$ $hk0$: $(h,k=2n)$ $h00$: $(h=4n)$ $0k0$: $(k=4n)$ $00l$: $(l=4n)$
8	a	2	$0,0,z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}+z.$	Special: as above, plus hkl: $h+k+l=2n+1$ or $4n$

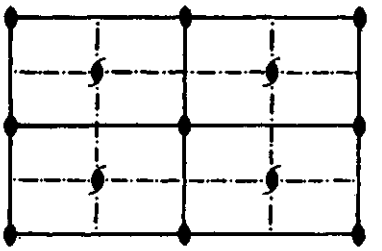
Symmetry of special projections

(001) pgg; $a'=a/2$, $b'=b/2$ (100) $cm1$; $b'=b/2$, $c'=c/2$ (010) $c1m$; $c'=c/2$, $a'=a/2$

$Imm2$ C_{2v}^{20}

No. 44 $I\,m\,m\,2$ $m\,m\,2$ Orthorhombic



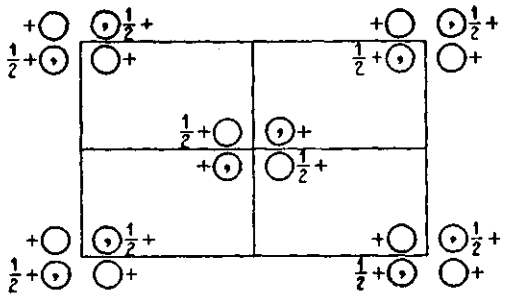


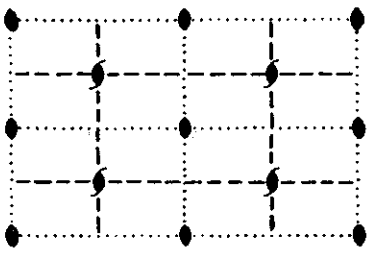
Origin on $mm2$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
				General:
8	e	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z.$	hkl: $h+k+l=2n$ $0kl$: $(k+l=2n)$ $h0l$: $(l+h=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above only
4	d	m	$0,y,z;\ 0,\bar{y},z.$	
4	c	m	$x,0,z;\ \bar{x},0,z.$	
2	b	mm	$0,\frac{1}{2},z.$	
2	a	mm	$0,0,z.$	

Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) $cm1$; $b'=b$, $c'=c$ (010) $c1m$; $c'=c$, $a'=a$





Origin on 2

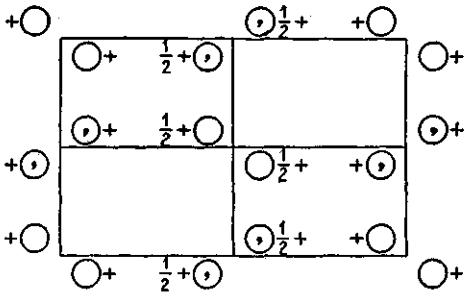
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
8	c	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z.$	General: hkl: $h+k+l=2n$ $0kl$: $k=2n$; $(l=2n)$ $h0l$: $h=2n$; $(l=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
4	b	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\frac{1}{2}+z.$	Special: as above, plus hkl: $l=2n$; $(h+k=2n)$
4	a	2	$0,0,z;\ 0,0,\frac{1}{2}+z.$	

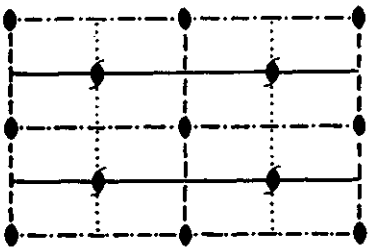
Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) $pm1$; $b'=b/2$, $c'=c/2$ (010) $p1m$; $c'=c/2$, $a'=a/2$

$Ima2$ C_{2v}^{22}

No. 46 $I\,m\,a\,2$ $m\,m\,2$ Orthorhombic





Origin on 2

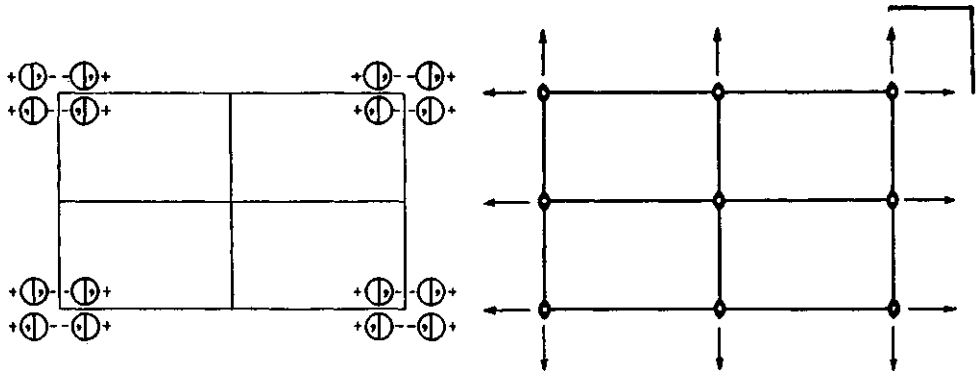
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
				General:
8	c	1	$x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,y,z;\ \frac{1}{2}+x,\bar{y},z.$	hkl: $h+k+l=2n$ $0kl$: $(k+l=2n)$ $h0l$: $h=2n;\ (l=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	b	m	$\frac{1}{4},y,z;\ \frac{3}{4},\bar{y},z.$	no extra conditions
4	a	2	$0,0,z;\ \frac{1}{2},0,z.$	hkl: $h=2n;\ (k+l=2n)$

Symmetry of special projections

(001) cmm; $a'=a,\ b'=b$ (100) $cm1$; $b'=b,\ c'=c$ (010) $p1m$; $c'=c/2,\ a'=a/2$

Orthorhombic $m\,m\,m$ $P\,2/m\,2/m\,2/m$ No. 47

$Pmmm$ D_{2h}^{1}



Origin at centre (mmm)

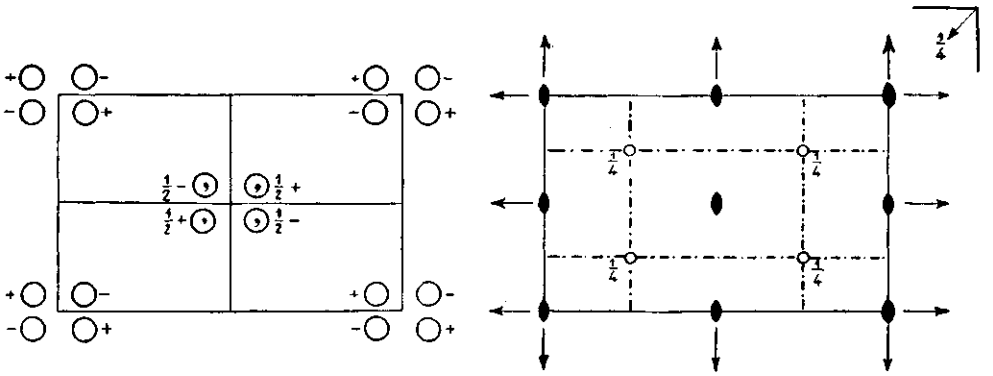
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions				Conditions limiting possible reflections
							General:
8	a	1	x,y,z; $\bar{x},\bar{y},z$; $x,\bar{y},\bar{z}$; $\bar{x},y,\bar{z}$; $\bar{x},\bar{y},\bar{z}$; $x,y,\bar{z}$; $\bar{x},y,z$; $x,\bar{y},z$.				No conditions
							Special:
4	z	m	$x,y,\frac{1}{2}$; $\bar{x},\bar{y},\frac{1}{2}$; $\bar{x},y,\frac{1}{2}$; $x,\bar{y},\frac{1}{2}$.				No conditions
4	y	m	$x,y,0$; $\bar{x},\bar{y},0$; $\bar{x},y,0$; $x,\bar{y},0$.				
4	x	m	$x,\frac{1}{2},z$; $\bar{x},\frac{1}{2},\bar{z}$; $x,\frac{1}{2},\bar{z}$; $\bar{x},\frac{1}{2},z$.				
4	w	m	$x,0,z$; $\bar{x},0,\bar{z}$; $x,0,\bar{z}$; $\bar{x},0,z$.				
4	v	m	$\frac{1}{2},y,z$; $\frac{1}{2},\bar{y},\bar{z}$; $\frac{1}{2},\bar{y},z$; $\frac{1}{2},y,\bar{z}$.				
4	u	m	$0,y,z$; $0,\bar{y},\bar{z}$; $0,\bar{y},z$; $0,y,\bar{z}$.				
2	t	mm	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	2	n	mm	$0,y,\frac{1}{2}$; $0,\bar{y},\frac{1}{2}$.
2	s	mm	$\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$.	2	m	mm	$0,y,0$; $0,\bar{y},0$.
2	r	mm	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$.	2	l	mm	$x,\frac{1}{2},\frac{1}{2}$; $\bar{x},\frac{1}{2},\frac{1}{2}$.
2	q	mm	$0,0,z$; $0,0,\bar{z}$.	2	k	mm	$x,\frac{1}{2},0$; $\bar{x},\frac{1}{2},0$.
2	p	mm	$\frac{1}{2},y,\frac{1}{2}$; $\frac{1}{2},\bar{y},\frac{1}{2}$.	2	j	mm	$x,0,\frac{1}{2}$; $\bar{x},0,\frac{1}{2}$.
2	o	mm	$\frac{1}{2},y,0$; $\frac{1}{2},\bar{y},0$.	2	i	mm	$x,0,0$; $\bar{x},0,0$.
1	h	mmm	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	1	d	mmm	$\frac{1}{2},0,\frac{1}{2}$.
1	g	mmm	$0,\frac{1}{2},\frac{1}{2}$.	1	c	mmm	$0,0,\frac{1}{2}$.
1	f	mmm	$\frac{1}{2},\frac{1}{2},0$.	1	b	mmm	$\frac{1}{2},0,0$.
1	e	mmm	$0,\frac{1}{2},0$.	1	a	mmm	$0,0,0$.

Symmetry of special projections

(001) pmm; $a'=a$, $b'=b$
(100) pmm; $b'=b$, $c'=c$
(010) pmm; $c'=c$, $a'=a$

$Pnnn$ D_{2h}^{2}

No. 48 $P\,2/n\,2/n\,2/n$ $m\,m\,m$ Orthorhombic



Origin at 222, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{1}$ (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	m	1	$x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z;\ \frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z;$ $x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z.$	hkl: No conditions $0kl$: $k+l=2n$ $h0l$: $l+h=2n$ $hk0$: $h+k=2n$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	l	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\bar{z};\ \frac{1}{2},0,\frac{1}{2}-z;\ \frac{1}{2},0,\frac{1}{2}+z.$	hkl: $h+k+l=2n$
4	k	2	$0,0,z;\ 0,0,\bar{z};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}-z;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}+z.$	
4	j	2	$\frac{1}{2},y,0;\ \frac{1}{2},\bar{y},0;\ 0,\frac{1}{2}-y,\frac{1}{2};\ 0,\frac{1}{2}+y,\frac{1}{2}.$	
4	i	2	$0,y,0;\ 0,\bar{y},0;\ \frac{1}{2},\frac{1}{2}-y,\frac{1}{2};\ \frac{1}{2},\frac{1}{2}+y,\frac{1}{2}.$	
4	h	2	$x,0,\frac{1}{2};\ \bar{x},0,\frac{1}{2};\ \frac{1}{2}-x,\frac{1}{2},0;\ \frac{1}{2}+x,\frac{1}{2},0.$	
4	g	2	$x,0,0;\ \bar{x},0,0;\ \frac{1}{2}-x,\frac{1}{2},\frac{1}{2};\ \frac{1}{2}+x,\frac{1}{2},\frac{1}{2}.$	
4	f	$\bar{1}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{3}{4}.$	hkl: $h+k,k+l,(l+h)=2n$
4	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\frac{3}{4},\frac{1}{4}.$	
2	d	222	$0,\frac{1}{2},0;\ \frac{1}{2},0,\frac{1}{2}.$	hkl: $h+k+l=2n$
2	c	222	$0,0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0.$	
2	b	222	$\frac{1}{2},0,0;\ 0,\frac{1}{2},\frac{1}{2}.$	
2	a	222	$0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	

Diagrams as on previous page but with origin shifted to $\bar{\frac{1}{4}},\bar{\frac{1}{4}},\bar{\frac{1}{4}}$

Origin at $\bar{1}$, at $\bar{\frac{1}{4}},\bar{\frac{1}{4}},\bar{\frac{1}{4}}$ from 222 (compare previous page for alternative origin)

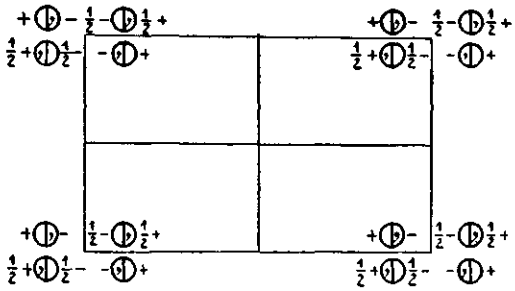
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	m	1	x,y,z; $\bar{x},\frac{1}{2}+y,\frac{1}{2}+z$; $\frac{1}{2}+x,\bar{y},\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\bar{x},\bar{y},\bar{z}$; $x,\frac{1}{2}-y,\frac{1}{2}-z$; $\frac{1}{2}-x,y,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}-y,z$.	hkl: No conditions $0kl$: $k+l=2n$ $h0l$: $l+h=2n$ $hk0$: $h+k=2n$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	l	2	$\frac{1}{4},\frac{3}{4},z$; $\frac{3}{4},\frac{1}{4},\bar{z}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}+z$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
4	k	2	$\frac{1}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{3}{4},\bar{z}$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}+z$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}-z$.	
4	j	2	$\frac{3}{4},y,\frac{1}{4}$; $\frac{1}{4},\bar{y},\frac{3}{4}$; $\frac{1}{4},\frac{1}{2}+y,\frac{3}{4}$; $\frac{3}{4},\frac{1}{2}-y,\frac{1}{4}$.	
4	i	2	$\frac{1}{4},y,\frac{1}{4}$; $\frac{3}{4},\bar{y},\frac{3}{4}$; $\frac{3}{4},\frac{1}{2}+y,\frac{3}{4}$; $\frac{1}{4},\frac{1}{2}-y,\frac{1}{4}$.	
4	h	2	$x,\frac{1}{4},\frac{3}{4}$; $\bar{x},\frac{3}{4},\frac{1}{4}$; $\frac{1}{2}+x,\frac{3}{4},\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{4},\frac{3}{4}$.	
4	g	2	$x,\frac{1}{4},\frac{1}{4}$; $\bar{x},\frac{3}{4},\frac{3}{4}$; $\frac{1}{2}+x,\frac{3}{4},\frac{3}{4}$; $\frac{1}{2}-x,\frac{1}{4},\frac{1}{4}$.	
4	f	$\bar{1}$	$0,0,0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	hkl: $h+k,k+l,(l+h)=2n$
4	e	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	
2	d	222	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$.	hkl: $h+k+l=2n$
2	c	222	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$.	
2	b	222	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$.	
2	a	222	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$.	

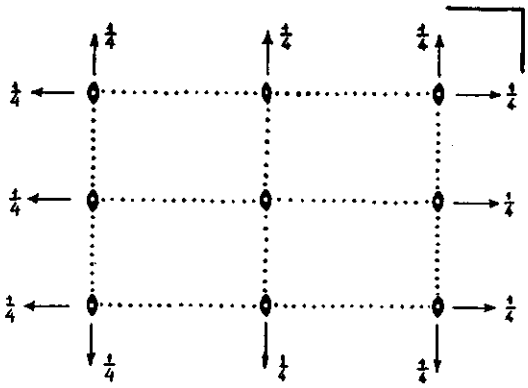
Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) cmm; $b'=b$, $c'=c$ (010) cmm; $c'=c$, $a'=a$

$Pccm$ D_{2h}^{3}

No. 49 $P\,2/c\,2/c\,2/m$ $m\,m\,m$ Orthorhombic



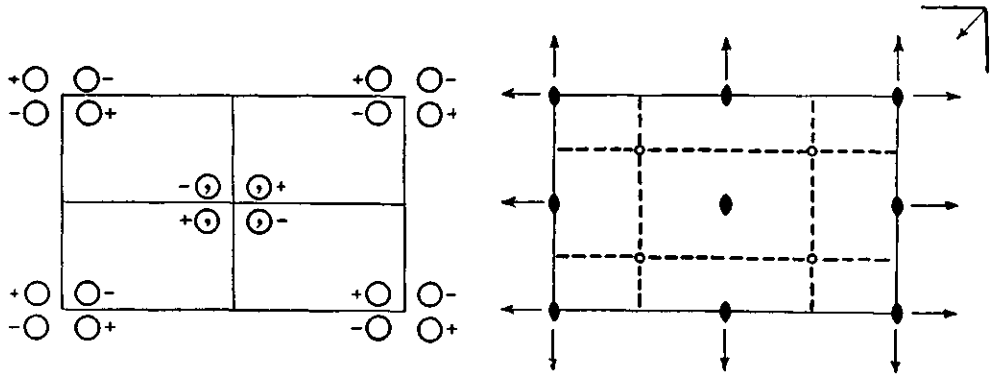


Origin at centre $(2/m)$

Number of positions, Wyckoff notation and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	r	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\frac{1}{2}+z$; $x,\bar{y},\frac{1}{2}+z$; $\bar{x},\bar{y},\bar{z}$; $x,y,\bar{z}$; $x,\bar{y},\frac{1}{2}-z$; $\bar{x},y,\frac{1}{2}-z$.	hkl: No conditions $0kl$: $l=2n$ $h0l$: $l=2n$ $hk0$: $h00$: $0k0$: No conditions $00l$: $(l=2n)$
				Special: as above, plus
4	q	m	$x,y,0$; $\bar{x},\bar{y},0$; $\bar{x},y,\frac{1}{2}$; $x,\bar{y},\frac{1}{2}$.	no extra conditions
4	p	2	$\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$; $\frac{1}{2},0,\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	(a) to (p) inclusive hkl: $l=2n$
4	o	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $0,\frac{1}{2},\frac{1}{2}+z$; $0,\frac{1}{2},\frac{1}{2}-z$.	
4	n	2	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	
4	m	2	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	
4	l	2	$\frac{1}{2},y,\frac{1}{4}$; $\frac{1}{2},\bar{y},\frac{1}{4}$; $\frac{1}{2},y,\frac{3}{4}$; $\frac{1}{2},\bar{y},\frac{3}{4}$.	
4	k	2	$0,y,\frac{1}{4}$; $0,\bar{y},\frac{1}{4}$; $0,y,\frac{3}{4}$; $0,\bar{y},\frac{3}{4}$.	
4	j	2	$x,\frac{1}{2},\frac{1}{4}$; $\bar{x},\frac{1}{2},\frac{1}{4}$; $x,\frac{1}{2},\frac{3}{4}$; $\bar{x},\frac{1}{2},\frac{3}{4}$.	
4	i	2	$x,0,\frac{1}{4}$; $\bar{x},0,\frac{1}{4}$; $x,0,\frac{3}{4}$; $\bar{x},0,\frac{3}{4}$.	
2	h	222	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},\frac{3}{4}$.	
2	g	222	$0,\frac{1}{2},\frac{1}{4}$; $0,\frac{1}{2},\frac{3}{4}$.	
2	f	222	$\frac{1}{2},0,\frac{1}{4}$; $\frac{1}{2},0,\frac{3}{4}$.	
2	e	222	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	
2	d	$2/m$	$\frac{1}{2},0,0$; $\frac{1}{2},0,\frac{1}{2}$.	
2	c	$2/m$	$0,\frac{1}{2},0$; $0,\frac{1}{2},\frac{1}{2}$.	
2	b	$2/m$	$\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
2	a	$2/m$	$0,0,0$; $0,0,\frac{1}{2}$.	

Symmetry of special projections

(001) pmm; $a'=a$, $b'=b$ (100) pmm; $b'=b$, $c'=c/2$ (010) pmm; $c'=c/2$, $a'=a$



Origin at 222, at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$ (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	*m*	1	$x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}-y,\bar{z};\ \frac{1}{2}+x,\frac{1}{2}+y,\bar{z};$ $x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \frac{1}{2}-x,\frac{1}{2}+y,z;\ \frac{1}{2}+x,\frac{1}{2}-y,z.$	*hkl*: No conditions 0*kl*: $k=2n$ *h*0*l*: $h=2n$ *hk*0: $h+k=2n$ *h*00: $(h=2n)$ 0*k*0: $(k=2n)$ 00*l*: No conditions
				Special: as above, plus
4	*l*	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\bar{z};\ \frac{1}{2},0,z;\ \frac{1}{2},0,\bar{z}.$	*hkl*: $h+k=2n$
4	*k*	2	$0,0,z;\ 0,0,\bar{z};\ \frac{1}{2},\frac{1}{2},z;\ \frac{1}{2},\frac{1}{2},\bar{z}.$	
4	*j*	2	$0,y,\frac{1}{2};\ 0,\bar{y},\frac{1}{2};\ \frac{1}{2},\frac{1}{2}-y,\frac{1}{2};\ \frac{1}{2},\frac{1}{2}+y,\frac{1}{2}.$	
4	*i*	2	$0,y,0;\ 0,\bar{y},0;\ \frac{1}{2},\frac{1}{2}-y,0;\ \frac{1}{2},\frac{1}{2}+y,0.$	
4	*h*	2	$x,0,\frac{1}{2};\ \bar{x},0,\frac{1}{2};\ \frac{1}{2}-x,\frac{1}{2},\frac{1}{2};\ \frac{1}{2}+x,\frac{1}{2},\frac{1}{2}.$	
4	*g*	2	$x,0,0;\ \bar{x},0,0;\ \frac{1}{2}-x,\frac{1}{2},0;\ \frac{1}{2}+x,\frac{1}{2},0.$	
4	*f*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2};\ \frac{3}{4},\frac{3}{4},\frac{1}{2};\ \frac{1}{4},\frac{3}{4},\frac{1}{2};\ \frac{3}{4},\frac{1}{4},\frac{1}{2}.$	*hkl*: $h=2n;\ k=2n$
4	*e*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0;\ \frac{3}{4},\frac{3}{4},0;\ \frac{1}{4},\frac{3}{4},0;\ \frac{3}{4},\frac{1}{4},0.$	
2	*d*	222	$0,0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	*hkl*: $h+k=2n$
2	*c*	222	$\frac{1}{2},0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2}.$	
2	*b*	222	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0.$	
2	*a*	222	$0,0,0;\ \frac{1}{2},\frac{1}{2},0.$	

$Pban$ D_{2h}^{4}

No. 50 $P\,2/b\,2/a\,2/n$ $m\,m\,m$ Orthorhombic

Diagrams as on previous page but with origin shifted to $\bar{\tfrac{1}{4}},\bar{\tfrac{1}{4}},0$

Origin at $\bar{1}$, at $\bar{\tfrac{1}{4}},\bar{\tfrac{1}{4}},0$ from 222 (compare previous page for alternative origin)

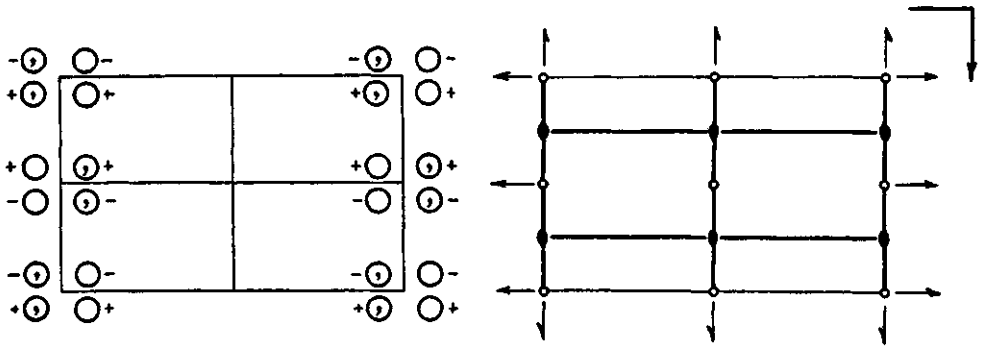
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	m	1	x,y,z; $\tfrac{1}{2}-x,\tfrac{1}{2}-y,z$; $\tfrac{1}{2}-x,y,\bar{z}$; $x,\tfrac{1}{2}-y,\bar{z}$; $\bar{x},\bar{y},\bar{z}$; $\tfrac{1}{2}+x,\tfrac{1}{2}+y,\bar{z}$; $\tfrac{1}{2}+x,\bar{y},z$; $\bar{x},\tfrac{1}{2}+y,z$.	hkl: No conditions $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: No conditions
				Special: as above, plus
4	l	2	$\tfrac{1}{4},\tfrac{3}{4},z$; $\tfrac{3}{4},\tfrac{1}{4},\bar{z}$; $\tfrac{1}{4},\tfrac{3}{4},\bar{z}$; $\tfrac{3}{4},\tfrac{1}{4},z$.	hkl: $h+k=2n$
4	k	2	$\tfrac{1}{4},\tfrac{1}{4},z$; $\tfrac{3}{4},\tfrac{3}{4},\bar{z}$; $\tfrac{1}{4},\tfrac{1}{4},\bar{z}$; $\tfrac{3}{4},\tfrac{3}{4},z$.	
4	j	2	$\tfrac{1}{4},y,\tfrac{1}{2}$; $\tfrac{3}{4},\bar{y},\tfrac{1}{2}$; $\tfrac{1}{4},\tfrac{1}{2}-y,\tfrac{1}{2}$; $\tfrac{3}{4},\tfrac{1}{2}+y,\tfrac{1}{2}$.	
4	i	2	$\tfrac{1}{4},y,0$; $\tfrac{3}{4},\bar{y},0$; $\tfrac{1}{4},\tfrac{1}{2}-y,0$; $\tfrac{3}{4},\tfrac{1}{2}+y,0$.	
4	h	2	$x,\tfrac{1}{4},\tfrac{1}{2}$; $\bar{x},\tfrac{3}{4},\tfrac{1}{2}$; $\tfrac{1}{2}-x,\tfrac{1}{4},\tfrac{1}{2}$; $\tfrac{1}{2}+x,\tfrac{3}{4},\tfrac{1}{2}$.	
4	g	2	$x,\tfrac{1}{4},0$; $\bar{x},\tfrac{3}{4},0$; $\tfrac{1}{2}-x,\tfrac{1}{4},0$; $\tfrac{1}{2}+x,\tfrac{3}{4},0$.	
4	f	$\bar{1}$	$0,0,\tfrac{1}{2}$; $\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}$; $0,\tfrac{1}{2},\tfrac{1}{2}$; $\tfrac{1}{2},0,\tfrac{1}{2}$.	hkl: $h=2n$; $k=2n$
4	e	$\bar{1}$	$0,0,0$; $\tfrac{1}{2},\tfrac{1}{2},0$; $\tfrac{1}{2},0,0$; $0,\tfrac{1}{2},0$.	
2	d	222	$\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{2}$; $\tfrac{3}{4},\tfrac{3}{4},\tfrac{1}{2}$.	hkl: $h+k=2n$
2	c	222	$\tfrac{3}{4},\tfrac{1}{4},\tfrac{1}{2}$; $\tfrac{1}{4},\tfrac{3}{4},\tfrac{1}{2}$.	
2	b	222	$\tfrac{3}{4},\tfrac{1}{4},0$; $\tfrac{1}{4},\tfrac{3}{4},0$.	
2	a	222	$\tfrac{1}{4},\tfrac{1}{4},0$; $\tfrac{3}{4},\tfrac{3}{4},0$.	

Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) pmm; $b'=b/2$, $c'=c$ (010) pmm; $c'=c$, $a'=a/2$

Orthorhombic $m\,m\,m$ $P\,2_1/m\,2/m\,2/a$ No. 51

$Pmma$
D_{2h}^{5}



Origin at centre ($2/m$)

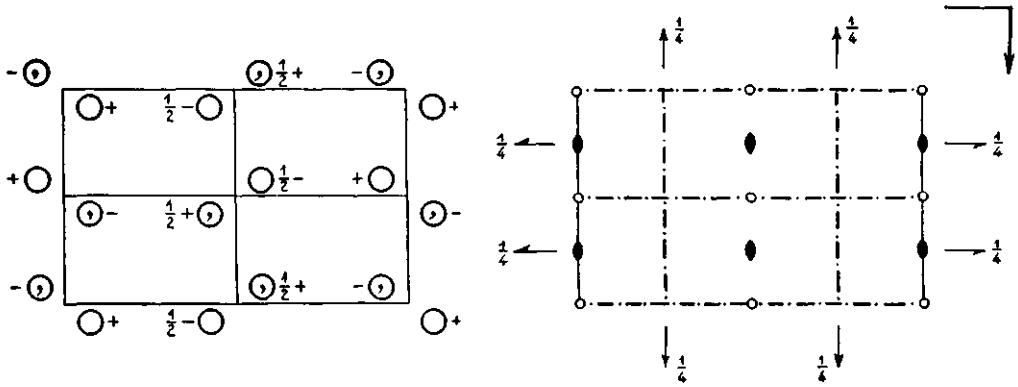
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	l	1	x,y,z; $\bar{x},y,\bar{z}$; $\frac{1}{2}-x,y,z$; $\frac{1}{2}+x,y,\bar{z}$; $\bar{x},\bar{y},\bar{z}$; $x,\bar{y},z$; $\frac{1}{2}+x,\bar{y},\bar{z}$; $\frac{1}{2}-x,\bar{y},z$.	hkl: No conditions $0kl$: No conditions $h0l$: No conditions $hk0$: $h=2n$ $h00$: ($h=2n$) $0k0$: No conditions $00l$: No conditions
				Special: as above, plus
4	k	m	$\frac{1}{4},y,z$; $\frac{1}{4},\bar{y},z$; $\frac{3}{4},\bar{y},\bar{z}$; $\frac{3}{4},y,\bar{z}$.	no extra conditions
4	j	m	$x,\frac{1}{2},z$; $\bar{x},\frac{1}{2},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2},\bar{z}$; $\frac{1}{2}-x,\frac{1}{2},z$.	
4	i	m	$x,0,z$; $\bar{x},0,\bar{z}$; $\frac{1}{2}+x,0,\bar{z}$; $\frac{1}{2}-x,0,z$.	
4	h	2	$0,y,\frac{1}{2}$; $0,\bar{y},\frac{1}{2}$; $\frac{1}{2},y,\frac{1}{2}$; $\frac{1}{2},\bar{y},\frac{1}{2}$.	hkl: $h=2n$
4	g	2	$0,y,0$; $0,\bar{y},0$; $\frac{1}{2},y,0$; $\frac{1}{2},\bar{y},0$.	
2	f	mm	$\frac{1}{4},\frac{1}{2},z$; $\frac{3}{4},\frac{1}{2},\bar{z}$.	no extra conditions
2	e	mm	$\frac{1}{4},0,z$; $\frac{3}{4},0,\bar{z}$.	
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h=2n$
2	c	$2/m$	$0,0,\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	
2	b	$2/m$	$0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$.	
2	a	$2/m$	$0,0,0$; $\frac{1}{2},0,0$.	

Symmetry of special projections

(001) pmm; $a'=a/2$, $b'=b$ (100) pmm; $b'=b$, $c'=c$ (010) pgm; $c'=c$, $a'=a$

$Pnna$ D_{2h}^{6}

No. 52 $P\,2/n\,2_1/n\,2/a$ $m\,m\,m$ Orthorhombic



Origin at $\bar{1}$

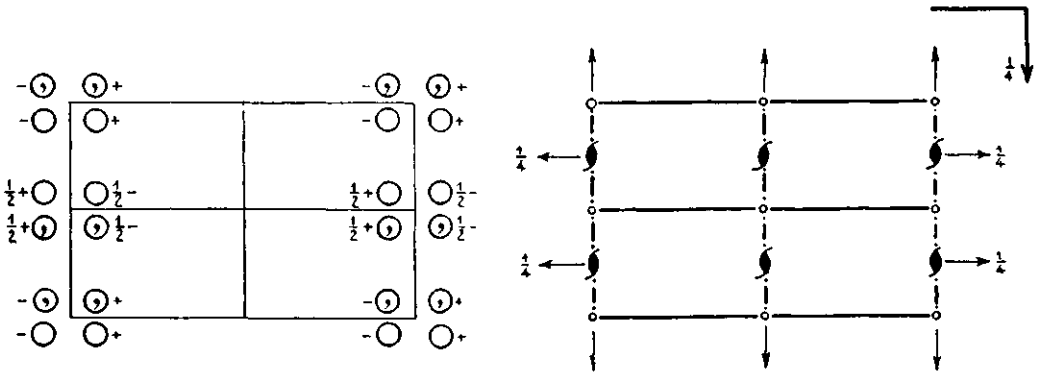
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	e	1	x,y,z; $\frac{1}{2}-x,\bar{y},z$; $x,\frac{1}{2}-y,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,y,\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$.	hkl: No conditions $0kl$: $k+l=2n$ $h0l$: $l+h=2n$ $hk0$: $h=2n$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	d	2	$x,\frac{1}{4},\frac{1}{4}$; $\bar{x},\frac{3}{4},\frac{3}{4}$; $\frac{1}{2}+x,\frac{1}{4},\frac{3}{4}$; $\frac{1}{2}-x,\frac{3}{4},\frac{1}{4}$.	hkl: $h+l=2n$
4	c	2	$\frac{1}{4},0,z$; $\frac{3}{4},0,\bar{z}$; $\frac{3}{4},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{4},\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
4	b	$\bar{1}$	$0,0,\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$.	hkl: $h=2n$; $k+l=2n$
4	a	$\bar{1}$	$0,0,0$; $\frac{1}{2},0,0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	

Symmetry of special projections

(001) pgm; $a'=a/2$, $b'=b$ (100) cmm; $b'=b$, $c'=c$ (010) cmm; $c'=c$, $a'=a$

Orthorhombic $m\,m\,m$ $P\,2/m\,2/n\,2_1/a$ No. 53

$Pmna$ D_{2h}^{7}



Origin at centre ($2/m$)

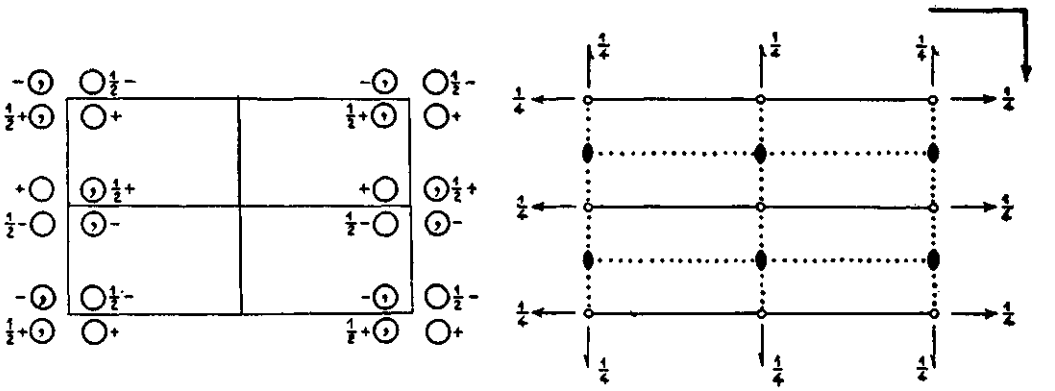
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	i	1	$x,y,z;\ x,\bar{y},\bar{z};\ \frac{1}{2}-x,y,\frac{1}{2}-z;\ \frac{1}{2}-x,\bar{y},\frac{1}{2}+z;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},y,z;\ \frac{1}{2}+x,\bar{y},\frac{1}{2}+z;\ \frac{1}{2}+x,y,\frac{1}{2}-z.$	hkl: No conditions $0kl$: No conditions $h0l$: $l+h=2n$ $hk0$: $h=2n$ $h00$: $(h=2n)$ $0k0$: No conditions $00l$: $(l=2n)$
				Special: as above, plus
4	h	m	$0,y,z;\ 0,\bar{y},\bar{z};\ \frac{1}{2},y,\frac{1}{2}-z;\ \frac{1}{2},\bar{y},\frac{1}{2}+z.$	no extra conditions
4	g	2	$\frac{1}{4},y,\frac{1}{4};\ \frac{3}{4},\bar{y},\frac{3}{4};\ \frac{3}{4},y,\frac{1}{4};\ \frac{1}{4},\bar{y},\frac{3}{4}.$	hkl: $h=2n$
4	f	2	$x,\frac{1}{2},0;\ \bar{x},\frac{1}{2},0;\ \frac{1}{2}+x,\frac{1}{2},\frac{1}{2};\ \frac{1}{2}-x,\frac{1}{2},\frac{1}{2}.$	hkl: $h+l=2n$
4	e	2	$x,0,0;\ \bar{x},0,0;\ \frac{1}{2}+x,0,\frac{1}{2};\ \frac{1}{2}-x,0,\frac{1}{2}.$	
2	d	$2/m$	$0,\frac{1}{2},0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	
2	c	$2/m$	$\frac{1}{2},\frac{1}{2},0;\ 0,\frac{1}{2},\frac{1}{2}.$	
2	b	$2/m$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}.$	
2	a	$2/m$	$0,0,0;\ \frac{1}{2},0,\frac{1}{2}.$	

Symmetry of special projections

(001) pmm; $a'=a/2$, $b'=b$ (100) pgm; $b'=b$, $c'=c$ (010) cmm; $c'=c$, $a'=a$

$Pcca$ D_{2h}^{8}

No. 54 $P\,2_1/c\,2/c\,2/a$ $m\,m\,m$ Orthorhombic



Origin at $\bar{1}$

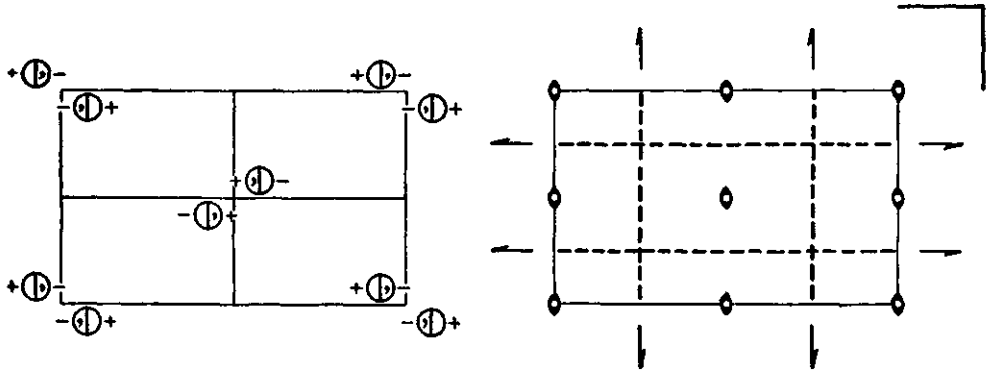
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	f	1	x,y,z; $\frac{1}{2}-x,\bar{y},z$; $\frac{1}{2}+x,\bar{y},\frac{1}{2}-z$; $\bar{x},y,\frac{1}{2}-z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,y,\bar{z}$; $\frac{1}{2}-x,y,\frac{1}{2}+z$; $x,\bar{y},\frac{1}{2}+z$.	hkl: No conditions $0kl$: $l=2n$ $h0l$: $l=2n$ $hk0$: $h=2n$ $h00$: $(h=2n)$ $0k0$: No conditions $00l$: $(l=2n)$
				Special: as above, plus
4	e	2	$\frac{1}{4},\frac{1}{2},z$; $\frac{3}{4},\frac{1}{2},\bar{z}$; $\frac{1}{4},\frac{1}{2},\frac{1}{2}+z$; $\frac{3}{4},\frac{1}{2},\frac{1}{2}-z$.	hkl: $l=2n$
4	d	2	$\frac{1}{4},0,z$; $\frac{3}{4},0,\bar{z}$; $\frac{1}{4},0,\frac{1}{2}+z$; $\frac{3}{4},0,\frac{1}{2}-z$.	
4	c	2	$0,y,\frac{1}{4}$; $0,\bar{y},\frac{3}{4}$; $\frac{1}{2},y,\frac{3}{4}$; $\frac{1}{2},\bar{y},\frac{1}{4}$.	hkl: $h+l=2n$
4	b	$\bar{1}$	$0,\frac{1}{2},0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h=2n$; $l=2n$
4	a	$\bar{1}$	$0,0,0$; $0,0,\frac{1}{2}$; $\frac{1}{2},0,0$; $\frac{1}{2},0,\frac{1}{2}$.	

Symmetry of special projections

(001) pmm; $a'=a/2$, $b'=b$ (100) pmm; $b'=b$, $c'=c/2$ (010) pgm; $c'=c/2$, $a'=a$

Orthorhombic $m\,m\,m$ $P\,2_1/b\,2_1/a\,2/m$ No. 55

$Pbam$
D_{2h}^{9}



Origin at centre $(2/m)$

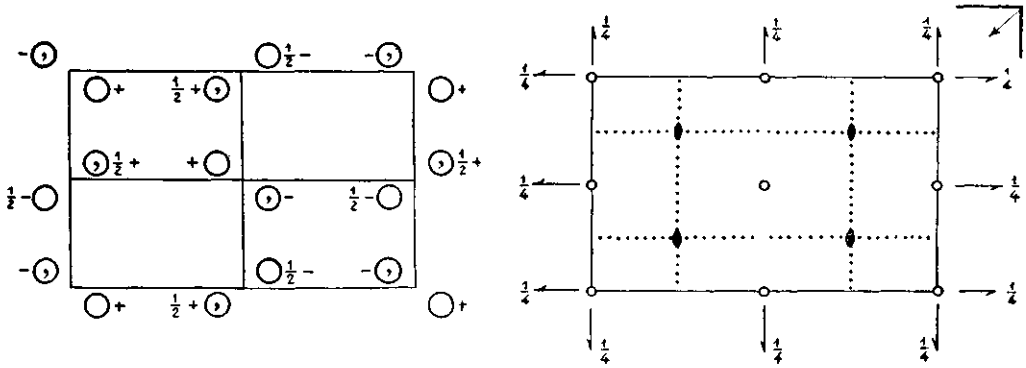
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	i	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$; $\bar{x},\bar{y},\bar{z}$; $x,y,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $\frac{1}{2}+x,\frac{1}{2}-y,z$.	hkl: No conditions $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: No conditions $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: No conditions
				Special: as above, plus
4	h	m	$x,y,\frac{1}{2}$; $\bar{x},\bar{y},\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}$.	no extra conditions
4	g	m	$x,y,0$; $\bar{x},\bar{y},0$; $\frac{1}{2}+x,\frac{1}{2}-y,0$; $\frac{1}{2}-x,\frac{1}{2}+y,0$.	
4	f	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$.	hkl: $h+k=2n$
4	e	2	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	
2	c	$2/m$	$0,\frac{1}{2},0$; $\frac{1}{2},0,0$.	
2	b	$2/m$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
2	a	$2/m$	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$.	

Symmetry of special projections

(001) pgg; $a'=a$, $b'=b$ (100) pmm; $b'=b/2$, $c'=c$ (010) pmm; $c'=c$, $a'=a/2$

$Pccn$ D_{2h}^{10}

No. 56 $P\,2_1/c\,2_1/c\,2/n$ $m\,m\,m$ Orthorhombic

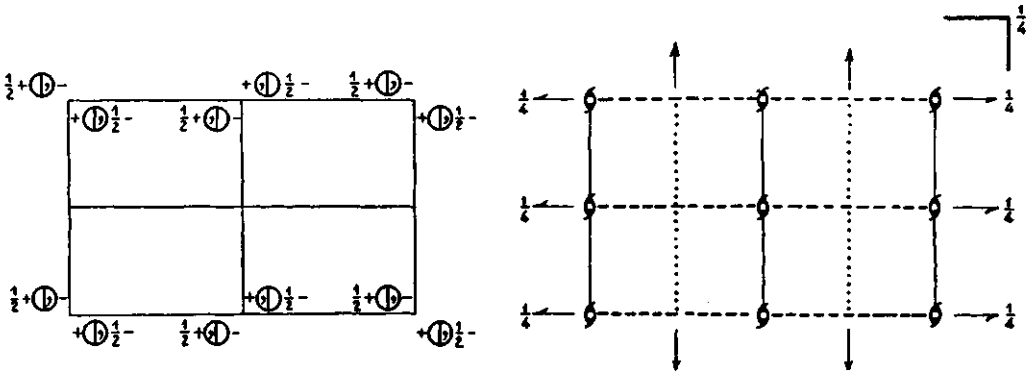


Origin at $\bar{1}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	e	1	x,y,z; $\frac{1}{2}-x,\frac{1}{2}-y,z$; $\frac{1}{2}+x,\bar{y},\frac{1}{2}-z$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}-x,y,\frac{1}{2}+z$; $x,\frac{1}{2}-y,\frac{1}{2}+z$.	hkl: No conditions $0kl$: $l=2n$ $h0l$: $l=2n$ $hk0$: $h+k=2n$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	d	2	$\frac{1}{4},\frac{3}{4},z$; $\frac{3}{4},\frac{1}{4},\bar{z}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}+z$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}-z$.	hkl: $l=2n$
4	c	2	$\frac{1}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{3}{4},\bar{z}$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}+z$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}-z$.	
4	b	$\bar{1}$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $0,\frac{1}{2},0$; $\frac{1}{2},0,0$.	hkl: $h+k,k+l,(l+h)=2n$
4	a	$\bar{1}$	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	

Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) pmg; $b'=b$, $c'=c/2$ (010) pgm; $c'=c/2$, $a'=a$



Origin at $\bar{1}$

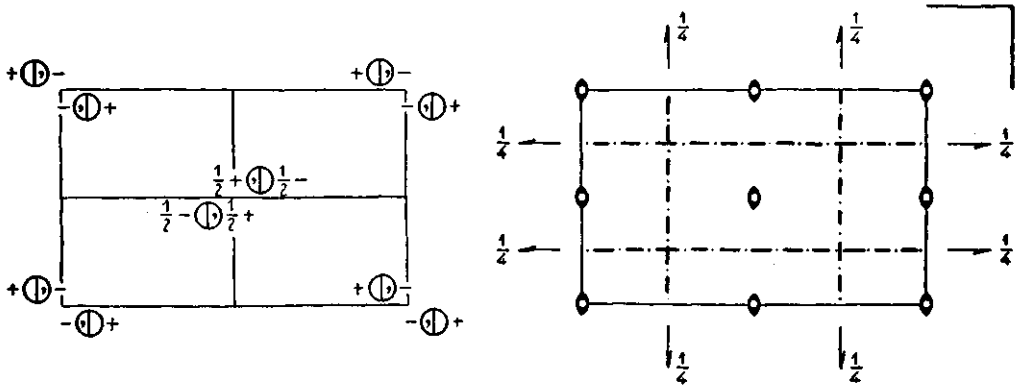
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	e	1	x,y,z; $\bar{x},\bar{y},\frac{1}{2}+z$; $x,\frac{1}{2}-y,\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$; $\bar{x},\bar{y},\bar{z}$; $x,y,\frac{1}{2}-z$; $\bar{x},\frac{1}{2}+y,z$; $x,\frac{1}{2}-y,\frac{1}{2}+z$.	hkl: No conditions $0kl$: $k=2n$ $h0l$: $l=2n$ $hk0$: No conditions $h00$: No conditions $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	d	m	$x,y,\frac{1}{4}$; $\bar{x},\bar{y},\frac{3}{4}$; $\bar{x},\frac{1}{2}+y,\frac{1}{4}$; $x,\frac{1}{2}-y,\frac{3}{4}$.	no extra conditions
4	c	2	$x,\frac{1}{4},0$; $\bar{x},\frac{3}{4},0$; $x,\frac{1}{4},\frac{1}{2}$; $\bar{x},\frac{3}{4},\frac{1}{2}$.	hkl: $l=2n$
4	b	$\bar{1}$	$\frac{1}{2},0,0$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $k=2n$; $l=2n$
4	a	$\bar{1}$	$0,0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$.	

Symmetry of special projections

(001) pgm; $a'=a$, $b'=b$ (100) pgm; $b'=b/2$, $c'=c$ (010) pmm; $c'=c/2$, $a'=a$

$Pnnm$ D_{2h}^{12}

No. 58 $P\,2_1/n\,2_1/n\,2/m$ $m\,m\,m$ Orthorhombic

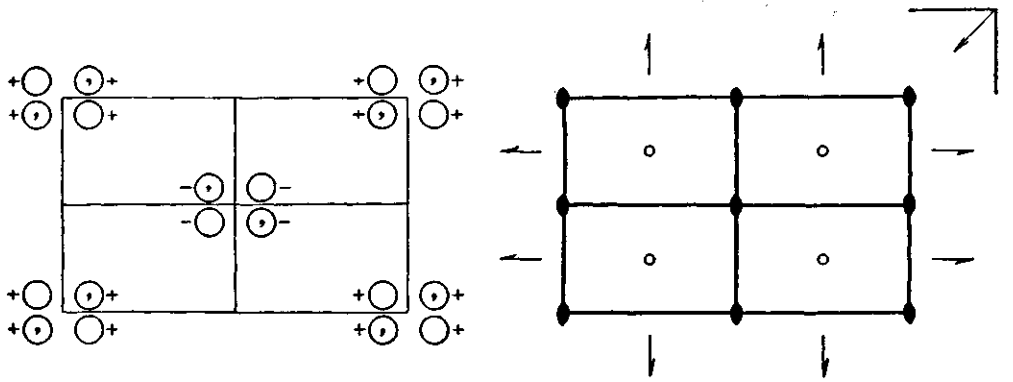


Origin at centre ($2/m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	h	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; $\bar{x},\bar{y},\bar{z}$; $x,y,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$.	hkl: No conditions $0kl$: $k+l=2n$ $h0l$: $l+h=2n$ $hk0$: No conditions $h00$: ($h=2n$) $0k0$: ($k=2n$) $00l$: ($l=2n$)
				Special: as above, plus
4	g	m	$x,y,0$; $\bar{x},\bar{y},0$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}$.	no extra conditions
4	f	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},0,\frac{1}{2}-z$; $\frac{1}{2},0,\frac{1}{2}+z$.	hkl: $h+k+l=2n$
4	e	2	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$.	
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$.	
2	c	$2/m$	$0,\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$.	
2	b	$2/m$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	
2	a	$2/m$	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	

Symmetry of special projections

(001) pgg; $a'=a$, $b'=b$ (100) cmm; $b'=b$, $c'=c$ (010) cmm; $c'=c$, $a'=a$



Origin at mmn, at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$ (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	g	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}-y,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$; $\bar{x},y,z$; $x,\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$.	hkl: No conditions $0kl$: No conditions $h0l$: No conditions $hk0$: $h+k=2n$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: No conditions
				Special: as above, plus
4	f	m	$x,0,z$; $\bar{x},0,z$; $\frac{1}{2}-x,\frac{1}{2},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2},\bar{z}$.	no extra conditions
4	e	m	$0,y,z$; $0,\bar{y},z$; $\frac{1}{2},\frac{1}{2}-y,\bar{z}$; $\frac{1}{2},\frac{1}{2}+y,\bar{z}$.	
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}$.	hkl: $h=2n$; $k=2n$
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$; $\frac{3}{4},\frac{3}{4},0$; $\frac{1}{4},\frac{3}{4},0$; $\frac{3}{4},\frac{1}{4},0$.	
2	b	mm	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$.	no extra conditions
2	a	mm	$0,0,z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	

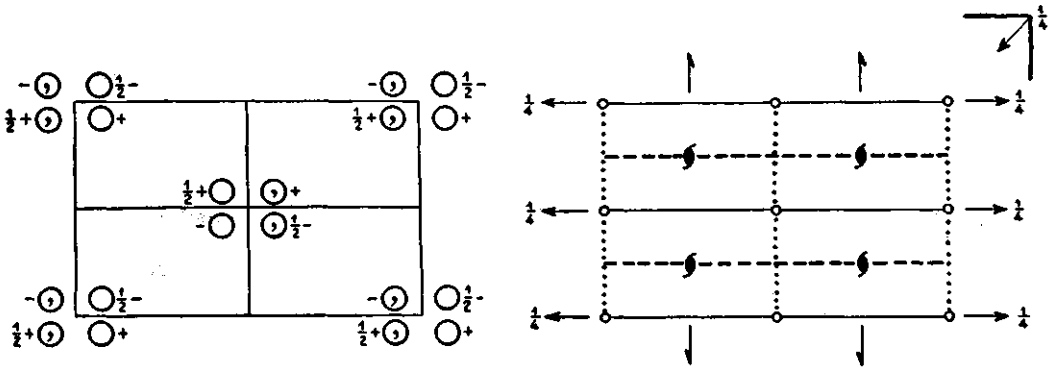
Diagrams as on previous page but with origin shifted to $\bar{\frac{1}{4}},\bar{\frac{1}{4}},0$

Origin at $\bar{1}$, at $\bar{\frac{1}{4}},\bar{\frac{1}{4}},0$ from *mmn* (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	g	1	$x,y,z;\ \frac{1}{2}-x,y,z;\ x,\frac{1}{2}-y,z;\ \frac{1}{2}-x,\frac{1}{2}-y,z;$ $\bar{x},\bar{y},\bar{z};\ \frac{1}{2}+x,\bar{y},\bar{z};\ \bar{x},\frac{1}{2}+y,\bar{z};\ \frac{1}{2}+x,\frac{1}{2}+y,\bar{z}.$	hkl: $0kl$: $h0l$: No conditions $hk0$: $h+k=2n$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: No conditions
				Special: as above, plus
4	f	m	$x,\frac{1}{4},z;\ \bar{x},\frac{3}{4},\bar{z};\ \frac{1}{2}-x,\frac{1}{4},z;\ \frac{1}{2}+x,\frac{3}{4},\bar{z}.$	no extra conditions
4	e	m	$\frac{1}{4},y,z;\ \frac{3}{4},\bar{y},\bar{z};\ \frac{1}{4},\frac{1}{2}-y,z;\ \frac{3}{4},\frac{1}{2}+y,\bar{z}.$	
4	d	$\bar{1}$	$0,0,\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	hkl: $h=2n$; $k=2n$
4	c	$\bar{1}$	$0,0,0;\ \frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ \frac{1}{2},\frac{1}{2},0.$	
2	b	mm	$\frac{1}{4},\frac{3}{4},z;\ \frac{3}{4},\frac{1}{4},\bar{z}.$	no extra conditions
2	a	mm	$\frac{1}{4},\frac{1}{4},z;\ \frac{3}{4},\frac{3}{4},\bar{z}.$	

Symmetry of special projections

(001) *cmm*; $a'=a$, $b'=b$ (100) *pmg*; $b'=b$, $c'=c$ (010) *pgm*; $c'=c$, $a'=a$



Origin at $\bar{1}$

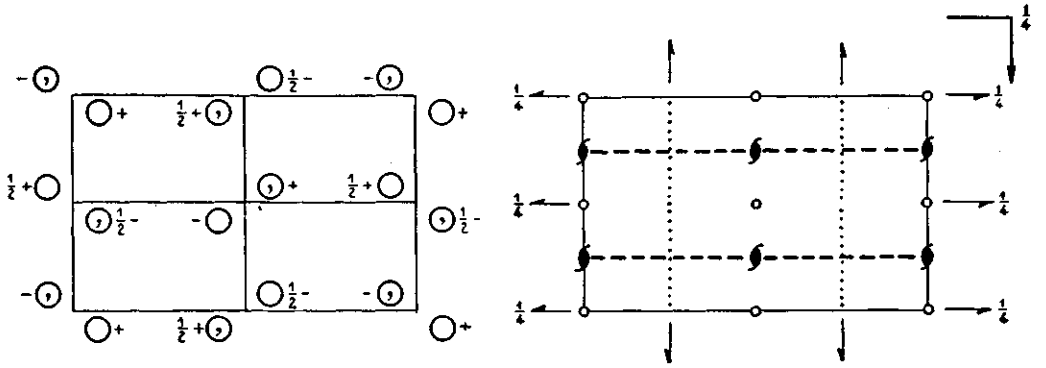
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	*d*	1	x,y,z; $\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\bar{x},y,\frac{1}{2}-z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $x,\bar{y},\frac{1}{2}+z$.	*hkl*: No conditions 0*kl*: $k=2n$ *h*0*l*: $l=2n$ *hk*0: $h+k=2n$ *h*00: $(h=2n)$ 0*k*0: $(k=2n)$ 00*l*: $(l=2n)$
				Special: as above, plus
4	*c*	2	$0,y,\frac{1}{4}$; $0,\bar{y},\frac{3}{4}$; $\frac{1}{2},\frac{1}{2}+y,\frac{1}{4}$; $\frac{1}{2},\frac{1}{2}-y,\frac{3}{4}$.	*hkl*: $h+k=2n$
4	*b*	$\bar{1}$	$0,\frac{1}{2},0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$; $\frac{1}{2},0,\frac{1}{2}$.	*hkl*: $h+k=2n$; $l=2n$
4	*a*	$\bar{1}$	$0,0,0$; $0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	

Symmetry of special projections

(001) *cmm*; $a'=a$, $b'=b$ (100) *pgm*; $b'=b/2$, $c'=c$ (010) *pgm*; $c'=c/2$, $a'=a$

$Pbca$ D_{2h}^{15}

No. 61 $P\,2_1/b\,2_1/c\,2_1/a$ $m\,m\,m$ Orthorhombic

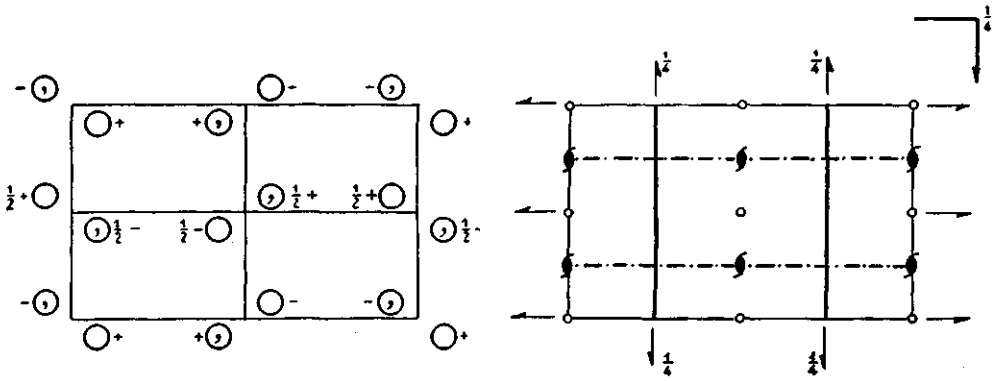


Origin at $\bar{1}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	c	1	x,y,z; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}-x,\bar{y},\frac{1}{2}+z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $x,\frac{1}{2}-y,\frac{1}{2}+z$; $\frac{1}{2}+x,y,\frac{1}{2}-z$.	hkl: No conditions $0kl$: $k=2n$ $h0l$: $l=2n$ $hk0$: $h=2n$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	b	$\bar{1}$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $0,\frac{1}{2},0$; $\frac{1}{2},0,0$.	hkl: $h+k,k+l,(l+h)=2n$
4	a	$\bar{1}$	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	

Symmetry of special projections

(001) pgm; $a'=a/2$, $b'=b$ (100) pgm; $b'=b/2$, $c'=c$ (010) pgm; $c'=c/2$, $a'=a$



Origin at $\bar{1}$

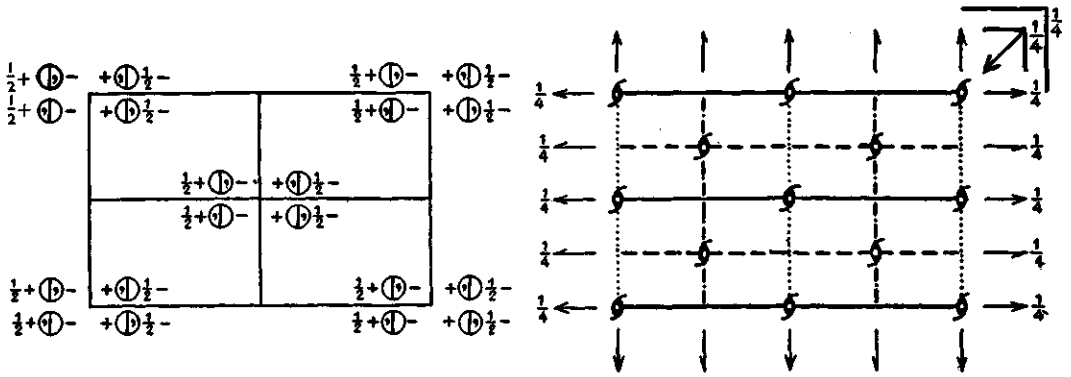
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	d	1	x,y,z; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z$; $\bar{x},\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}-x,\bar{y},\frac{1}{2}+z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $x,\frac{1}{2}-y,z$; $\frac{1}{2}+x,y,\frac{1}{2}-z$.	hkl: No conditions $0kl$: $k+l=2n$ $h0l$: No conditions $hk0$: $h=2n$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	c	m	$x,\frac{1}{4},z$; $\bar{x},\frac{3}{4},\bar{z}$; $\frac{1}{2}-x,\frac{3}{4},\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{4},\frac{1}{2}-z$.	no extra conditions
4	b	$\bar{1}$	$0,0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$; $\frac{1}{2},\frac{1}{2},0$.	hkl: $h+l=2n$; $k=2n$
4	a	$\bar{1}$	$0,0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	

Symmetry of special projections

(001) pgm; $a'=a/2$, $b'=b$ (100) cmm; $b'=b$, $c'=c$ (010) pgg; $c'=c$, $a'=a$

$Cmcm$ D_{2h}^{17}

No. 63 $C\,2/m\,2/c\,2_1/m$ $m\,m\,m$ Orthorhombic

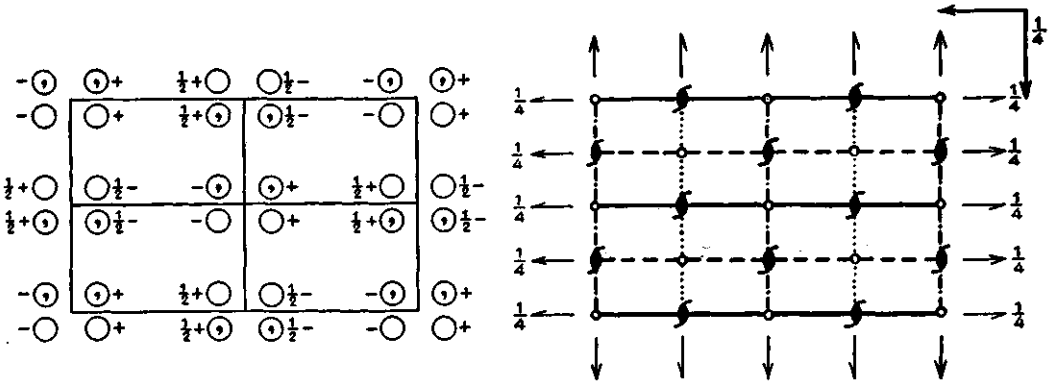


Origin at centre ($2/m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	General:
16	h	1	$x,y,z;\ x,\bar{y},\bar{z};\ x,y,\frac{1}{2}-z;\ x,\bar{y},\frac{1}{2}+z;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},y,z;\ \bar{x},\bar{y},\frac{1}{2}+z;\ \bar{x},y,\frac{1}{2}-z.$	hkl: $h+k=2n$ $0kl$: $(k=2n)$ $h0l$: $l=2n$; $(h=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
8	g	m	$x,y,\frac{1}{4};\ \bar{x},y,\frac{1}{4};\ x,\bar{y},\frac{3}{4};\ \bar{x},\bar{y},\frac{3}{4}.$	no extra conditions
8	f	m	$0,y,z;\ 0,\bar{y},\bar{z};\ 0,y,\frac{1}{2}-z;\ 0,\bar{y},\frac{1}{2}+z.$	
8	e	2	$x,0,0;\ \bar{x},0,0;\ x,0,\frac{1}{2};\ \bar{x},0,\frac{1}{2}.$	hkl: $l=2n$
8	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0;\ \frac{1}{4},\frac{3}{4},0;\ \frac{1}{4},\frac{1}{4},\frac{1}{2};\ \frac{1}{4},\frac{3}{4},\frac{1}{2}.$	hkl: $h,l=2n$; $(k=2n)$
4	c	mm	$0,y,\frac{1}{4};\ 0,\bar{y},\frac{3}{4}.$	no extra conditions
4	b	$2/m$	$0,\frac{1}{2},0;\ 0,\frac{1}{2},\frac{1}{2}.$	hkl: $l=2n$
4	a	$2/m$	$0,0,0;\ 0,0,\frac{1}{2}.$	

Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) pgm; $b'=b/2$, $c'=c$ (010) pmm; $c'=c/2$, $a'=a/2$



Origin at centre ($2/m$)

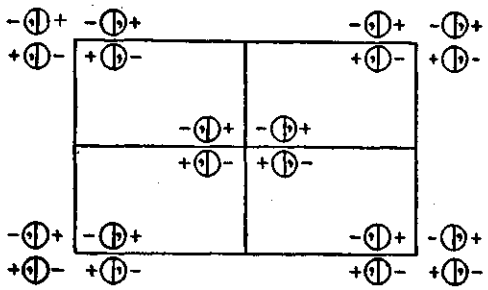
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
16	g	1	$x,y,z;\ x,\bar{y},\bar{z};\ x,\frac{1}{2}-y,\frac{1}{2}+z;\ x,\frac{1}{2}+y,\frac{1}{2}-z;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},y,z;\ \bar{x},\frac{1}{2}+y,\frac{1}{2}-z;\ \bar{x},\frac{1}{2}-y,\frac{1}{2}+z.$	hkl: $h+k=2n$ $0kl$: $(k=2n)$ $h0l$: $l=2n$; $(h=2n)$ $hk0$: $h=2n$; $(k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
8	f	m	$0,y,z;\ 0,\bar{y},\bar{z};\ \frac{1}{2},y,\frac{1}{2}-z;\ \frac{1}{2},\bar{y},\frac{1}{2}+z.$	no extra conditions
8	e	2	$\frac{1}{4},y,\frac{1}{4};\ \frac{3}{4},\bar{y},\frac{3}{4};\ \frac{3}{4},y,\frac{1}{4};\ \frac{1}{4},\bar{y},\frac{3}{4}.$	hkl: $h=2n$; $(k=2n)$
8	d	2	$x,0,0;\ \bar{x},0,0;\ x,\frac{1}{2},\frac{1}{2};\ \bar{x},\frac{1}{2},\frac{1}{2}.$	hkl: $k+l=2n$; $(l+h=2n)$
8	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0;\ \frac{1}{4},\frac{3}{4},0;\ \frac{1}{4},\frac{1}{4},\frac{1}{2};\ \frac{1}{4},\frac{3}{4},\frac{1}{2}.$	hkl: $h,l=2n$; $(k=2n)$
4	b	$2/m$	$\frac{1}{2},0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	hkl: $k+l=2n$; $(l+h=2n)$
4	a	$2/m$	$0,0,0;\ 0,\frac{1}{2},\frac{1}{2}.$	hkl: $k+l=2n$; $(l+h=2n)$

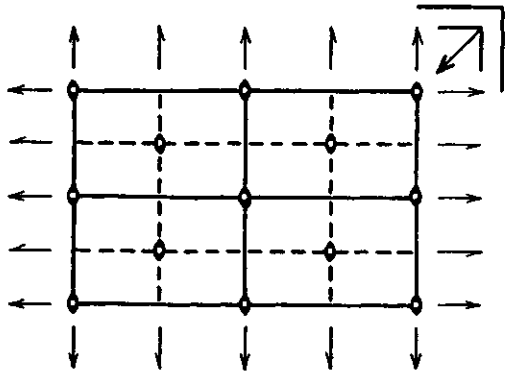
Symmetry of special projections

(001) pmm; $a'=a/2$, $b'=b/2$ (100) pgm; $b'=b/2$, $c'=c$ (010) pmm; $c'=c/2$, $a'=a/2$

$Cmmm$ D_{2h}^{19}

No. 65 $C\,2/m\,2/m\,2/m$ $m\,m\,m$ Orthorhombic



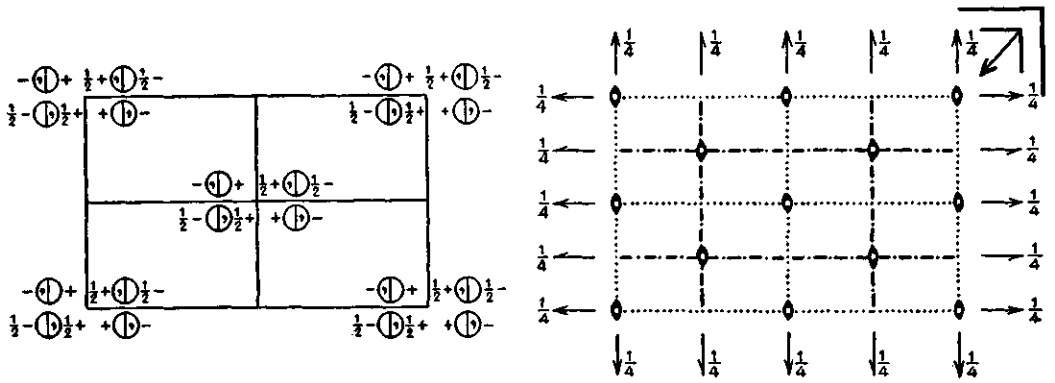


Origin at centre (mmm)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	
16	r	1	$x,y,z;\ \bar{x},\bar{y},z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};$ $\bar{x},\bar{y},\bar{z};\ x,y,\bar{z};\ \bar{x},y,z;\ x,\bar{y},z.$	General: hkl: $h+k=2n$; $0kl$: $(k=2n)$; $h0l$: $(h=2n)$; $hk0$: $(h+k=2n)$; $h00$: $(h=2n)$; $0k0$: $(k=2n)$; $00l$: No conditions
				Special: as above, plus
8	q	m	$x,y,\frac{1}{2};\ \bar{x},\bar{y},\frac{1}{2};\ \bar{x},y,\frac{1}{2};\ x,\bar{y},\frac{1}{2}.$	no extra conditions
8	p	m	$x,y,0;\ \bar{x},\bar{y},0;\ \bar{x},y,0;\ x,\bar{y},0.$	
8	o	m	$x,0,z;\ \bar{x},0,\bar{z};\ \bar{x},0,z;\ x,0,\bar{z}.$	
8	n	m	$0,y,z;\ 0,\bar{y},\bar{z};\ 0,\bar{y},z;\ 0,y,\bar{z}.$	
8	m	2	$\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\bar{z};\ \frac{1}{4},\frac{3}{4},z;\ \frac{1}{4},\frac{3}{4},\bar{z}.$	hkl: $h=2n$; $(k=2n)$
4	l	mm	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\bar{z}.$	(g) to (l) inclusive no extra conditions
4	k	mm	$0,0,z;\ 0,0,\bar{z}.$	
4	j	mm	$0,y,\frac{1}{2};\ 0,\bar{y},\frac{1}{2}.$	
4	i	mm	$0,y,0;\ 0,\bar{y},0.$	
4	h	mm	$x,0,\frac{1}{2};\ \bar{x},0,\frac{1}{2}.$	
4	g	mm	$x,0,0;\ \bar{x},0,0.$	
4	f	$2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{2};\ \frac{1}{4},\frac{3}{4},\frac{1}{2}.$	hkl: $h=2n$; $(k=2n)$
4	e	$2/m$	$\frac{1}{4},\frac{1}{4},0;\ \frac{1}{4},\frac{3}{4},0.$	
2	d	mmm	$0,0,\frac{1}{2}.$	(a) to (d) inclusive no extra conditions
2	c	mmm	$\frac{1}{2},0,\frac{1}{2}.$	
2	b	mmm	$\frac{1}{2},0,0.$	
2	a	mmm	$0,0,0.$	

Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) pmm; $b'=b/2$, $c'=c$ (010) pmm; $c'=c$, $a'=a/2$



Origin at centre (2/*m* at *ccm*)

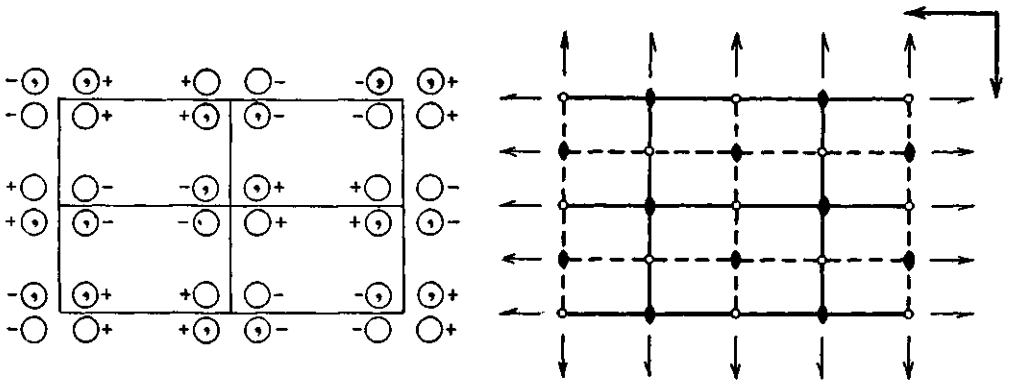
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	Conditions limiting possible reflections
				General:
16	*m*	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}-z;\ x,\bar{y},\frac{1}{2}-z;$ $\bar{x},\bar{y},\bar{z};\ x,y,\bar{z};\ x,\bar{y},\frac{1}{2}+z;\ \bar{x},y,\frac{1}{2}+z.$	hkl: $h+k=2n$ $0kl$: $l=2n$; $(k=2n)$ $h0l$: $l=2n$; $(h=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus no extra conditions
8	*l*	*m*	$x,y,0;\ \bar{x},\bar{y},0;\ \bar{x},y,\frac{1}{2};\ x,\bar{y},\frac{1}{2}.$	
8	*k*	2	$\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\bar{z};\ \frac{1}{4},\frac{3}{4},\frac{1}{2}+z;\ \frac{1}{4},\frac{3}{4},\frac{1}{2}-z.$	hkl: $k+l, (l+h)=2n$
8	*j*	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\bar{z};\ 0,\frac{1}{2},\frac{1}{2}+z;\ 0,\frac{1}{2},\frac{1}{2}-z.$	hkl: $l=2n$
8	*i*	2	$0,0,z;\ 0,0,\bar{z};\ 0,0,\frac{1}{2}+z;\ 0,0,\frac{1}{2}-z.$	
8	*h*	2	$0,y,\frac{1}{4};\ 0,\bar{y},\frac{1}{4};\ 0,y,\frac{3}{4};\ 0,\bar{y},\frac{3}{4}.$	
8	*g*	2	$x,0,\frac{1}{4};\ \bar{x},0,\frac{1}{4};\ x,0,\frac{3}{4};\ \bar{x},0,\frac{3}{4}.$	
4	*f*	2/*m*	$\frac{1}{4},\frac{3}{4},0;\ \frac{1}{4},\frac{1}{4},\frac{1}{2}.$	hkl: $k+l, (l+h)=2n$
4	*e*	2/*m*	$\frac{1}{4},\frac{1}{4},0;\ \frac{1}{4},\frac{3}{4},\frac{1}{2}.$	
4	*d*	2/*m*	$0,\frac{1}{2},0;\ 0,\frac{1}{2},\frac{1}{2}.$	hkl: $l=2n$
4	*c*	2/*m*	$0,0,0;\ 0,0,\frac{1}{2}.$	
4	*b*	222	$0,\frac{1}{2},\frac{1}{4};\ 0,\frac{1}{2},\frac{3}{4}.$	
4	*a*	222	$0,0,\frac{1}{4};\ 0,0,\frac{3}{4}.$	

Symmetry of special projections

(001) *cmm*; $a'=a$, $b'=b$ (100) *pmm*; $b'=b/2$, $c'=c/2$ (010) *pmm*; $c'=c/2$, $a'=a/2$

$Cmma$ D_{2h}^{21}

No. 67 $C\,2/m\,2/m\,2/a$ $m\,m\,m$ Orthorhombic

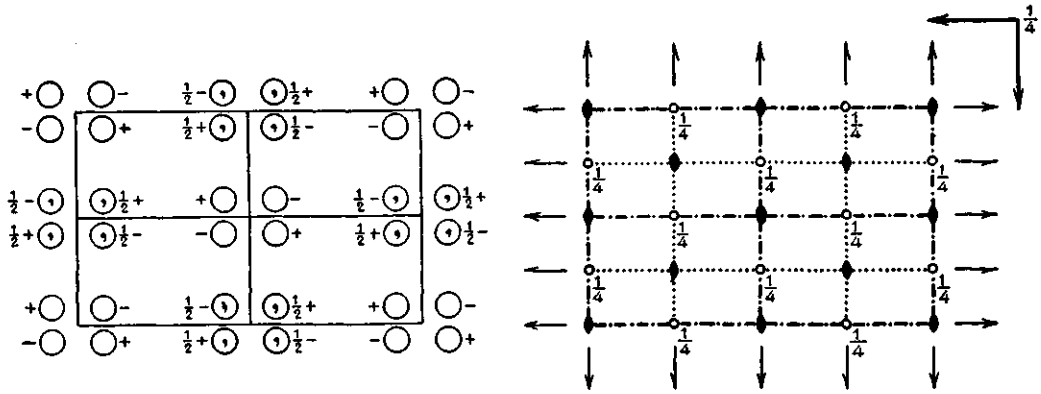


Origin at centre ($2/m$ at maa)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},0)+$	
16	o	1	$x,y,z;\ x,\bar{y},\bar{z};\ \tfrac{1}{2}-x,y,\bar{z};\ \tfrac{1}{2}-x,\bar{y},z;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},y,z;\ \tfrac{1}{2}+x,\bar{y},z;\ \tfrac{1}{2}+x,y,\bar{z}.$	General: hkl: $h+k=2n$; $0kl$: $(k=2n)$; $h0l$: $(h=2n)$; $hk0$: $h=2n$; $(k=2n)$; $h00$: $(h=2n)$; $0k0$: $(k=2n)$; $00l$: No conditions
				Special: as above, plus
8	n	m	$x,\tfrac{1}{4},z;\ \bar{x},\tfrac{3}{4},\bar{z};\ x,\tfrac{3}{4},\bar{z};\ \bar{x},\tfrac{1}{4},z.$	no extra conditions
8	m	m	$0,y,z;\ 0,\bar{y},\bar{z};\ \tfrac{1}{2},y,\bar{z};\ \tfrac{1}{2},\bar{y},z.$	
8	l	2	$\tfrac{1}{4},0,z;\ \tfrac{1}{4},0,\bar{z};\ \tfrac{3}{4},0,z;\ \tfrac{3}{4},0,\bar{z}.$	hkl: $h=2n$; $(k=2n)$
8	k	2	$\tfrac{1}{4},y,\tfrac{1}{2};\ \tfrac{1}{4},\bar{y},\tfrac{1}{2};\ \tfrac{3}{4},y,\tfrac{1}{2};\ \tfrac{3}{4},\bar{y},\tfrac{1}{2}.$	
8	j	2	$\tfrac{1}{4},y,0;\ \tfrac{1}{4},\bar{y},0;\ \tfrac{3}{4},y,0;\ \tfrac{3}{4},\bar{y},0.$	
8	i	2	$x,0,\tfrac{1}{2};\ \bar{x},0,\tfrac{1}{2};\ x,\tfrac{1}{2},\tfrac{1}{2};\ \bar{x},\tfrac{1}{2},\tfrac{1}{2}.$	
8	h	2	$x,0,0;\ \bar{x},0,0;\ x,\tfrac{1}{2},0;\ \bar{x},\tfrac{1}{2},0.$	
4	g	mm	$0,\tfrac{1}{4},z;\ 0,\tfrac{3}{4},\bar{z}.$	no extra conditions
4	f	$2/m$	$\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{2};\ \tfrac{3}{4},\tfrac{1}{4},\tfrac{1}{2}.$	(c) to (f) inclusive hkl: $h=2n$; $(k=2n)$
4	e	$2/m$	$\tfrac{1}{4},\tfrac{1}{4},0;\ \tfrac{3}{4},\tfrac{1}{4},0.$	
4	d	$2/m$	$0,0,\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2}.$	
4	c	$2/m$	$0,0,0;\ \tfrac{1}{2},0,0.$	
4	b	222	$\tfrac{1}{4},0,\tfrac{1}{2};\ \tfrac{3}{4},0,\tfrac{1}{2}.$	hkl: $h=2n$; $(k=2n)$
4	a	222	$\tfrac{1}{4},0,0;\ \tfrac{3}{4},0,0.$	

Symmetry of special projections

(001) pmm; $a'=a/2$, $b'=b/2$ (100) pmm; $b'=b/2$, $c'=c$ (010) pmm; $c'=c$, $a'=a/2$



Origin at 222, at $0,\frac{1}{4},\frac{1}{4}$ from $\bar{1}$ on *nca* (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
16	*i*	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},\frac{1}{2}-y,\frac{1}{2}-z;\ x,\frac{1}{2}-y,\frac{1}{2}+z;$ $x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\frac{1}{2}+y,\frac{1}{2}+z;\ x,\frac{1}{2}+y,\frac{1}{2}-z.$	hkl: $h+k=2n$ $0kl$: $l=2n$; $(k=2n)$ $h0l$: $l=2n$; $(h=2n)$ $hk0$: $h=2n$; $(k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
8	*h*	2	$\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{3}{4},\bar{z};\ \frac{1}{4},\frac{1}{4},\frac{1}{2}+z;\ \frac{1}{4},\frac{3}{4},\frac{1}{2}-z.$	hkl: $l=2n$
8	*g*	2	$0,0,z;\ 0,0,\bar{z};\ 0,\frac{1}{2},\frac{1}{2}+z;\ 0,\frac{1}{2},\frac{1}{2}-z.$	hkl: $k+l=2n$; $(l+h=2n)$
8	*f*	2	$0,y,0;\ 0,\bar{y},0;\ \frac{1}{2},y,\frac{1}{2};\ \frac{1}{2},\bar{y},\frac{1}{2}.$	
8	*e*	2	$x,0,0;\ \bar{x},0,0;\ x,\frac{1}{2},\frac{1}{2};\ \bar{x},\frac{1}{2},\frac{1}{2}.$	
8	*d*	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4};\ 0,\frac{3}{4},\frac{1}{4};\ 0,\frac{1}{4},\frac{3}{4};\ 0,\frac{3}{4},\frac{3}{4}.$	hkl: $h,l=2n$; $(k=2n)$
8	*c*	$\bar{1}$	$\frac{1}{4},0,\frac{1}{4};\ \frac{3}{4},0,\frac{1}{4};\ \frac{1}{4},0,\frac{3}{4};\ \frac{3}{4},0,\frac{3}{4}.$	
4	*b*	222	$0,0,\frac{1}{2};\ 0,\frac{1}{2},0.$	hkl: $k+l=2n$; $(l+h=2n)$
4	*a*	222	$0,0,0;\ 0,\frac{1}{2},\frac{1}{2}.$	

$Ccca$ D_{2h}^{22}

No. 68 $C\,2/c\,2/c\,2/a$ $m\,m\,m$ Orthorhombic

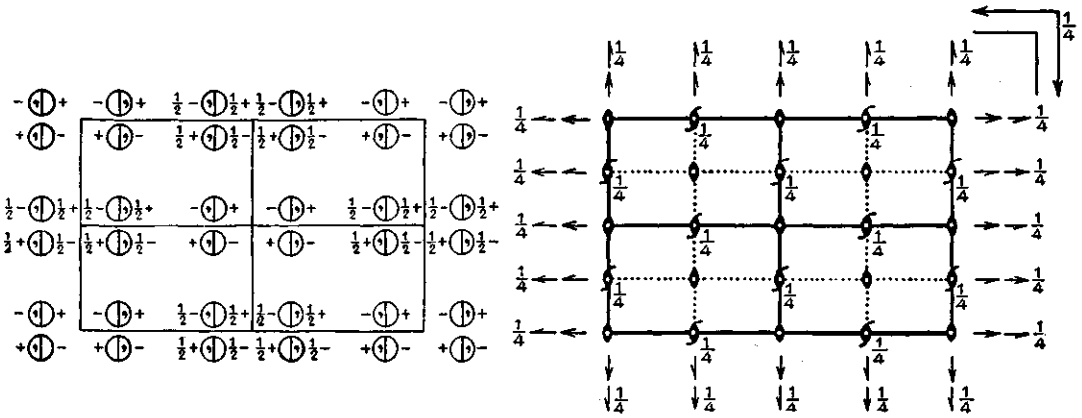
Diagrams as on previous page but with origin shifted to $0,\bar{\tfrac{1}{4}},\bar{\tfrac{1}{4}}$

Origin at $\bar{1}$ on *nca*, at $0,\bar{\tfrac{1}{4}},\bar{\tfrac{1}{4}}$ from 222 (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},0)+$	Conditions limiting possible reflections
				General:
16	i	1	$x,y,z;\ \tfrac{1}{2}-x,y,\tfrac{1}{2}+z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{1}{2}+z;\ \bar{x},\tfrac{1}{2}-y,z;$ $\bar{x},\bar{y},\bar{z};\ \tfrac{1}{2}+x,\bar{y},\tfrac{1}{2}-z;\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{2}-z;\ x,\tfrac{1}{2}+y,\bar{z}.$	hkl: $h+k=2n$ $0kl$: $l=2n$; $(k=2n)$ $h0l$: $l=2n$; $(h=2n)$ $hk0$: $h=2n$; $(k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
8	h	2	$\tfrac{1}{4},0,z;\ \tfrac{3}{4},0,\bar{z};\ \tfrac{1}{4},0,\tfrac{1}{2}+z;\ \tfrac{3}{4},0,\tfrac{1}{2}-z.$	hkl: $l=2n$
8	g	2	$0,\tfrac{1}{4},z;\ 0,\tfrac{3}{4},\bar{z};\ \tfrac{1}{2},\tfrac{1}{4},\tfrac{1}{2}+z;\ \tfrac{1}{2},\tfrac{3}{4},\tfrac{1}{2}-z.$	hkl: $k+l=2n$; $(l+h=2n)$
8	f	2	$0,y,\tfrac{1}{4};\ 0,\bar{y},\tfrac{3}{4};\ \tfrac{1}{2},y,\tfrac{3}{4};\ \tfrac{1}{2},\bar{y},\tfrac{1}{4}.$	
8	e	2	$x,\tfrac{1}{4},\tfrac{1}{4};\ \bar{x},\tfrac{3}{4},\tfrac{3}{4};\ x,\tfrac{3}{4},\tfrac{3}{4};\ \bar{x},\tfrac{1}{4},\tfrac{1}{4}.$	
8	d	$\bar{1}$	$0,0,0;\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2};\ 0,\tfrac{1}{2},0.$	hkl: $h,l=2n$; $(k=2n)$
8	c	$\bar{1}$	$\tfrac{1}{4},\tfrac{3}{4},0;\ \tfrac{1}{4},\tfrac{1}{4},0;\ \tfrac{1}{4},\tfrac{3}{4},\tfrac{1}{2};\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{2}.$	
4	b	222	$0,\tfrac{1}{4},\tfrac{3}{4};\ 0,\tfrac{3}{4},\tfrac{1}{4}.$	hkl: $k+l=2n$; $(l+h=2n)$
4	a	222	$0,\tfrac{1}{4},\tfrac{1}{4};\ 0,\tfrac{3}{4},\tfrac{3}{4}.$	

Symmetry of special projections

(001) *pmm*; $a'=a/2$, $b'=b/2$ (100) *pmm*; $b'=b/2$, $c'=c/2$ (010) *pmm*; $c'=c/2$, $a'=a/2$



Origin at centre (*mmm*)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	Conditions limiting possible reflections
				General:
32	*p*	1	$x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},y,z;\ x,\bar{y},z;\ x,y,\bar{z}.$	hkl: $h+k, k+l, (l+h)=2n$ $0kl$: $(k, l=2n)$ $h0l$: $(l, h=2n)$ $hk0$: $(h, k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
16	*o*	*m*	$x,y,0;\ \bar{x},\bar{y},0;\ \bar{x},y,0;\ x,\bar{y},0.$	no extra conditions
16	*n*	*m*	$x,0,z;\ \bar{x},0,\bar{z};\ \bar{x},0,z;\ x,0,\bar{z}.$	
16	*m*	*m*	$0,y,z;\ 0,\bar{y},\bar{z};\ 0,\bar{y},z;\ 0,y,\bar{z}.$	
16	*l*	2	$x,\frac{1}{4},\frac{1}{4};\ \bar{x},\frac{1}{4},\frac{1}{4};\ x,\frac{1}{4},\frac{3}{4};\ \bar{x},\frac{1}{4},\frac{3}{4}.$	hkl: $h=2n$; $(k, l=2n)$
16	*k*	2	$\frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\bar{y},\frac{1}{4};\ \frac{1}{4},y,\frac{3}{4};\ \frac{1}{4},\bar{y},\frac{3}{4}.$	
16	*j*	2	$\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\bar{z};\ \frac{1}{4},\frac{3}{4},z;\ \frac{1}{4},\frac{3}{4},\bar{z}.$	
8	*i*	*mm*	$0,0,z;\ 0,0,\bar{z}.$	no extra conditions
8	*h*	*mm*	$0,y,0;\ 0,\bar{y},0.$	
8	*g*	*mm*	$x,0,0;\ \bar{x},0,0.$	

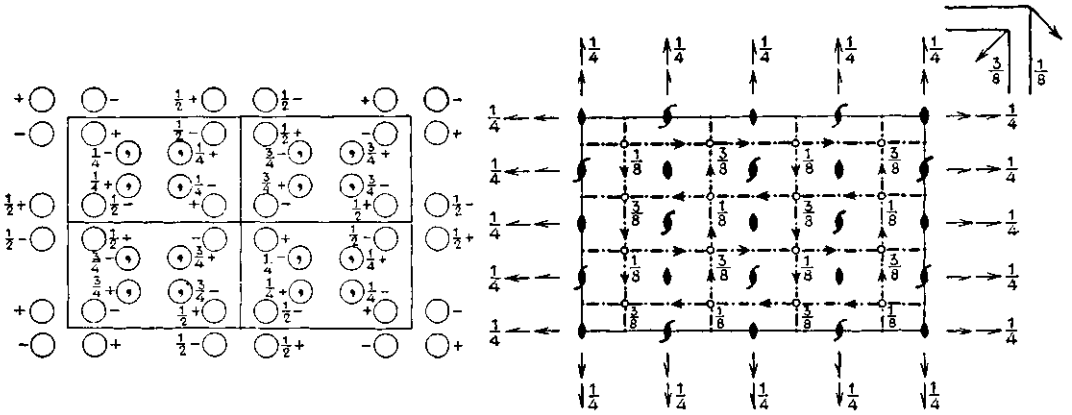
(*continued on next page*)

$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$

8	f	222	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{3}{4}.$	hkl: $h=2n$; $(k,l=2n)$
8	e	$2/m$	$\frac{1}{4},\frac{1}{4},0;\ \frac{1}{4},\frac{1}{4},\frac{1}{2}.$	
8	d	$2/m$	$\frac{1}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{1}{2},\frac{1}{4}.$	
8	c	$2/m$	$0,\frac{1}{4},\frac{1}{4};\ \frac{1}{2},\frac{1}{4},\frac{1}{4}.$	
4	b	mmm	$0,0,\frac{1}{2}.$	no extra conditions
4	a	mmm	$0,0,0.$	

Symmetry of special projections

(001) pmm; $a'=a/2$, $b'=b/2$ (100) pmm; $b'=b/2$, $c'=c/2$ (010) pmm; $c'=c/2$, $a'=a/2$



Origin at 222, at $\bar{\tfrac{1}{8}},\bar{\tfrac{1}{8}},\bar{\tfrac{1}{8}}$ from $\bar{1}$ (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0)+$	
				General:
32	h	1	$x,y,z;\ \bar{x},y,\bar{z};\ \tfrac{1}{4}-x,\tfrac{1}{4}-y,\tfrac{1}{4}-z;\ \tfrac{1}{4}+x,\tfrac{1}{4}-y,\tfrac{1}{4}+z;$ $x,\bar{y},\bar{z};\ \bar{x},\bar{y},z;\ \tfrac{1}{4}-x,\tfrac{1}{4}+y,\tfrac{1}{4}+z;\ \tfrac{1}{4}+x,\tfrac{1}{4}+y,\tfrac{1}{4}-z.$	hkl: $h+k,k+l,(l+h)=2n$ $0kl$: $k+l=4n$; $(k,l=2n)$ $h0l$: $l+h=4n$; $(l,h=2n)$ $hk0$: $h+k=4n$; $(h,k=2n)$ $h00$: $(h=4n)$ $0k0$: $(k=4n)$ $00l$: $(l=4n)$
				Special: as above, plus
16	g	2	$0,0,z;\ 0,0,\bar{z};\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}-z;\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}+z.$	hkl: $h+k+l=2n+1$ or $4n$
16	f	2	$0,y,0;\ 0,\bar{y},0;\ \tfrac{1}{4},\tfrac{1}{4}-y,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{4}+y,\tfrac{1}{4}.$	
16	e	2	$x,0,0;\ \bar{x},0,0;\ \tfrac{1}{4}-x,\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{1}{4}+x,\tfrac{1}{4},\tfrac{1}{4}.$	
16	d	$\bar{1}$	$\tfrac{5}{8},\tfrac{5}{8},\tfrac{5}{8};\ \tfrac{5}{8},\tfrac{7}{8},\tfrac{7}{8};\ \tfrac{7}{8},\tfrac{5}{8},\tfrac{7}{8};\ \tfrac{7}{8},\tfrac{7}{8},\tfrac{5}{8}.$	hkl: $h,k,l=2n+1$ or $4n$ or $4n+2$ (not mixed)
16	c	$\bar{1}$	$\tfrac{1}{8},\tfrac{1}{8},\tfrac{1}{8};\ \tfrac{1}{8},\tfrac{3}{8},\tfrac{3}{8};\ \tfrac{3}{8},\tfrac{1}{8},\tfrac{3}{8};\ \tfrac{3}{8},\tfrac{3}{8},\tfrac{1}{8}.$	
8	b	222	$0,0,\tfrac{1}{2};\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{3}{4}.$	hkl: $h+k+l=2n+1$ or $4n$
8	a	222	$0,0,0;\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}.$	

$Fddd$ D_{2h}^{24}

No. 70 $F\,2/d\,2/d\,2/d$ $m\,m\,m$ Orthorhombic

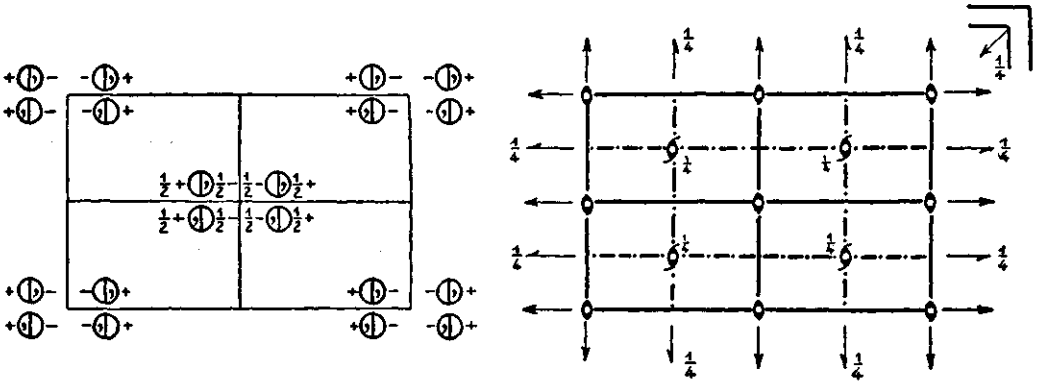
Diagrams as on previous page but with origin shifted to $\frac{1}{8},\frac{1}{8},\frac{1}{8}$

Origin at $\bar{1}$, at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from 222 (compare previous page for alternative origin)

Number of positions, Wyckoff notation and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
32	h	1	$x,y,z;\ x,\frac{1}{4}-y,\frac{1}{4}-z;\ \frac{1}{4}-x,y,\frac{1}{4}-z;\ \frac{1}{4}-x,\frac{1}{4}-y,z;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},\frac{1}{4}+y,\frac{1}{4}+z;\ \frac{1}{4}+x,\bar{y},\frac{1}{4}+z;\ \frac{1}{4}+x,\frac{1}{4}+y,\bar{z}.$	hkl: $h+k,k+l,(l+h)=2n$ $0kl$: $k+l=4n$; $(k,l=2n)$ $h0l$: $l+h=4n$; $(l,h=2n)$ $hk0$: $h+k=4n$; $(h,k=2n)$ $h00$: $(h=4n)$ $0k0$: $(k=4n)$ $00l$: $(l=4n)$
				Special: as above, plus
16	g	2	$\frac{1}{8},\frac{1}{8},z;\ \frac{1}{8},\frac{1}{8},\frac{1}{4}-z;\ \frac{7}{8},\frac{7}{8},\bar{z};\ \frac{7}{8},\frac{7}{8},\frac{3}{4}+z.$	hkl: $h+k+l=2n+1$ or $4n$
16	f	2	$\frac{1}{8},y,\frac{1}{8};\ \frac{1}{8},\frac{1}{4}-y,\frac{1}{8};\ \frac{7}{8},\bar{y},\frac{7}{8};\ \frac{7}{8},\frac{3}{4}+y,\frac{7}{8}.$	
16	e	2	$x,\frac{1}{8},\frac{1}{8};\ \frac{1}{4}-x,\frac{1}{8},\frac{1}{8};\ \bar{x},\frac{7}{8},\frac{7}{8};\ \frac{3}{4}+x,\frac{7}{8},\frac{7}{8}.$	
16	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2};\ \frac{1}{2},\frac{3}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{2},\frac{3}{4};\ \frac{3}{4},\frac{3}{4},\frac{1}{2}.$	hkl: $h,k,l=2n+1$ or $4n$ or $4n+2$ not mixed
16	c	$\bar{1}$	$0,0,0;\ 0,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},0.$	
8	b	222	$\frac{1}{8},\frac{1}{8},\frac{5}{8};\ \frac{7}{8},\frac{7}{8},\frac{3}{8}.$	hkl: $h+k+l=2n+1$ or $4n$
8	a	222	$\frac{1}{8},\frac{1}{8},\frac{1}{8};\ \frac{7}{8},\frac{7}{8},\frac{7}{8}.$	

Symmetry of special projections

(001) cmm; $a'=a/2,\ b'=b/2$ (100) cmm; $b'=b/2,\ c'=c/2$ (010) cmm; $c'=c/2,\ a'=a/2$



Origin at centre (*mmm*)

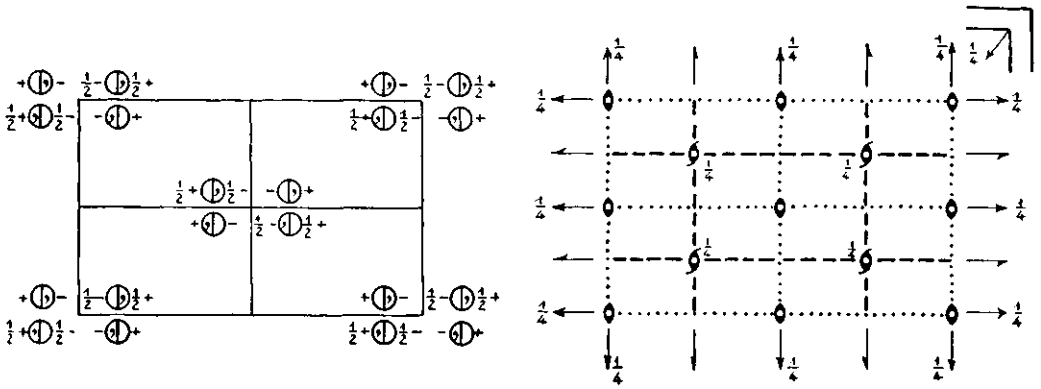
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
				General:
16	*o*	1	$x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},y,z;\ x,\bar{y},z;\ x,y,\bar{z}.$	*hkl*: $h+k+l=2n$ 0*kl*: $(k+l=2n)$ *h*0*l*: $(l+h=2n)$ *hk*0: $(h+k=2n)$ *h*00: $(h=2n)$ 0*k*0: $(k=2n)$ 00*l*: $(l=2n)$
				Special: as above, plus
8	*n*	*m*	$x,y,0;\ \bar{x},\bar{y},0;\ \bar{x},y,0;\ x,\bar{y},0.$	no extra conditions
8	*m*	*m*	$x,0,z;\ \bar{x},0,\bar{z};\ \bar{x},0,z;\ x,0,\bar{z}.$	
8	*l*	*m*	$0,y,z;\ 0,\bar{y},\bar{z};\ 0,\bar{y},z;\ 0,y,\bar{z}.$	
8	*k*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{3}{4},\frac{3}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{1}{4};\ \frac{3}{4},\frac{1}{4},\frac{1}{4}.$	*hkl*: $h,k,(l)=2n$
4	*j*	*mm*	$\frac{1}{2},0,z;\ \frac{1}{2},0,\bar{z}.$	(*a*) to (*j*) inclusive no extra conditions
4	*i*	*mm*	$0,0,z;\ 0,0,\bar{z}.$	
4	*h*	*mm*	$0,y,\frac{1}{2};\ 0,\bar{y},\frac{1}{2}.$	
2	*d*	*mmm*	$\frac{1}{2},0,\frac{1}{2}.$	
2	*c*	*mmm*	$\frac{1}{2},\frac{1}{2},0.$	
4	*g*	*mm*	$0,y,0;\ 0,\bar{y},0.$	
4	*f*	*mm*	$x,\frac{1}{2},0;\ \bar{x},\frac{1}{2},0.$	
4	*e*	*mm*	$x,0,0;\ \bar{x},0,0.$	
2	*b*	*mmm*	$0,\frac{1}{2},\frac{1}{2}.$	
2	*a*	*mmm*	$0,0,0.$	

Symmetry of special projections

(001) *cmm*; $a'=a,\ b'=b$ (100) *cmm*; $b'=b,\ c'=c$ (010) *cmm*; $c'=c,\ a'=a$

$Ibam$ D_{2h}^{26}

No. 72 $I\,2/b\,2/a\,2/m$ $m\,m\,m$ Orthorhombic



Origin at centre $(2/m)$

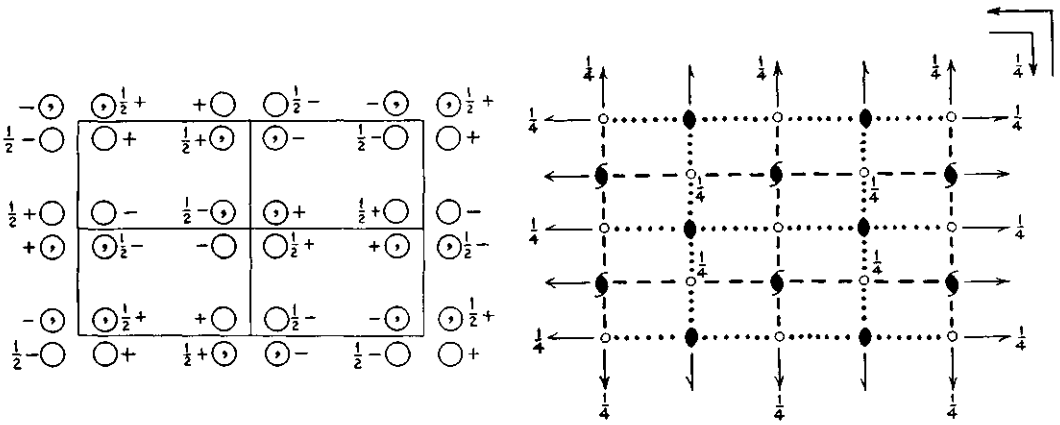
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
				General:
16	k	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}-z;\ x,\bar{y},\frac{1}{2}-z;$ $\bar{x},\bar{y},\bar{z};\ x,y,\bar{z};\ x,\bar{y},\frac{1}{2}+z;\ \bar{x},y,\frac{1}{2}+z.$	hkl: $h+k+l=2n$ $0kl$: $k=2n$; $(l=2n)$ $h0l$: $h=2n$; $(l=2n)$ $hk0$: $(h+k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
8	j	m	$x,y,0;\ \bar{x},\bar{y},0;\ \bar{x},y,\frac{1}{2};\ x,\bar{y},\frac{1}{2}.$	no extra conditions
8	i	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\bar{z};\ 0,\frac{1}{2},\frac{1}{2}-z;\ 0,\frac{1}{2},\frac{1}{2}+z.$	hkl: $l=2n$; $(h+k=2n)$
8	h	2	$0,0,z;\ 0,0,\bar{z};\ 0,0,\frac{1}{2}-z;\ 0,0,\frac{1}{2}+z.$	
8	g	2	$0,y,\frac{1}{4};\ 0,\bar{y},\frac{1}{4};\ 0,y,\frac{3}{4};\ 0,\bar{y},\frac{3}{4}.$	
8	f	2	$x,0,\frac{1}{4};\ \bar{x},0,\frac{1}{4};\ x,0,\frac{3}{4};\ \bar{x},0,\frac{3}{4}.$	
8	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{1}{4};\ \frac{3}{4},\frac{3}{4},\frac{1}{4};\ \frac{3}{4},\frac{1}{4},\frac{1}{4}.$	hkl: $h,k,(l)=2n$
4	d	$2/m$	$\frac{1}{2},0,0;\ \frac{1}{2},0,\frac{1}{2}.$	hkl: $l=2n$; $(h+k=2n)$
4	c	$2/m$	$0,0,0;\ 0,0,\frac{1}{2}.$	
4	b	222	$\frac{1}{2},0,\frac{1}{4};\ \frac{1}{2},0,\frac{3}{4}.$	
4	a	222	$0,0,\frac{1}{4};\ 0,0,\frac{3}{4}.$	

Symmetry of special projections

(001) cmm; $a'=a$, $b'=b$ (100) pmm; $b'=b/2$, $c'=c/2$ (010) pmm; $c'=c/2$, $a'=a/2$

Orthorhombic $m\,m\,m$ $I\,2/b\,2/c\,2/a$ No. 73

$Ibca$ D_{2h}^{27}



Origin at $\bar{1}$ at cab

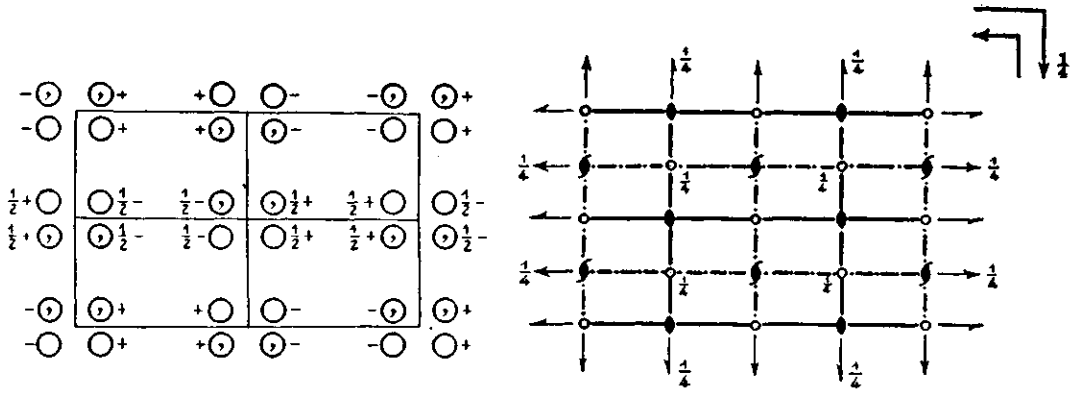
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
				General:
16	f	1	$x,y,z;\ x,\bar{y},\frac{1}{2}-z;\ \frac{1}{2}-x,y,\bar{z};\ \bar{x},\frac{1}{2}-y,z;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},y,\frac{1}{2}+z;\ \frac{1}{2}+x,\bar{y},z;\ x,\frac{1}{2}+y,\bar{z}.$	hkl: $h+k+l=2n$ $0kl$: $k=2n$; $(l=2n)$ $h0l$: $l=2n$; $(h=2n)$ $hk0$: $h=2n$; $(k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
8	e	2	$0,\frac{1}{4},z;\ 0,\frac{3}{4},\bar{z};\ \frac{1}{2},\frac{3}{4},z;\ \frac{1}{2},\frac{1}{4},\bar{z}.$	hkl: $l=2n$; $(h+k=2n)$
8	d	2	$\frac{1}{4},y,0;\ \frac{3}{4},\bar{y},0;\ \frac{3}{4},y,\frac{1}{2};\ \frac{1}{4},\bar{y},\frac{1}{2}.$	hkl: $k=2n$; $(l+h=2n)$
8	c	2	$x,0,\frac{1}{4};\ \bar{x},0,\frac{3}{4};\ x,\frac{1}{2},\frac{3}{4};\ \bar{x},\frac{1}{2},\frac{1}{4}.$	hkl: $h=2n$; $(k+l=2n)$
8	b	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\frac{3}{4},\frac{1}{4}.$	hkl: $h,k,(l)=2n$
8	a	$\bar{1}$	$0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0.$	

Symmetry of special projections

(001) pmm; $a'=a/2$, $b'=b/2$ (100) pmm; $b'=b/2$, $c'=c/2$ (010) pmm; $c'=c/2$, $a'=a/2$

$Imma$ D_{2h}^{28}

No. 74 | $I\,2/m\,2/m\,2/a$ | $m\,m\,m$ | Orthorhombic



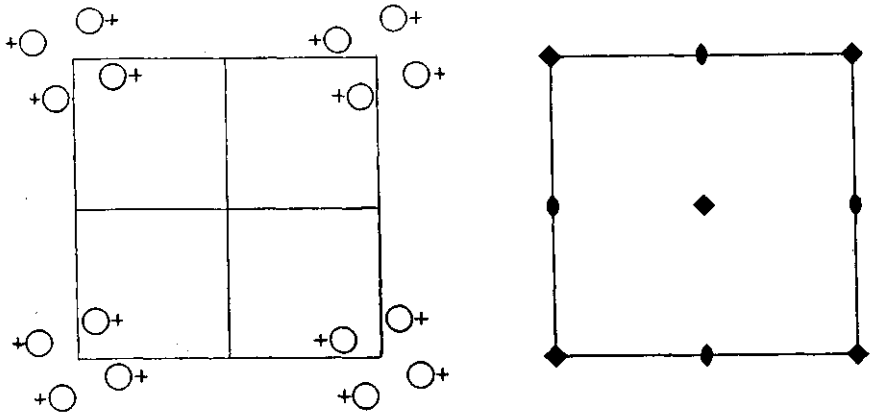
Origin at centre ($2/m2_11$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
				General:
16	j	1	$x,y,z;\ x,\bar{y},\bar{z};\ x,\frac{1}{2}+y,\bar{z};\ x,\frac{1}{2}-y,z;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},y,z;\ \bar{x},\frac{1}{2}-y,z;\ \bar{x},\frac{1}{2}+y,\bar{z}.$	hkl: $h+k+l=2n$ $0kl$: $(k+l=2n)$ $h0l$: $(l+h=2n)$ $hk0$: $h=2n;\ (k=2n)$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
8	i	m	$x,\frac{1}{4},z;\ \bar{x},\frac{3}{4},\bar{z};\ \bar{x},\frac{1}{4},z;\ x,\frac{3}{4},\bar{z}.$	no extra conditions
8	h	m	$0,y,z;\ 0,\bar{y},\bar{z};\ 0,\frac{1}{2}+y,\bar{z};\ 0,\frac{1}{2}-y,z.$	
8	g	2	$\frac{1}{4},y,\frac{1}{4};\ \frac{3}{4},\bar{y},\frac{3}{4};\ \frac{3}{4},y,\frac{1}{4};\ \frac{1}{4},\bar{y},\frac{3}{4}.$	hkl: $h=2n;\ (k+l=2n)$
8	f	2	$x,0,0;\ \bar{x},0,0;\ x,\frac{1}{2},0;\ \bar{x},\frac{1}{2},0.$	hkl: $k=2n;\ (l+h=2n)$
4	e	mm	$0,\frac{1}{4},z;\ 0,\frac{3}{4},\bar{z}.$	no extra conditions
4	d	$2/m$	$\frac{1}{4},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{4},\frac{3}{4}.$	hkl: $h=2n;\ (k+l=2n)$
4	c	$2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{3}{4},\frac{1}{4},\frac{1}{4}.$	
4	b	$2/m$	$0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2}.$	hkl: $k=2n;\ (l+h=2n)$
4	a	$2/m$	$0,0,0;\ 0,\frac{1}{2},0.$	

Symmetry of special projections

(001) pmm; $a'=a/2,\ b'=b/2$ | (100) cmm; $b'=b,\ c'=c$ | (010) cmm; $c'=c,\ a'=a$

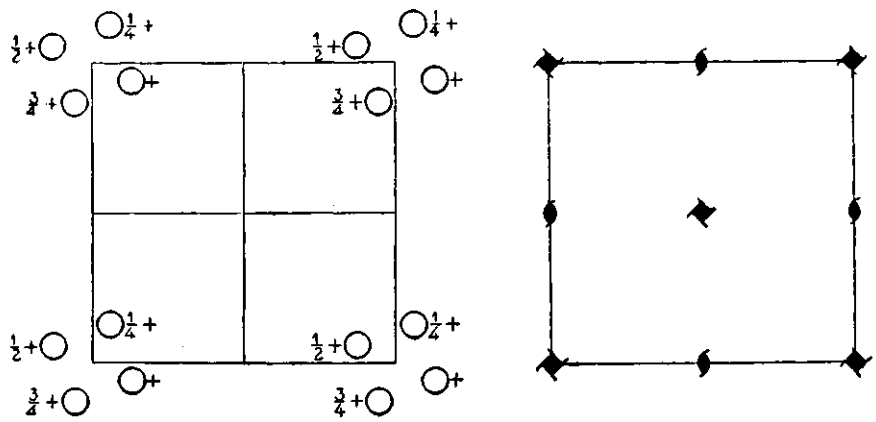
Tetragonal 4 $P\,4$ No. 75 $P4$ C_4^1



Origin on 4

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	d	1	$x,y,z;\ \bar{x},\bar{y},z;\ y,\bar{x},z;\ \bar{y},x,z.$	hkl: No conditions $00l$: No conditions
				Special:
2	c	2	$0,\frac{1}{2},z;\ \frac{1}{2},0,z.$	hkl: $h+k=2n$
1	b	4	$\frac{1}{2},\frac{1}{2},z.$	No conditions
1	a	4	$0,0,z.$	No conditions

Tetragonal 4 $P\,4_1$ No. 76 $P4_1$ C_4^2

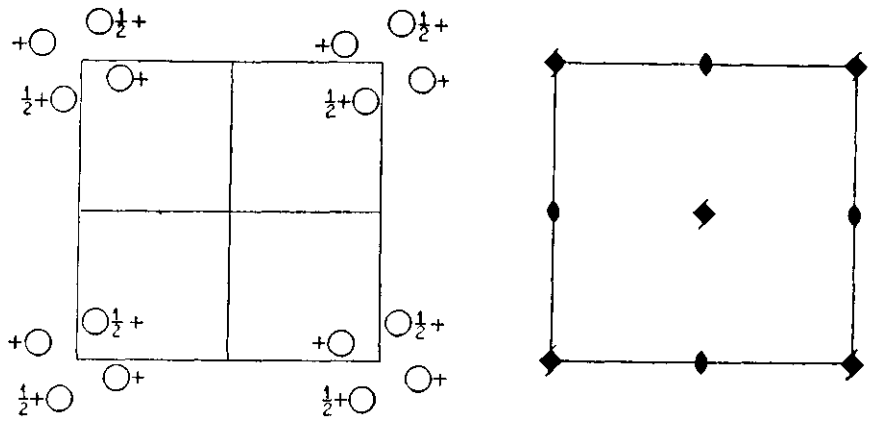


Origin on 4_1

				General:
4	a	1	$x,y,z;\ \bar{x},\bar{y},\frac{1}{2}+z;\ \bar{y},x,\frac{1}{4}+z;\ y,\bar{x},\frac{3}{4}+z.$	hkl: No conditions $00l$: $l=4n$

$P4_2$ C_4^3

No. 77 $P\,4_2$ 4 Tetragonal

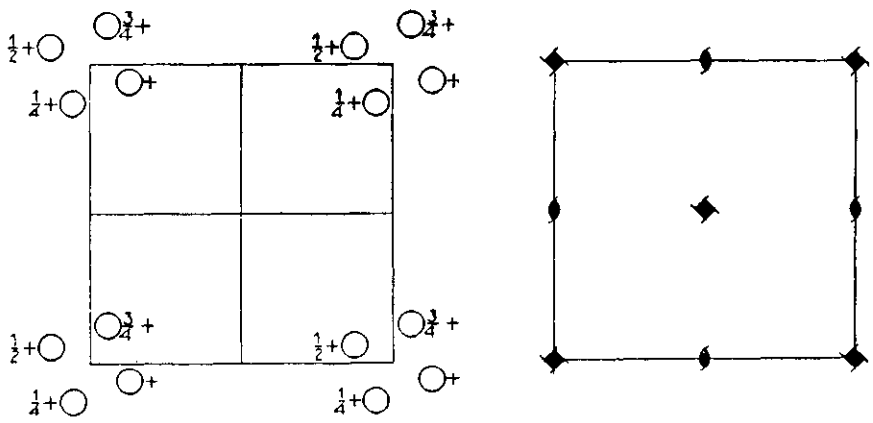


Origin on 4_2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	d	1	$x,y,z;\quad \bar{x},\bar{y},z;\quad \bar{y},x,\frac{1}{2}+z;\quad y,\bar{x},\frac{1}{2}+z.$	hkl: No conditions $00l$: $l=2n$
				Special: as above, plus
2	c	2	$0,\frac{1}{2},z;\quad \frac{1}{2},0,\frac{1}{2}+z.$	hkl: $h+k+l=2n$
2	b	2	$\frac{1}{2},\frac{1}{2},z;\quad \frac{1}{2},\frac{1}{2},\frac{1}{2}+z.$	hkl: $l=2n$
2	a	2	$0,0,z;\quad 0,0,\frac{1}{2}+z.$	

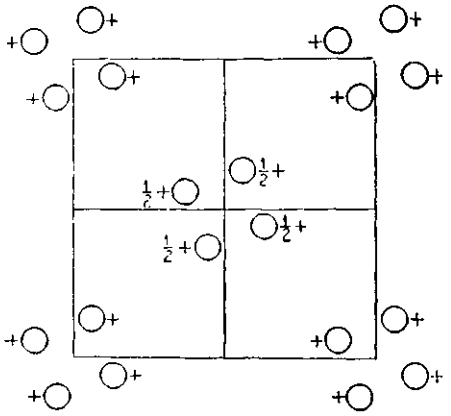
$P4_3$ C_4^4

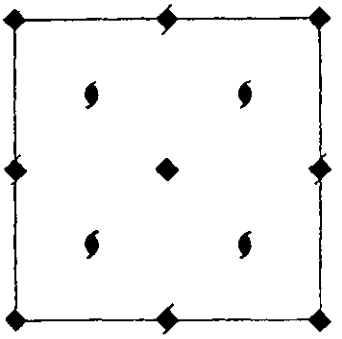
No. 78 $P\,4_3$ 4 Tetragonal



Origin on 4_3

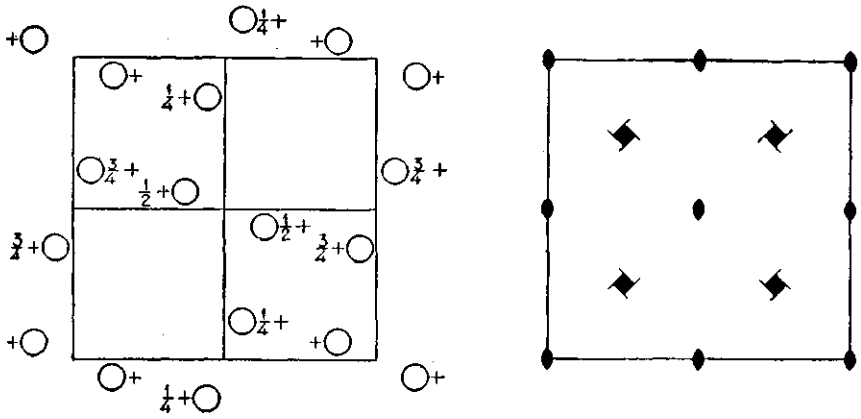
				General:
4	a	1	$x,y,z;\quad \bar{x},\bar{y},\frac{1}{2}+z;\quad \bar{y},x,\frac{3}{4}+z;\quad y,\bar{x},\frac{1}{4}+z.$	hkl: No conditions $00l$: $l=4n$





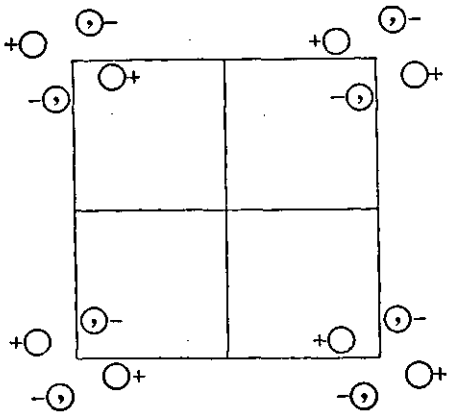
Origin on 4

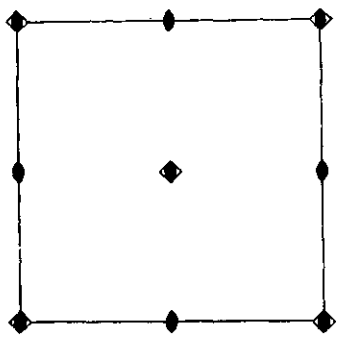
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
8	c	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{y},x,z;\ y,\bar{x},z.$	hkl: $h+k+l=2n$ $00l$: $(l=2n)$
				Special: as above, plus
4	b	2	$0,\frac{1}{2},z;\ \frac{1}{2},0,z.$	hkl: $l=2n$; $(h+k=2n)$
2	a	4	$0,0,z.$	no extra conditions



Origin on 2

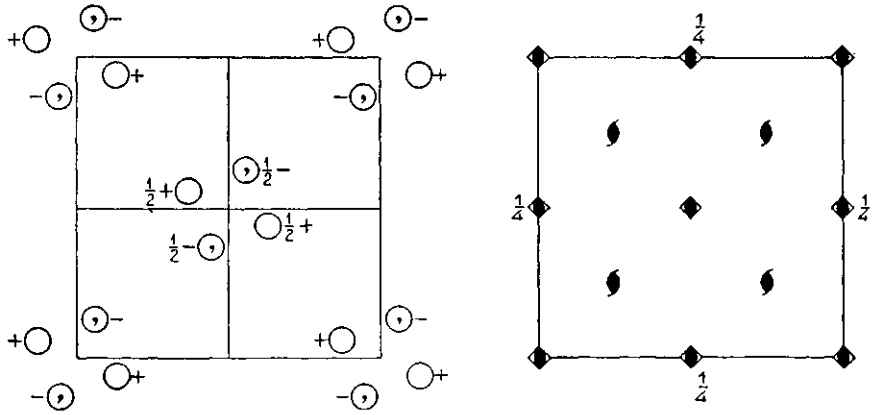
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
				General:
8	b	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{y},\frac{1}{2}+x,\frac{1}{4}+z;\ y,\frac{1}{2}-x,\frac{1}{4}+z.$	hkl: $h+k+l=2n$ $00l$: $l=4n$
				Special: as above, plus
4	a	2	$0,0,z;\ 0,\frac{1}{2},\frac{1}{4}+z.$	hkl: $2k+l=2n+1$ or $4n$





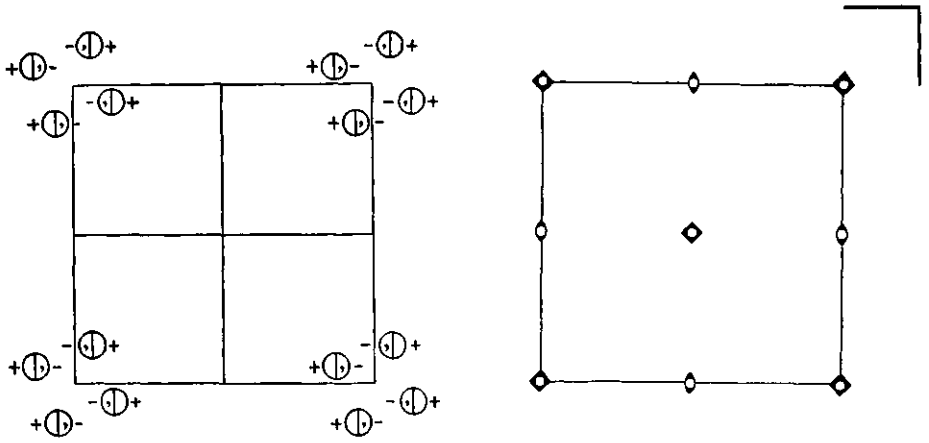
Origin at $\bar{4}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	h	1	x,y,z; $\bar{x},\bar{y},z$; $y,\bar{x},\bar{z}$; $\bar{y},x,\bar{z}$.	hkl: No conditions
				Special:
2	g	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$.	$hk0$: $h+k=2n$
2	f	2	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	No conditions
2	e	2	$0,0,z$; $0,0,\bar{z}$.	
1	d	$\bar{4}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
1	c	$\bar{4}$	$\frac{1}{2},\frac{1}{2},0$.	
1	b	$\bar{4}$	$0,0,\frac{1}{2}$.	
1	a	$\bar{4}$	$0,0,0$.	



Origin at $\bar{4}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
8	g	1	$x,y,z;\ \bar{x},\bar{y},z;\ y,\bar{x},\bar{z};\ \bar{y},x,\bar{z}.$	hkl: $h+k+l=2n$
4	f	2	$0,\frac{1}{2},z;\ \frac{1}{2},0,\bar{z}.$	Special: as above only
4	e	2	$0,0,z;\ 0,0,\bar{z}.$	
2	d	$\bar{4}$	$0,\frac{1}{2},\frac{3}{4}.$	
2	c	$\bar{4}$	$0,\frac{1}{2},\frac{1}{4}.$	
2	b	$\bar{4}$	$0,0,\frac{1}{2}.$	
2	a	$\bar{4}$	$0,0,0.$	

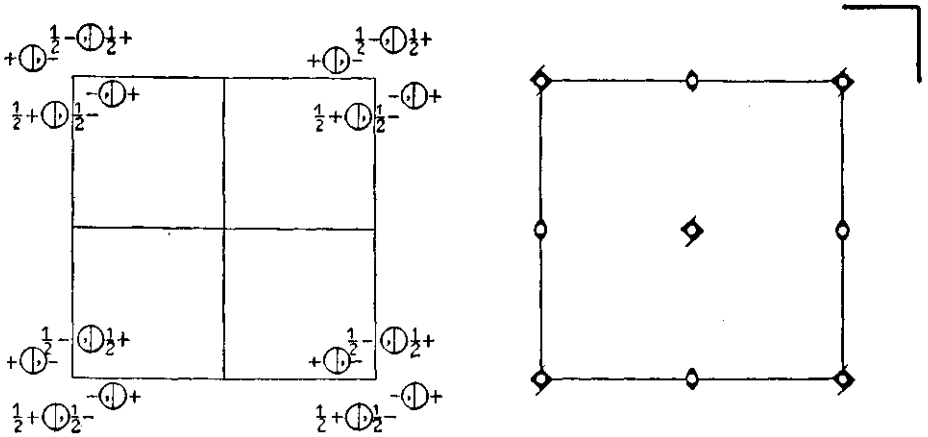


Origin at centre (4/m)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	l	1	x,y,z; $\bar{x},\bar{y},z$; $x,y,\bar{z}$; $\bar{x},\bar{y},\bar{z}$; $\bar{y},x,z$; $y,\bar{x},z$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$.	hkl: $hk0$: $00l$: No conditions
				Special:
4	k	m	$x,y,\frac{1}{2}$; $\bar{x},\bar{y},\frac{1}{2}$; $\bar{y},x,\frac{1}{2}$; $y,\bar{x},\frac{1}{2}$.	No conditions
4	j	m	$x,y,0$; $\bar{x},\bar{y},0$; $\bar{y},x,0$; $y,\bar{x},0$.	No conditions
4	i	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,z$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},0,\bar{z}$.	hkl: $h+k=2n$
2	h	4	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	No conditions
2	g	4	$0,0,z$; $0,0,\bar{z}$.	No conditions
2	f	$2/m$	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	hkl: $h+k=2n$
2	e	$2/m$	$0,\frac{1}{2},0$; $\frac{1}{2},0,0$.	hkl: $h+k=2n$
1	d	$4/m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	No conditions
1	c	$4/m$	$\frac{1}{2},\frac{1}{2},0$.	No conditions
1	b	$4/m$	$0,0,\frac{1}{2}$.	No conditions
1	a	$4/m$	$0,0,0$.	No conditions

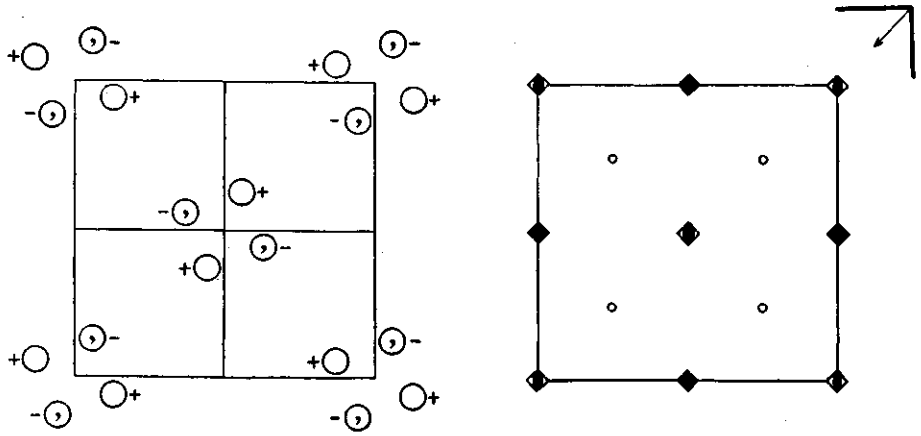
$P4_2/m$ C_{4h}^2

No. 84 $P4_2/m$ $4/m$ Tetragonal



Origin at centre $(2/m)$ on 4_2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	k	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{y},x,\frac{1}{2}+z$; $y,\bar{x},\frac{1}{2}+z$; $x,y,\bar{z}$; $\bar{x},\bar{y},\bar{z}$; $\bar{y},x,\frac{1}{2}-z$; $y,\bar{x},\frac{1}{2}-z$.	hkl: No conditions $hk0$: No conditions $00l$: $l=2n$
				Special: as above, plus
4	j	m	$x,y,0$; $\bar{x},\bar{y},0$; $\bar{y},x,\frac{1}{2}$; $y,\bar{x},\frac{1}{2}$.	no extra conditions
4	i	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},0,\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $h+k+l=2n$
4	h	2	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $l=2n$
4	g	2	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	
2	f	$\bar{4}$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},\frac{3}{4}$.	
2	e	$\bar{4}$	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$.	hkl: $h+k+l=2n$
2	c	$2/m$	$0,\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$.	
2	b	$2/m$	$\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $l=2n$
2	a	$2/m$	$0,0,0$; $0,0,\frac{1}{2}$.	

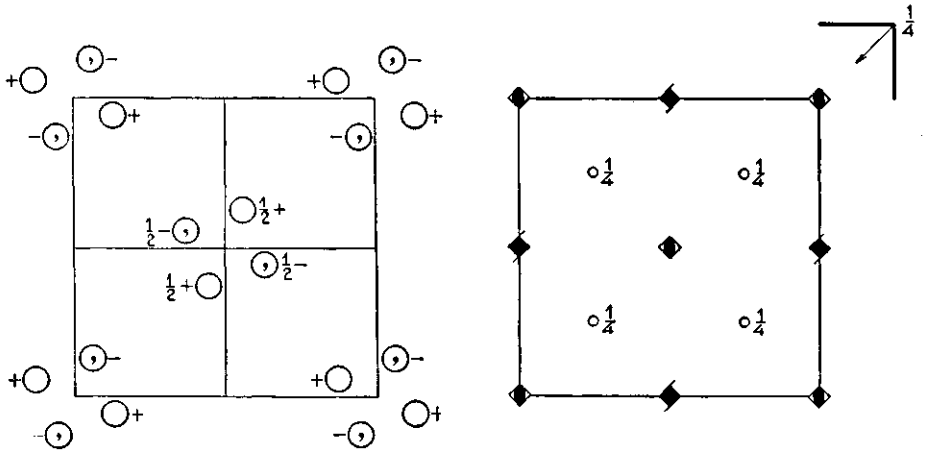


Origin at $\bar{4}$ at $\bar{1}_{\frac{1}{4}},\frac{1}{4},0$ from $\bar{1}$ (compare below for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	g	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}-y,\bar{z}$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}+x,z$; $\frac{1}{2}+y,\frac{1}{2}-x,z$.	hkl: No conditions $hk0$: $h+k=2n$ $00l$: No conditions
				Special: as above, plus
4	f	2	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	hkl: $h+k=2n$
4	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}$.	hkl: $h,k=2n$
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$; $\frac{3}{4},\frac{3}{4},0$; $\frac{1}{4},\frac{3}{4},0$; $\frac{3}{4},\frac{1}{4},0$.	
2	c	4	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$.	no extra conditions
2	b	$\bar{4}$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h+k=2n$ (a and b)
2	a	$\bar{4}$	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$.	

Origin at $\bar{1}$ at $\frac{1}{4},\bar{1}_{\frac{1}{4}},0$ from $\bar{4}$ (compare above for alternative origin)

8	g	1	x,y,z; $\frac{1}{2}-x,\frac{1}{2}-y,z$; $\frac{1}{2}-y,x,z$; $y,\frac{1}{2}-x,z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}+y,\bar{x},\bar{z}$; $\bar{y},\frac{1}{2}+x,\bar{z}$.	General and special conditions as above
4	f	2	$\frac{1}{4},\frac{3}{4},z$; $\frac{3}{4},\frac{1}{4},\bar{z}$; $\frac{1}{4},\frac{3}{4},\bar{z}$; $\frac{3}{4},\frac{1}{4},z$.	
4	e	$\bar{1}$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	
4	d	$\bar{1}$	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$; $0,\frac{1}{2},0$; $\frac{1}{2},0,0$.	
2	c	4	$\frac{1}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{3}{4},\bar{z}$.	
2	b	$\bar{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}$.	
2	a	$\bar{4}$	$\frac{1}{4},\frac{3}{4},0$; $\frac{3}{4},\frac{1}{4},0$.	

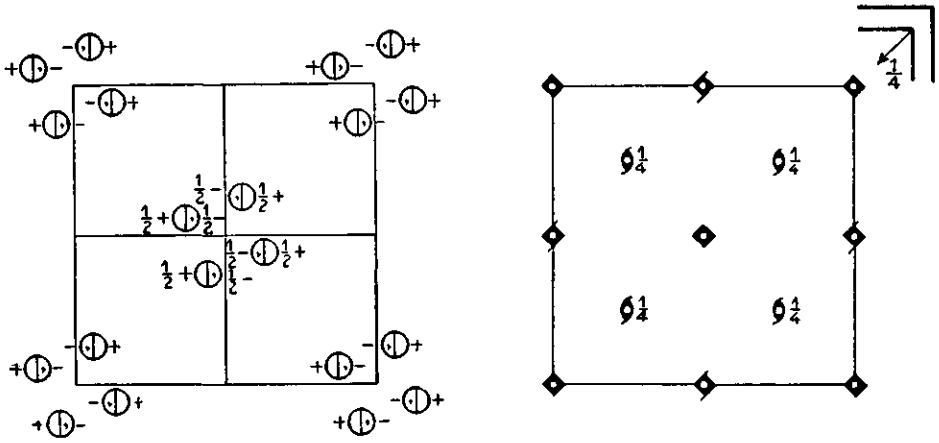


Origin at $\bar{4}$ at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{1}$ (compare below for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	g	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$.	hkl: No conditions $hk0$: $h+k=2n$ $00l$: $l=2n$
				Special: as above, plus
4	f	2	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
4	e	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},0,\bar{z}$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $l=2n$
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{4}$;	hkl: $h+k=2n$ $k+l=2n$ and $(l+h=2n)$
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$.	
2	b	$\bar{4}$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	2 a $\bar{4}$ $0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$. — hkl: $h+k+l=2n$ (a and b)

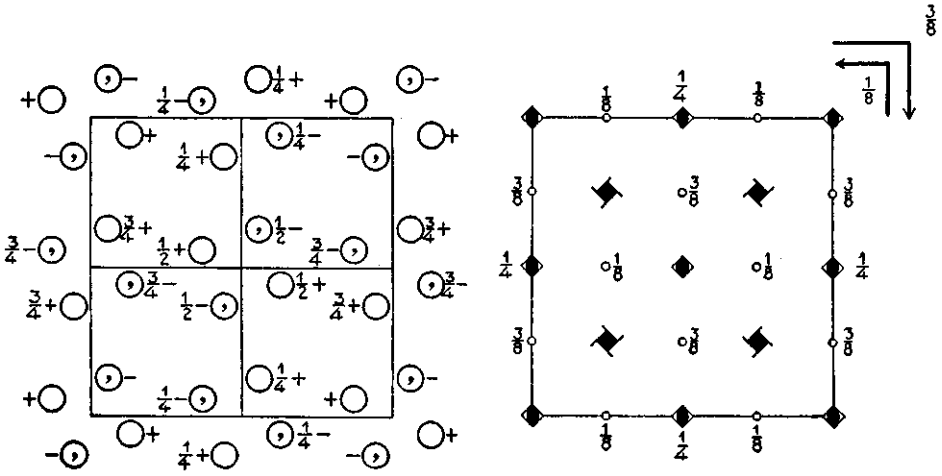
Origin at $\bar{1}$ at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{4}$ (compare above for alternative origin)

8	g	1	x,y,z; $\frac{1}{2}-x,\frac{1}{2}-y,z$; $\bar{y},\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+y,\bar{x},\frac{1}{2}+z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $y,\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}-y,x,\frac{1}{2}-z$.	General and special conditions as above
4	f	2	$\frac{1}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{3}{4},\bar{z}$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}+z$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}-z$.	
4	e	2	$\frac{3}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{3}{4},\bar{z}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}+z$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}-z$.	
4	d	$\bar{1}$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $0,\frac{1}{2},0$; $\frac{1}{2},0,0$.	
4	c	$\bar{1}$	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	
2	b	$\bar{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$. 2 a $\bar{4}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$.	



Origin at centre ($4/m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
16	i	1	$x,y,z;\ \bar{x},\bar{y},z;\ x,y,\bar{z};\ \bar{x},\bar{y},\bar{z};$ $\bar{y},x,z;\ y,\bar{x},z;\ \bar{y},x,\bar{z};\ y,\bar{x},\bar{z}.$	hkl: $h+k+l=2n$ $hk0$: $(h+k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
8	h	m	$x,y,0;\ \bar{x},\bar{y},0;\ \bar{y},x,0;\ y,\bar{x},0.$	no extra conditions
8	g	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\bar{z};\ \frac{1}{2},0,z;\ \frac{1}{2},0,\bar{z}.$	hkl: $l=2n$; $(h+k=2n)$
8	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{3}{4},\frac{3}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{1}{4};\ \frac{3}{4},\frac{1}{4},\frac{1}{4}.$	hkl: $h,k,(l)=2n$
4	e	4	$0,0,z;\ 0,0,\bar{z}.$	no extra conditions
4	d	$\bar{4}$	$0,\frac{1}{2},\frac{1}{4};\ \frac{1}{2},0,\frac{1}{4}.$	hkl: $l=2n$; $(h+k=2n)$
4	c	$2/m$	$0,\frac{1}{2},0;\ \frac{1}{2},0,0.$	
2	b	$4/m$	$0,0,\frac{1}{2}.$	no extra conditions
2	a	$4/m$	$0,0,0.$	



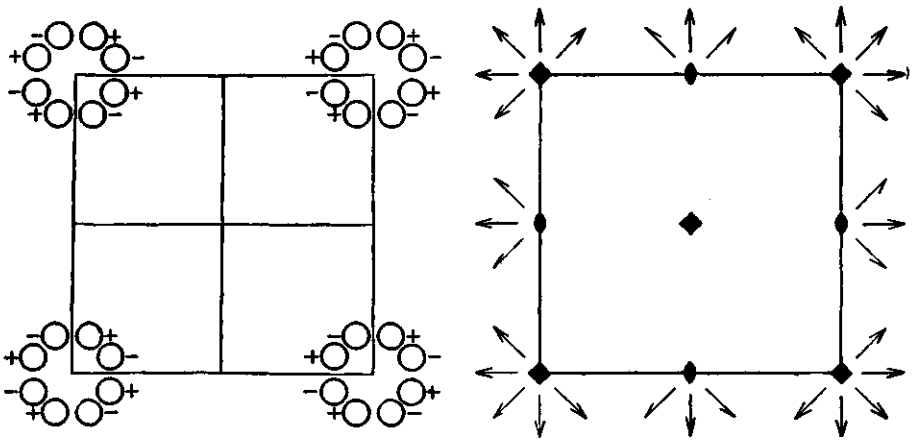
Origin at $\bar{4}$ at $0,\bar{\frac{1}{4}},\bar{\frac{1}{8}}$ from $\bar{1}$ (compare below for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
16	f	1	$x,y,z;\ \bar{x},\bar{y},z;\ x,\frac{1}{2}+y,\frac{1}{4}-z;\ \bar{x},\frac{1}{2}-y,\frac{1}{4}-z;$ $\bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ \bar{y},\frac{1}{2}+x,\frac{1}{4}+z;\ y,\frac{1}{2}-x,\frac{1}{4}+z.$	General: hkl: $h+k+l=2n$ $hk0$: $h,(k)=2n$ $00l$: $l=4n$
				Special: as above, plus
8	e	2	$0,0,z;\ 0,0,\bar{z};\ 0,\frac{1}{2},\frac{1}{4}+z;\ 0,\frac{1}{2},\frac{1}{4}-z.$	hkl: $2k+l=2n+1$ or $4n$
8	d	$\bar{1}$	$0,\frac{1}{4},\frac{5}{8};\ 0,\frac{3}{4},\frac{5}{8};\ \frac{1}{4},0,\frac{3}{8};\ \frac{3}{4},0,\frac{3}{8}.$	hkl: $l,(h+k)=2n+1$ or $[h,k,(l)=2n$ and $h+k+l=4n]$
8	c	$\bar{1}$	$0,\frac{1}{4},\frac{1}{8};\ 0,\frac{3}{4},\frac{1}{8};\ \frac{1}{4},0,\frac{7}{8};\ \frac{3}{4},0,\frac{7}{8}.$	
4	b	$\bar{4}$	$0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{3}{4}.$ 4 a $\bar{4}$ $0,0,0;\ 0,\frac{1}{2},\frac{1}{4}.$	(a and b) hkl: $2k+l=2n+1$ or $4n$

Origin at $\bar{1}$ at $0,\frac{1}{4},\frac{1}{8}$ from $\bar{4}$ (compare above for alternative origin)

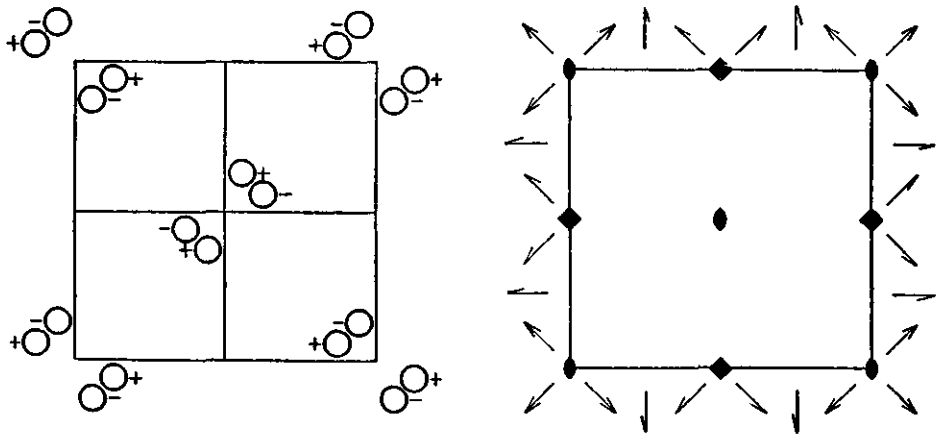
$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$

16	f	1	$x,y,z;\ \bar{x},\frac{1}{2}-y,z;\ \frac{3}{4}-y,\frac{1}{4}+x,\frac{1}{4}+z;\ \frac{1}{4}+y,\frac{1}{4}-x,\frac{1}{4}+z;$ $\bar{x},\bar{y},\bar{z};\ x,\frac{1}{2}+y,\bar{z};\ \frac{1}{4}+y,\frac{3}{4}-x,\frac{3}{4}-z;\ \frac{3}{4}-y,\frac{3}{4}+x,\frac{3}{4}-z.$	General and special conditions as above
8	e	2	$0,\frac{1}{4},z;\ 0,\frac{3}{4},\bar{z};\ 0,\frac{1}{4},\frac{1}{4}-z;\ 0,\frac{3}{4},\frac{3}{4}+z.$	
8	d	$\bar{1}$	$0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{4},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{4},\frac{3}{4}.$	
8	c	$\bar{1}$	$0,0,0;\ 0,\frac{1}{2},0;\ \frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{3}{4},\frac{1}{4},\frac{1}{4}.$	
4	b	$\bar{4}$	$0,\frac{1}{4},\frac{5}{8};\ 0,\frac{3}{4},\frac{3}{8}.$ 4 a $\bar{4}$ $0,\frac{1}{4},\frac{1}{8};\ 0,\frac{3}{4},\frac{7}{8}.$	



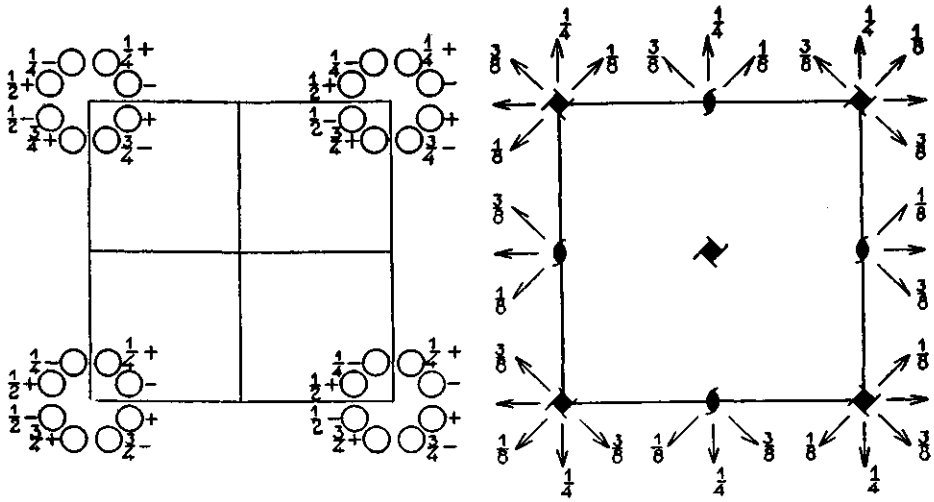
Origin at 422

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	*p*	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\bar{z}$; $x,\bar{y},\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $y,x,\bar{z}$; $y,\bar{x},z$; $\bar{y},x,z$.	No conditions
				Special:
4	*o*	2	$x,\frac{1}{2},0$; $\bar{x},\frac{1}{2},0$; $\frac{1}{2},x,0$; $\frac{1}{2},\bar{x},0$.	No conditions
4	*n*	2	$x,0,\frac{1}{2}$; $\bar{x},0,\frac{1}{2}$; $0,x,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$.	
4	*m*	2	$x,\frac{1}{2},\frac{1}{2}$; $\bar{x},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},x,\frac{1}{2}$; $\frac{1}{2},\bar{x},\frac{1}{2}$.	
4	*l*	2	$x,0,0$; $\bar{x},0,0$; $0,x,0$; $0,\bar{x},0$.	
4	*k*	2	$x,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $\bar{x},x,\frac{1}{2}$; $x,\bar{x},\frac{1}{2}$.	
4	*j*	2	$x,x,0$; $\bar{x},\bar{x},0$; $\bar{x},x,0$; $x,\bar{x},0$.	
4	*i*	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$.	*hkl*: $h+k=2n$
2	*h*	4	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	No conditions
2	*g*	4	$0,0,z$; $0,0,\bar{z}$.	
2	*f*	222	$\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$.	*hkl*: $h+k=2n$
2	*e*	222	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$.	
1	*d*	42	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	No conditions
1	*c*	42	$\frac{1}{2},\frac{1}{2},0$.	
1	*b*	42	$0,0,\frac{1}{2}$.	
1	*a*	42	$0,0,0$.	



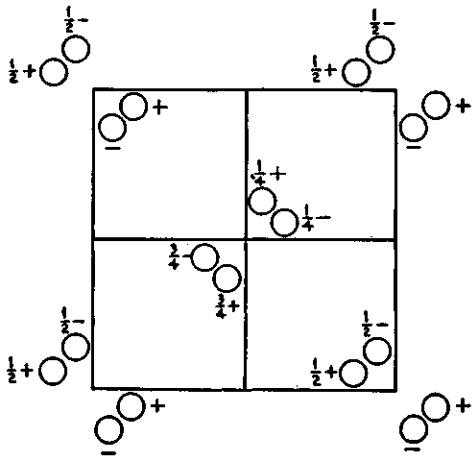
Origin at 222 ([001]⟨110⟩)

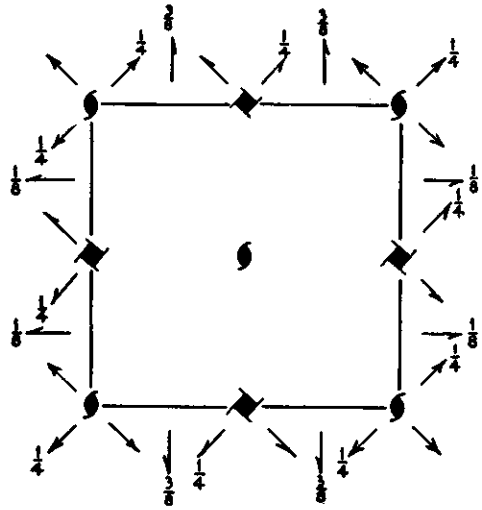
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	g	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}-x,z$; $\frac{1}{2}-y,\frac{1}{2}+x,z$.	hkl: No conditions $00l$: No conditions $h00$: $h=2n$
				Special: as above, plus
4	f	2	$x,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}$.	$0kl$: $k=2n$
4	e	2	$x,x,0$; $\bar{x},\bar{x},0$; $\frac{1}{2}+x,\frac{1}{2}-x,0$; $\frac{1}{2}-x,\frac{1}{2}+x,0$.	
4	d	2	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	hkl: $h+k=2n$
2	c	4	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$.	$hk0$: $h+k=2n$
2	b	222	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h+k=2n$
2	a	222	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$.	



Origin at 4_121 ([001] [010])

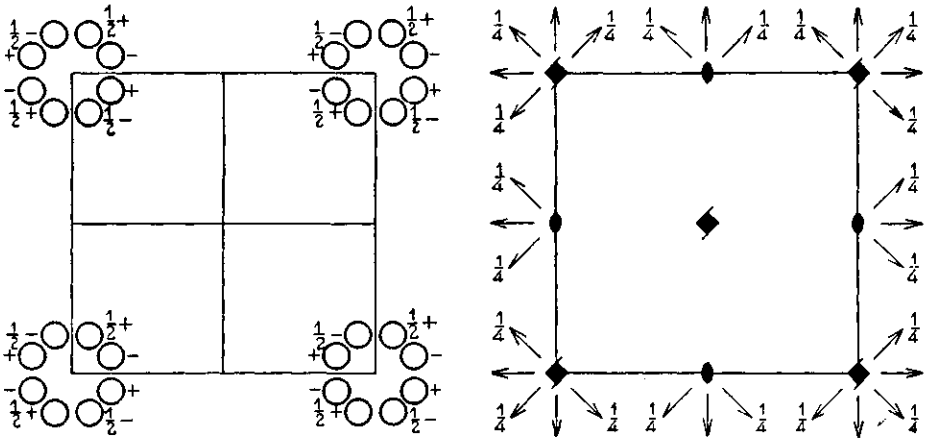
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	d	1	x,y,z; $\bar{x},\bar{y},\frac{1}{2}+z$; $\bar{y},x,\frac{1}{4}+z$; $y,\bar{x},\frac{3}{4}+z$; $\bar{x},y,\bar{z}$; $x,\bar{y},\frac{1}{2}-z$; $\bar{y},\bar{x},\frac{1}{4}-z$; $y,x,\frac{3}{4}-z$.	hkl: No conditions $00l$: $l=4n$ $h00$: No conditions
				Special: as above, plus
4	c	2	$x,x,\frac{3}{8}$; $\bar{x},\bar{x},\frac{7}{8}$; $x,\bar{x},\frac{1}{8}$; $\bar{x},x,\frac{5}{8}$.	$0kl$: $l=2n+1$ or $4n$
4	b	2	$\frac{1}{2},x,0$; $\frac{1}{2},\bar{x},\frac{1}{2}$; $x,\frac{1}{2},\frac{3}{4}$; $\bar{x},\frac{1}{2},\frac{1}{4}$.	hhl: $l=2n+1$ or $4n$
4	a	2	$0,x,0$; $0,\bar{x},\frac{1}{2}$; $x,0,\frac{3}{4}$; $\bar{x},0,\frac{1}{4}$.	





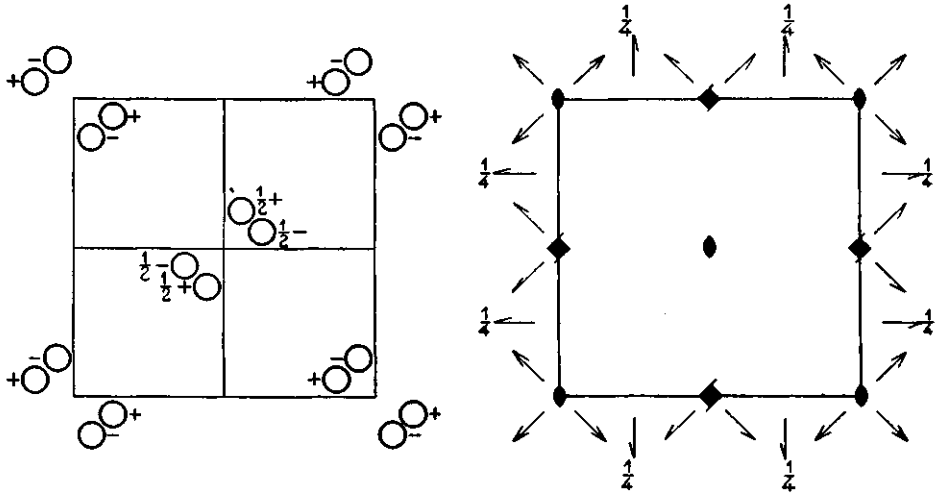
Origin at 2_12 ([001] [110])

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	b	1	x,y,z; $\bar{x},\bar{y},\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{4}+z$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{3}{4}+z$; $y,x,\bar{z}$; $\bar{y},\bar{x},\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{4}-z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{3}{4}-z$.	hkl: No conditions $00l$: $l=4n$ $h00$: $h=2n$
				Special: as above, plus
4	a	2	$x,x,0$; $\bar{x},\bar{x},\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{4}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{3}{4}$.	$0kl$: $2k+l=2n+1$ or $4n$



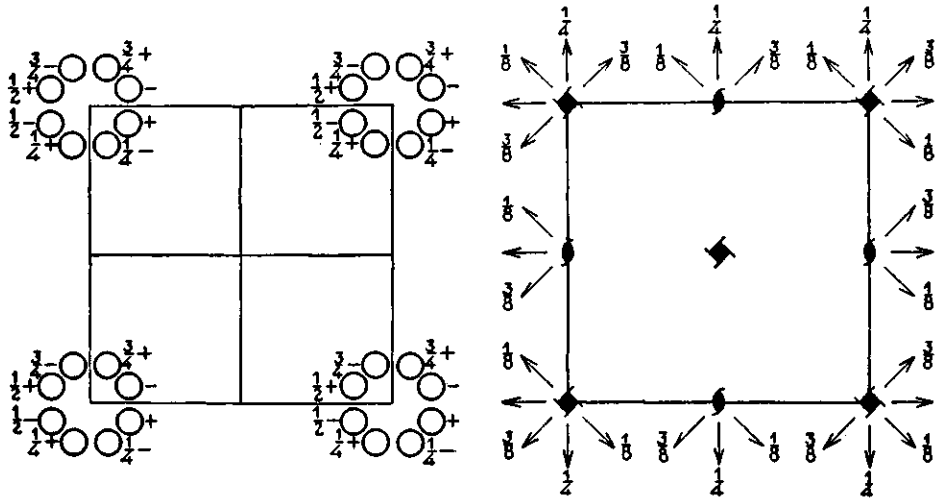
Origin at 4_221

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	p	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{y},x,\frac{1}{2}+z$; $y,\bar{x},\frac{1}{2}+z$; $\bar{x},y,\bar{z}$; $x,\bar{y},\bar{z}$; $y,x,\frac{1}{2}-z$; $\bar{y},\bar{x},\frac{1}{2}-z$.	hkl: No conditions $00l$: $l=2n$ $h00$: No conditions
				Special: as above, plus
4	o	2	$x,x,\frac{3}{4}$; $\bar{x},\bar{x},\frac{3}{4}$; $\bar{x},x,\frac{1}{4}$; $x,\bar{x},\frac{1}{4}$.	$0kl$: $l=2n$
4	n	2	$x,x,\frac{1}{4}$; $\bar{x},\bar{x},\frac{1}{4}$; $\bar{x},x,\frac{3}{4}$; $x,\bar{x},\frac{3}{4}$.	
4	m	2	$x,\frac{1}{2},0$; $\bar{x},\frac{1}{2},0$; $\frac{1}{2},x,\frac{1}{2}$; $\frac{1}{2},\bar{x},\frac{1}{2}$.	hhl: $l=2n$
4	l	2	$x,0,\frac{1}{2}$; $\bar{x},0,\frac{1}{2}$; $0,x,0$; $0,\bar{x},0$.	
4	k	2	$x,\frac{1}{2},\frac{1}{2}$; $\bar{x},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},x,0$; $\frac{1}{2},\bar{x},0$.	
4	j	2	$x,0,0$; $\bar{x},0,0$; $0,x,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$.	
4	i	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},0,\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $h+k+l=2n$
4	h	2	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $l=2n$
4	g	2	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	
2	f	222	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},\frac{3}{4}$.	
2	e	222	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	
2	d	222	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$.	hkl: $h+k+l=2n$
2	c	222	$0,\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$.	
2	b	222	$\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $l=2n$
2	a	222	$0,0,0$; $0,0,\frac{1}{2}$.	



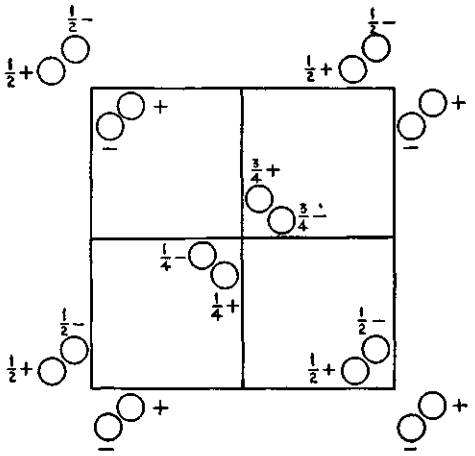
Origin at 222 ([001]⟨110⟩)

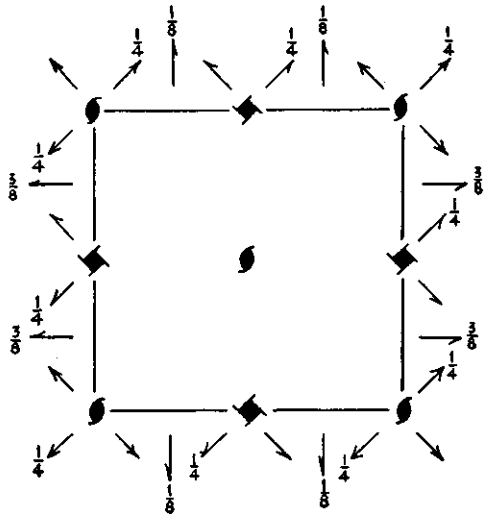
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	g	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z$; $y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$.	hkl: No conditions $00l$: $l=2n$ $h00$: $h=2n$
				Special: as above, plus
4	f	2	$x,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2}-x,0$; $\frac{1}{2}-x,\frac{1}{2}+x,0$.	$0kl$: $k+l=2n$
4	e	2	$x,x,0$; $\bar{x},\bar{x},0$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}$.	
4	d	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$; $0,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $l=2n$ $hk0$: $h+k=2n$
4	c	2	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
2	b	222	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	
2	a	222	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	



Origin at 4_321 ([001] [010])

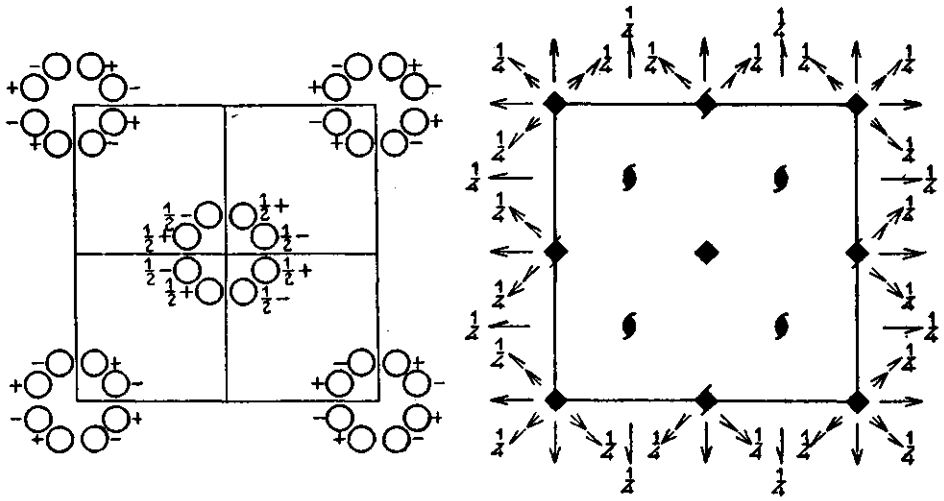
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	d	1	x,y,z; $\bar{x},\bar{y},\frac{1}{2}+z$; $\bar{y},x,\frac{3}{4}+z$; $y,\bar{x},\frac{1}{4}+z$; $\bar{x},y,\bar{z}$; $x,\bar{y},\frac{1}{2}-z$; $\bar{y},\bar{x},\frac{3}{4}-z$; $y,x,\frac{1}{4}-z$.	hkl: No conditions $00l$: $l=4n$ $h00$: No conditions
				Special: as above, plus
4	c	2	$x,x,\frac{5}{8}$; $\bar{x},\bar{x},\frac{1}{8}$; $x,\bar{x},\frac{7}{8}$; $\bar{x},x,\frac{3}{8}$.	$0kl$: $l=2n+1$ or $4n$
4	b	2	$\frac{1}{2},x,0$; $\frac{1}{2},\bar{x},\frac{1}{2}$; $x,\frac{1}{2},\frac{1}{4}$; $\bar{x},\frac{1}{2},\frac{3}{4}$.	hhl: $l=2n+1$ or $4n$
4	a	2	$0,x,0$; $0,\bar{x},\frac{1}{2}$; $x,0,\frac{1}{4}$; $\bar{x},0,\frac{3}{4}$.	





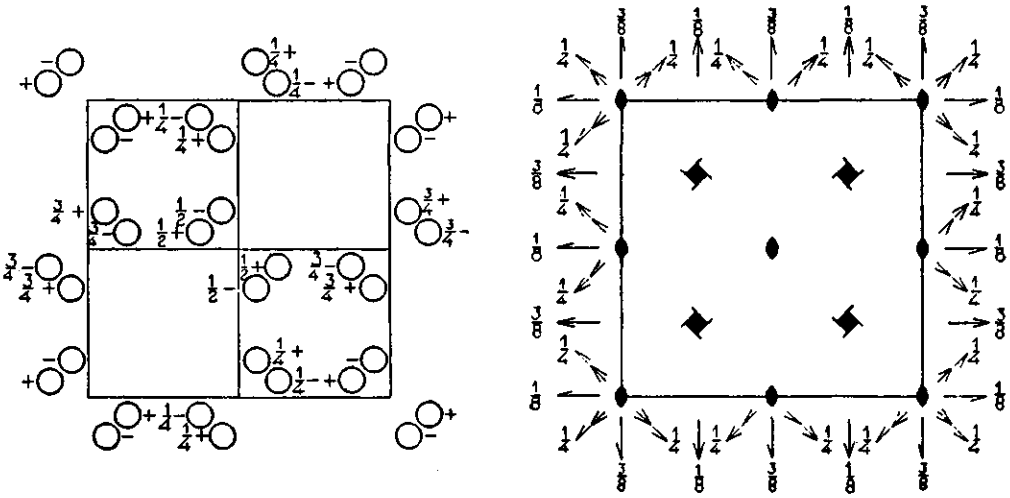
Origin at 2_12 ([001] [110])

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
8	b	1	x,y,z; $\bar{x},\bar{y},\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{3}{4}+z$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{4}+z$; $y,x,\bar{z}$; $\bar{y},\bar{x},\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{3}{4}-z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{4}-z$.	General: hkl: No conditions $00l$: $l=4n$ $h00$: $h=2n$
4	a	2	$x,x,0$; $\bar{x},\bar{x},\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{4}$.	Special: as above, plus $0kl$: $2k+l=2n+1$ or $4n$



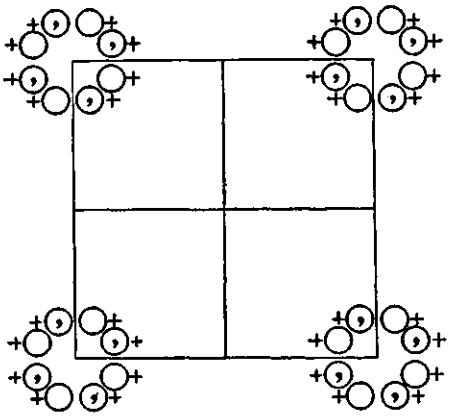
Origin at 422

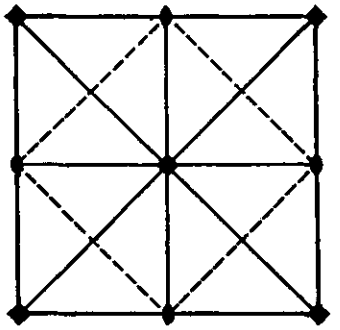
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
16	*k*	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\bar{z};\ x,\bar{y},\bar{z};$ $y,x,\bar{z};\ \bar{y},\bar{x},\bar{z};\ \bar{y},x,z;\ y,\bar{x},z.$	hkl: $h+k+l=2n$ $00l$: $(l=2n)$ $h00$: $(h=2n)$
				Special: as above, plus
8	*j*	2	$x,\frac{1}{2}+x,\frac{1}{4};\ \bar{x},\frac{1}{2}-x,\frac{1}{4};\ x,\frac{1}{2}-x,\frac{3}{4};\ \bar{x},\frac{1}{2}+x,\frac{3}{4}.$	$0kl$: $k,(l)=2n$
8	*i*	2	$x,0,\frac{1}{2};\ \bar{x},0,\frac{1}{2};\ 0,x,\frac{1}{2};\ 0,\bar{x},\frac{1}{2}.$	no extra conditions
8	*h*	2	$x,0,0;\ \bar{x},0,0;\ 0,x,0;\ 0,\bar{x},0.$	
8	*g*	2	$x,x,0;\ \bar{x},\bar{x},0;\ x,\bar{x},0;\ \bar{x},x,0.$	
8	*f*	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\bar{z};\ \frac{1}{2},0,z;\ \frac{1}{2},0,\bar{z}.$	hkl: $l=2n$; $(h+k=2n)$
4	*e*	4	$0,0,z;\ 0,0,\bar{z}.$	no extra conditions
4	*d*	222	$0,\frac{1}{2},\frac{1}{4};\ \frac{1}{2},0,\frac{1}{4}.$	hkl: $l=2n$; $(h+k=2n)$
4	*c*	222	$0,\frac{1}{2},0;\ \frac{1}{2},0,0.$	
2	*b*	42	$0,0,\frac{1}{2}.$	no extra conditions
2	*a*	42	$0,0,0.$	



Origin at 222 ([001]⟨110⟩)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
16	g	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},\frac{1}{2}+y,\frac{1}{4}-z;\ x,\frac{1}{2}-y,\frac{1}{4}-z;$ $y,x,\bar{z};\ \bar{y},\bar{x},\bar{z};\ \bar{y},\frac{1}{2}+x,\frac{1}{4}+z;\ y,\frac{1}{2}-x,\frac{1}{4}+z.$	hkl: $h+k+l=2n$ $00l$: $l=4n$ $h00$: $(h=2n)$
				Special: as above, plus
8	f	2	$x,\frac{1}{4},\frac{1}{8};\ \bar{x},\frac{3}{4},\frac{1}{8};\ \frac{1}{4},x,\frac{7}{8};\ \frac{3}{4},\bar{x},\frac{7}{8}.$	hhl: $l=4n$
8	e	2	$\bar{x},x,0;\ x,\bar{x},0;\ x,\frac{1}{2}+x,\frac{1}{4};\ \bar{x},\frac{1}{2}-x,\frac{1}{4}.$	$0kl$: $(k+l=2n)$; $2k+l=2n+1$ or $4n$
8	d	2	$x,x,0;\ \bar{x},\bar{x},0;\ \bar{x},\frac{1}{2}+x,\frac{1}{4};\ x,\frac{1}{2}-x,\frac{1}{4}.$	
8	c	2	$0,0,z;\ 0,0,\bar{z};\ 0,\frac{1}{2},\frac{1}{4}+z;\ 0,\frac{1}{2},\frac{1}{4}-z.$	hkl: $2k+l=2n+1$ or $4n$
4	b	222	$0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{3}{4}.$	
4	a	222	$0,0,0;\ 0,\frac{1}{2},\frac{1}{4}.$	



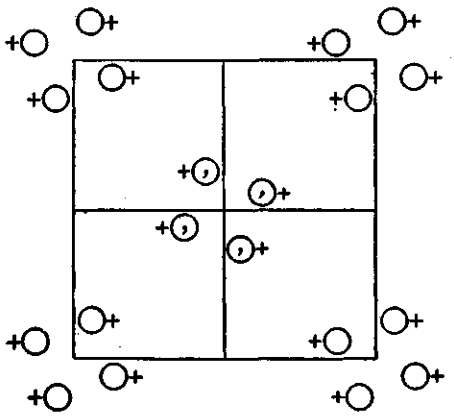


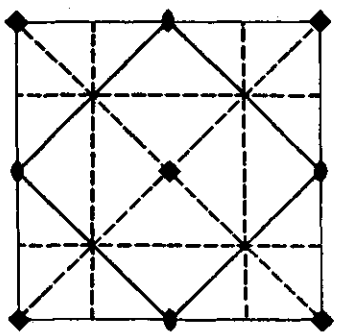
Origin on $4mm$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	g	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,z$; $x,\bar{y},z$; y,x,z; $\bar{y},\bar{x},z$; $\bar{y},x,z$; $y,\bar{x},z$.	No conditions
				Special:
4	f	m	$x,\frac{1}{2},z$; $\bar{x},\frac{1}{2},z$; $\frac{1}{2},x,z$; $\frac{1}{2},\bar{x},z$.	No conditions
4	e	m	$x,0,z$; $\bar{x},0,z$; $0,x,z$; $0,\bar{x},z$.	
4	d	m	x,x,z; $\bar{x},\bar{x},z$; $\bar{x},x,z$; $x,\bar{x},z$.	
2	c	mm	$\frac{1}{2},0,z$; $0,\frac{1}{2},z$.	hkl: $h+k=2n$
1	b	$4mm$	$\frac{1}{2},\frac{1}{2},z$.	No conditions
1	a	$4mm$	$0,0,z$	

$P4bm$ C_{4v}^{2}

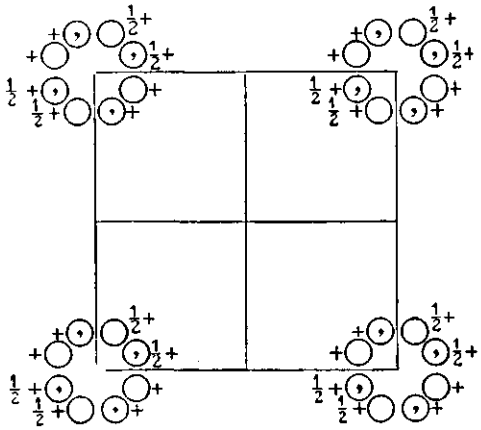
No. 100 $P\,4\,b\,m$ $4\,m\,m$ Tetragonal

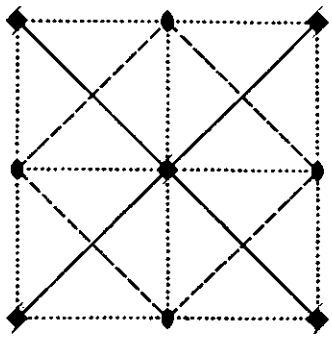




Origin on 4

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	d	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,z$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $\bar{y},x,z$; $y,\bar{x},z$; $\frac{1}{2}+y,\frac{1}{2}+x,z$; $\frac{1}{2}-y,\frac{1}{2}-x,z$.	hkl: No conditions $0kl$: $k=2n$ hhl: No conditions
				Special: as above, plus
4	c	m	$x,\frac{1}{2}+x,z$; $\bar{x},\frac{1}{2}-x,z$; $\frac{1}{2}+x,\bar{x},z$; $\frac{1}{2}-x,x,z$.	no extra conditions
2	b	mm	$\frac{1}{2},0,z$; $0,\frac{1}{2},z$.	hkl: $h+k=2n$
2	a	4	$0,0,z$; $\frac{1}{2},\frac{1}{2},z$.	



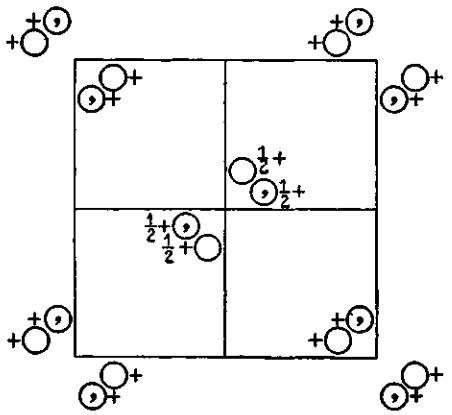


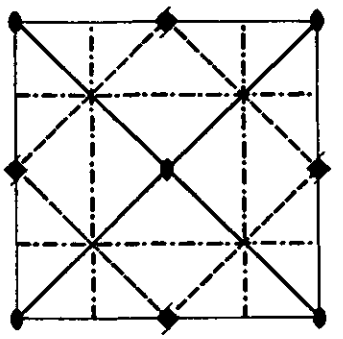
Origin on 4_2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	e	1	$x,y,z;\ \bar{x},\bar{y},z;\ x,\bar{y},\frac{1}{2}+z;\ \bar{x},y,\frac{1}{2}+z;$ $y,x,z;\ \bar{y},\bar{x},z;\ y,\bar{x},\frac{1}{2}+z;\ \bar{y},x,\frac{1}{2}+z.$	hkl: No conditions $0kl$: $l=2n$ hhl: No conditions
				Special: as above, plus
4	d	m	$x,x,z;\ \bar{x},\bar{x},z;\ x,\bar{x},\frac{1}{2}+z;\ \bar{x},x,\frac{1}{2}+z.$	no extra conditions
4	c	2	$0,\frac{1}{2},z;\ \frac{1}{2},0,z;\ 0,\frac{1}{2},\frac{1}{2}+z;\ \frac{1}{2},0,\frac{1}{2}+z.$	hkl: $h+k=2n$; $l=2n$
2	b	mm	$\frac{1}{2},\frac{1}{2},z;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}+z.$	hkl: $l=2n$
2	a	mm	$0,0,z;\ 0,0,\frac{1}{2}+z.$	

$P4_2nm$ C_{4v}^{4}

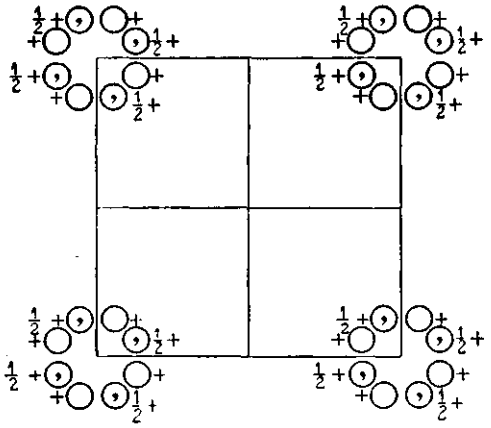
No. 102 $P\,4_2\,n\,m$ $4\,m\,m$ Tetragonal

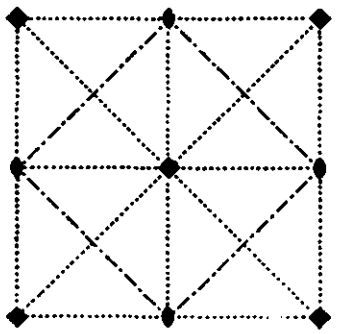




Origin on mm

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	d	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; y,x,z; $\bar{y},\bar{x},z$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$.	hkl: No conditions $0kl$: $k+l=2n$ hhl: No conditions
				Special: as above, plus
4	c	m	x,x,z; $\bar{x},\bar{x},z$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}+z$.	no extra conditions
4	b	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,z$; $0,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}+z$.	hkl: $h+k=2n$; $l=2n$
2	a	mm	$0,0,z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$.	hkl: $h+k+l=2n$



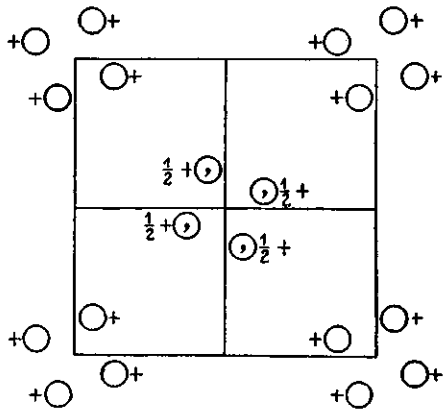


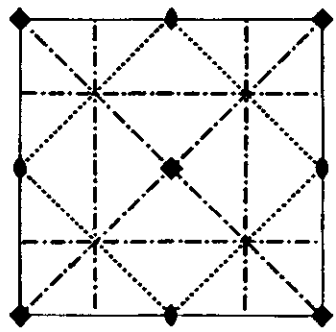
Origin on 4

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	*d*	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\frac{1}{2}+z$; $x,\bar{y},\frac{1}{2}+z$; $\bar{y},x,z$; $y,\bar{x},z$; $y,x,\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}+z$.	*hkl*: No conditions 0*kl*: $l=2n$ *hhl*: $l=2n$
				Special: as above, plus
4	*c*	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,z$; $0,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}+z$.	*hkl*: $h+k=2n$; $l=2n$
2	*b*	4	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$.	*hkl*: $l=2n$
2	*a*	4	$0,0,z$; $0,0,\frac{1}{2}+z$.	

$P4nc$ C_{4v}^{6}

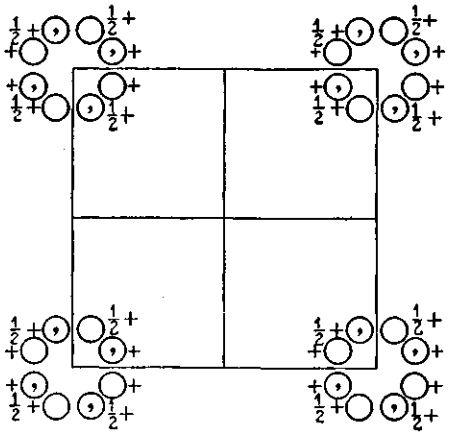
No. 104 $P\,4\,n\,c$ $4\,m\,m$ Tetragonal

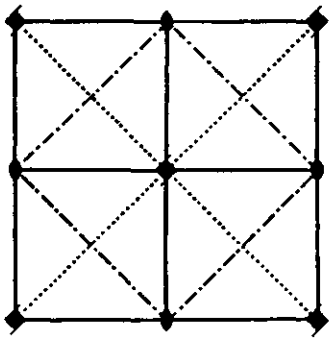




Origin on 4

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	c	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $\bar{y},x,z$; $y,\bar{x},z$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$.	hkl: No conditions $0kl$: $k+l=2n$ hhl: $l=2n$
				Special:
4	b	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,z$; $0,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}+z$.	hkl: $h+k=2n$; $l=2n$
2	a	4	$0,0,z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$.	hkl: $h+k+l=2n$



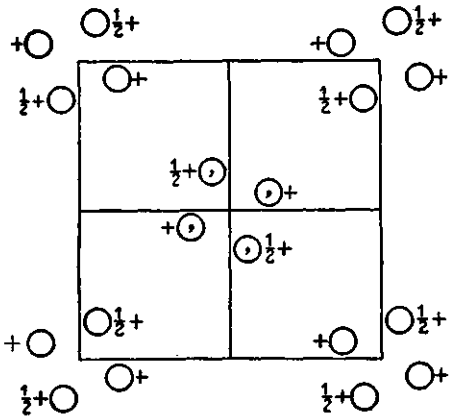


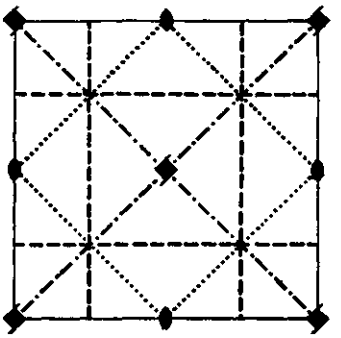
Origin on 4_2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	f	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{y},x,\frac{1}{2}+z$; $y,\bar{x},\frac{1}{2}+z$; $\bar{x},y,z$; $x,\bar{y},z$; $y,x,\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}+z$.	hkl: No conditions $0kl$: No conditions hhl: $l=2n$
				Special: as above, plus
4	e	m	$x,\frac{1}{2},z$; $\bar{x},\frac{1}{2},z$; $\frac{1}{2},x,\frac{1}{2}+z$; $\frac{1}{2},\bar{x},\frac{1}{2}+z$.	no extra conditions
4	d	m	$x,0,z$; $\bar{x},0,z$; $0,x,\frac{1}{2}+z$; $0,\bar{x},\frac{1}{2}+z$.	
2	c	mm	$0,\frac{1}{2},z$; $\frac{1}{2},0,\frac{1}{2}+z$.	hkl: $h+k+l=2n$
2	b	mm	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$.	hkl: $l=2n$
2	a	mm	$0,0,z$; $0,0,\frac{1}{2}+z$.	

$P4_2bc$ C_{4v}^{8}

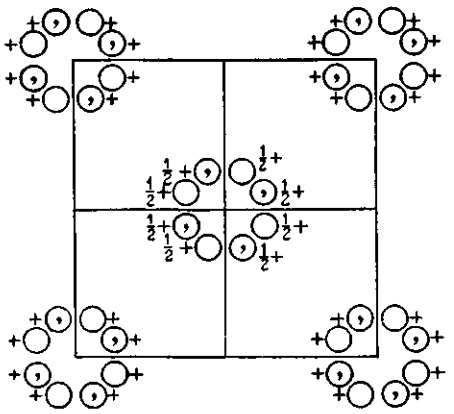
No. 106 $P\,4_2\,b\,c$ $4\,m\,m$ Tetragonal

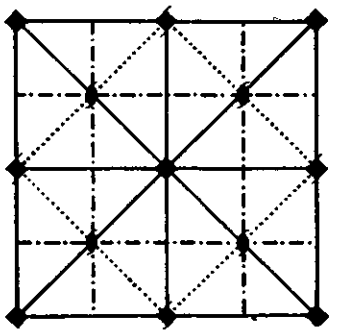




Origin on 4_2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	c	1	x,y,z; $\frac{1}{2}+x,\frac{1}{2}-y,z$; $\bar{y},x,\frac{1}{2}+z$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $y,\bar{x},\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$.	hkl: No conditions $0kl$: $k=2n$ hhl: $l=2n$
				Special: as above, plus
4	b	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,z$; $0,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}+z$.	hkl: $h+k=2n$; $l=2n$
4	a	2	$0,0,z$; $\frac{1}{2},\frac{1}{2},z$; $0,0,\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$.	

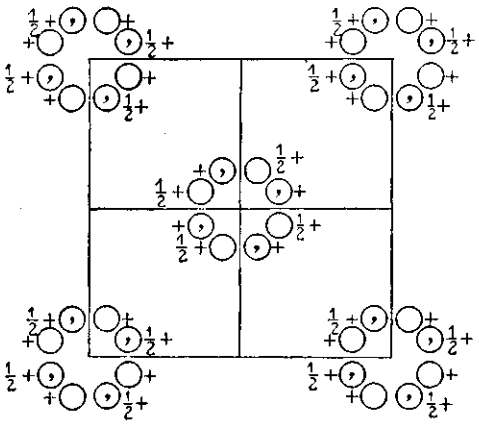


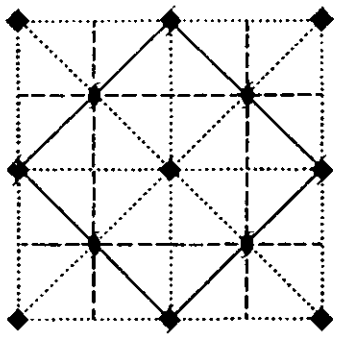


Origin on $4mm$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
16	*e*	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z;$ $y,x,z;\ \bar{y},\bar{x},z;\ y,\bar{x},z;\ \bar{y},x,z.$	hkl: $h+k+l=2n$ $0kl$: $(k+l=2n)$ hhl: $(l=2n)$
				Special: as above, plus
8	*d*	*m*	$x,0,z;\ \bar{x},0,z;\ 0,x,z;\ 0,\bar{x},z.$	no extra conditions
8	*c*	*m*	$x,x,z;\ \bar{x},\bar{x},z;\ \bar{x},x,z;\ x,\bar{x},z.$	no extra conditions
4	*b*	*mm*	$0,\frac{1}{2},z;\ \frac{1}{2},0,z.$	hkl: $l=2n$; $(h+k=2n)$
2	*a*	$4mm$	$0,0,z.$	no extra conditions

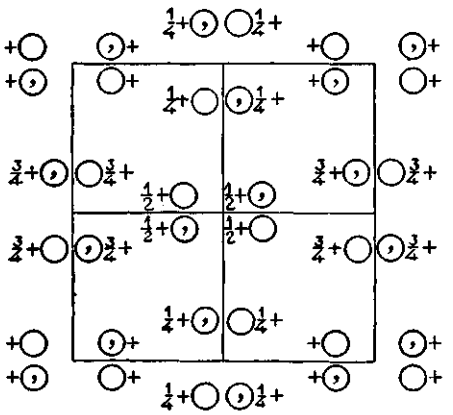
No. 108 $I4cm$ $4mm$ Tetragonal

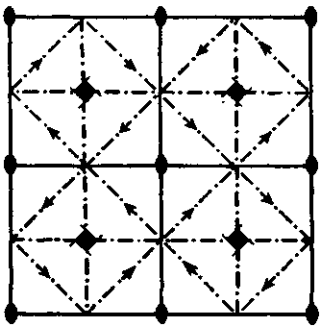




Origin on 4

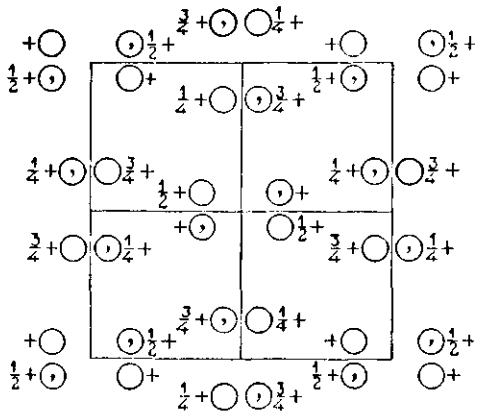
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
				General:
16	d	1	$x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}+y,z;\ \frac{1}{2}+x,\frac{1}{2}-y,z;$ $\bar{y},x,z;\ y,\bar{x},z;\ \frac{1}{2}+y,\frac{1}{2}+x,z;\ \frac{1}{2}-y,\frac{1}{2}-x,z.$	hkl: $h+k+l=2n$ $0kl$: $l,(k)=2n$ hhl: $(l=2n)$
				Special: as above, plus
8	c	m	$x,\frac{1}{2}+x,z;\ \bar{x},\frac{1}{2}-x,z;\ \frac{1}{2}+x,\bar{x},z;\ \frac{1}{2}-x,x,z.$	no extra conditions
4	b	mm	$\frac{1}{2},0,z;\ 0,\frac{1}{2},z.$	hkl: $l=2n$; $(h+k=2n)$
4	a	4	$0,0,z;\ \frac{1}{2},\frac{1}{2},z.$	

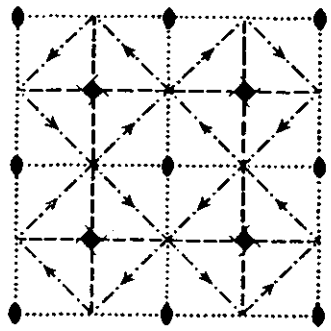




Origin on mm

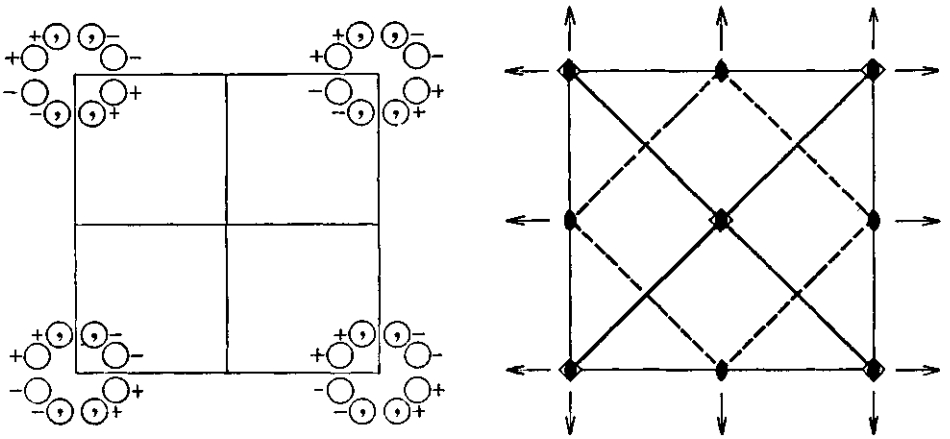
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+$	Conditions limiting possible reflections
				General:
16	c	1	$x,y,z;\ \bar{x},\bar{y},z;\ y,\tfrac{1}{2}+x,\tfrac{1}{4}+z;\ \bar{y},\tfrac{1}{2}-x,\tfrac{1}{4}+z;$ $\bar{x},y,z;\ x,\bar{y},z;\ \bar{y},\tfrac{1}{2}+x,\tfrac{1}{4}+z;\ y,\tfrac{1}{2}-x,\tfrac{1}{4}+z.$	hkl: $h+k+l=2n$ $0kl$: $(k+l=2n)$ hhl: $2h+l=4n$; $(l=2n)$
				Special: as above, plus
8	b	m	$0,y,z;\ 0,\bar{y},z;\ y,\tfrac{1}{2},\tfrac{1}{4}+z;\ \bar{y},\tfrac{1}{2},\tfrac{1}{4}+z.$	no extra conditions
4	a	mm	$0,0,z;\ 0,\tfrac{1}{2},\tfrac{1}{4}+z.$	hkl: $2k+l=2n+1$ or $4n$





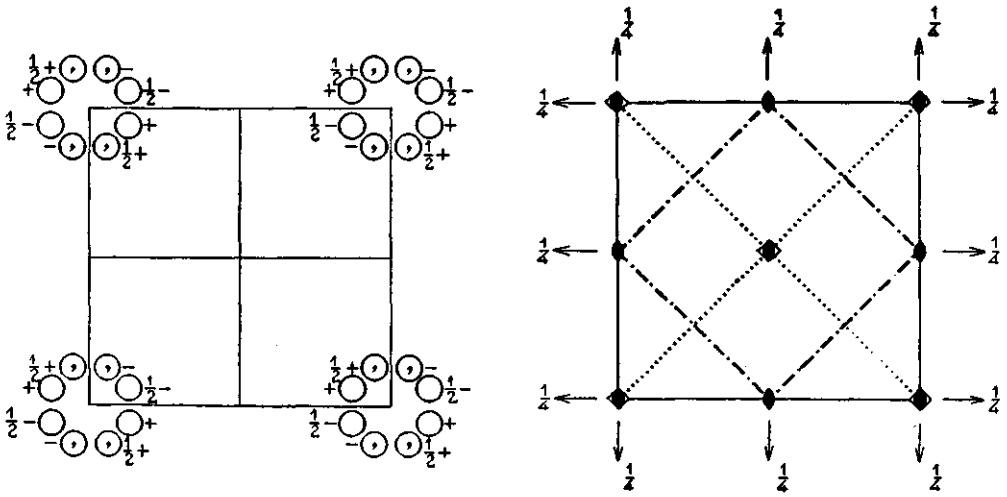
Origin on 2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+$	Conditions limiting possible reflections
				General:
16	b	1	$x,y,z;\ \bar{x},y,\tfrac{1}{2}+z;\ y,\tfrac{1}{2}-x,\tfrac{1}{4}+z;\ y,\tfrac{1}{2}+x,\tfrac{3}{4}+z;$ $\bar{x},\bar{y},z;\ x,\bar{y},\tfrac{1}{2}+z;\ \bar{y},\tfrac{1}{2}+x,\tfrac{1}{4}+z;\ \bar{y},\tfrac{1}{2}-x,\tfrac{3}{4}+z.$	hkl: $h+k+l=2n$ $0kl$: $l,(k)=2n$ hhl: $2h+l=4n$; $(l=2n)$
				Special: as above, plus
8	a	2	$0,0,z;\ \tfrac{1}{2},\tfrac{1}{2},z;\ 0,\tfrac{1}{2},\tfrac{1}{4}+z;\ \tfrac{1}{2},0,\tfrac{1}{4}+z.$	hkl: $l=2n$; $2k+l=4n$



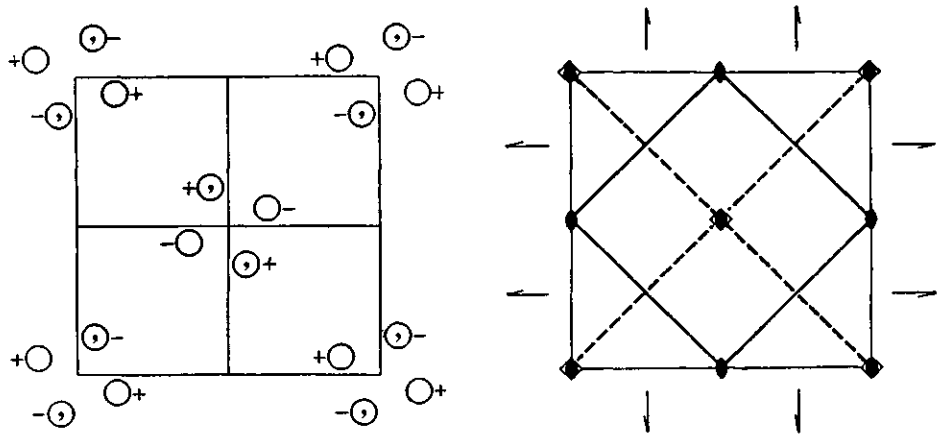
Origin at $\bar{4}2m$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	o	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\bar{z}$; $x,\bar{y},\bar{z}$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; y,x,z; $\bar{y},\bar{x},z$.	hkl: $0kl$: hhl: $h00$: $hh0$: No conditions
				Special: as above, plus
4	n	m	x,x,z; $\bar{x},\bar{x},z$; $\bar{x},x,\bar{z}$; $x,\bar{x},\bar{z}$.	no extra conditions
4	m	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,z$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},0,\bar{z}$.	hkl: $h+k=2n$
4	l	2	$x,\frac{1}{2},0$; $\bar{x},\frac{1}{2},0$; $\frac{1}{2},x,0$; $\frac{1}{2},\bar{x},0$.	no extra conditions
4	k	2	$x,0,\frac{1}{2}$; $\bar{x},0,\frac{1}{2}$; $0,x,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$.	
4	j	2	$x,\frac{1}{2},\frac{1}{2}$; $\bar{x},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},x,\frac{1}{2}$; $\frac{1}{2},\bar{x},\frac{1}{2}$.	
4	i	2	$x,0,0$; $\bar{x},0,0$; $0,x,0$; $0,\bar{x},0$.	
2	h	mm	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	
2	g	mm	$0,0,z$; $0,0,\bar{z}$.	
2	f	222	$\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$.	hkl: $h+k=2n$
2	e	222	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$.	
1	d	$\bar{4}2m$	$\frac{1}{2},\frac{1}{2},0$.	no extra conditions
1	c	$\bar{4}2m$	$0,0,\frac{1}{2}$.	
1	b	$\bar{4}2m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
1	a	$\bar{4}2m$	$0,0,0$.	



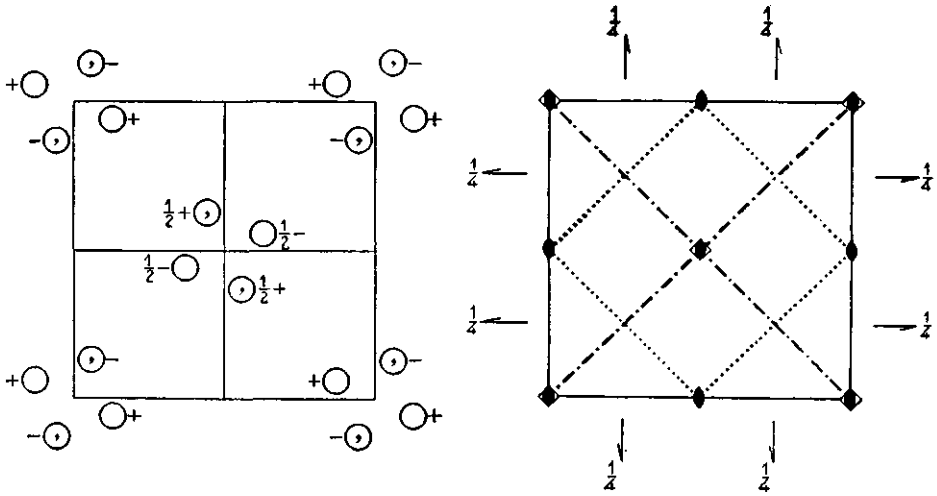
Origin at $\bar{4}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	n	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\frac{1}{2}-z$; $x,\bar{y},\frac{1}{2}-z$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; $y,x,\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}+z$.	hkl: No conditions $0kl$: No conditions hhl: $l=2n$ $h00$: No conditions $hh0$: No conditions
				Special: as above, plus
4	m	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$; $\frac{1}{2},0,\frac{1}{2}+z$; $0,\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
4	l	2	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $l=2n$
4	k	2	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	
4	j	2	$0,x,\frac{1}{4}$; $0,\bar{x},\frac{1}{4}$; $x,0,\frac{3}{4}$; $\bar{x},0,\frac{3}{4}$.	no extra conditions
4	i	2	$x,\frac{1}{2},\frac{1}{4}$; $\bar{x},\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},x,\frac{3}{4}$; $\frac{1}{2},\bar{x},\frac{3}{4}$.	
4	h	2	$\frac{1}{2},x,\frac{1}{4}$; $\frac{1}{2},\bar{x},\frac{1}{4}$; $x,\frac{1}{2},\frac{3}{4}$; $\bar{x},\frac{1}{2},\frac{3}{4}$.	
4	g	2	$x,0,\frac{1}{4}$; $\bar{x},0,\frac{1}{4}$; $0,x,\frac{3}{4}$; $0,\bar{x},\frac{3}{4}$.	
2	f	$\bar{4}$	$\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $l=2n$
2	e	$\bar{4}$	$0,0,0$; $0,0,\frac{1}{2}$.	
2	d	222	$0,\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},0,\frac{3}{4}$.	hkl: $h+k+l=2n$
2	c	222	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},\frac{3}{4}$.	hkl: $l=2n$
2	b	222	$\frac{1}{2},0,\frac{1}{4}$; $0,\frac{1}{2},\frac{3}{4}$.	hkl: $h+k+l=2n$
2	a	222	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	hkl: $l=2n$



Origin at $\bar{4}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	f	1	x,y,z; $\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\bar{y},x,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,z$; $y,\bar{x},\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}-x,z$.	hkl: No conditions $0kl$: No conditions hhl: No conditions $h00$: $h=2n$ $hh0$: No conditions
				Special: as above, plus
4	e	m	$x,\frac{1}{2}+x,z$; $\bar{x},\frac{1}{2}-x,z$; $\frac{1}{2}+x,\bar{x},\bar{z}$; $\frac{1}{2}-x,x,\bar{z}$.	no extra conditions
4	d	2	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	hkl: $h+k=2n$
2	c	mm	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$.	$hk0$: $h+k=2n$
2	b	$\bar{4}$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h+k=2n$
2	a	$\bar{4}$	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$.	

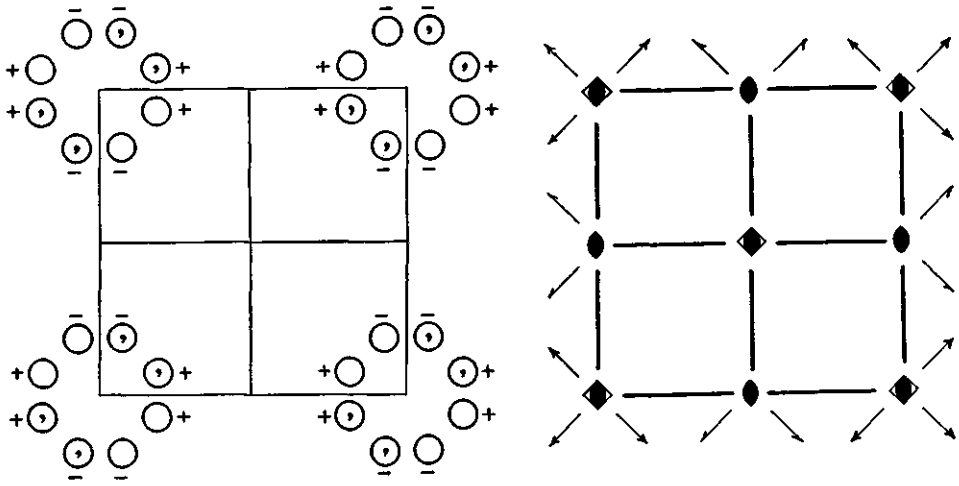


Origin at $\bar{4}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	e	1	x,y,z; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z$; $\bar{y},x,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $y,\bar{x},\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$.	hkl: No conditions $0kl$: No conditions hhl: $l=2n$ $h00$: $h=2n$ $hh0$: No conditions
				Special: as above, plus
4	d	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$; $0,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $l=2n$ $hk0$: $h+k=2n$
4	c	2	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
2	b	$\bar{4}$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	
2	a	$\bar{4}$	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	

Tetragonal $\bar{4}m2$ $P\bar{4}m2$ No. 115

$P\bar{4}m2$
D_{2d}^{5}

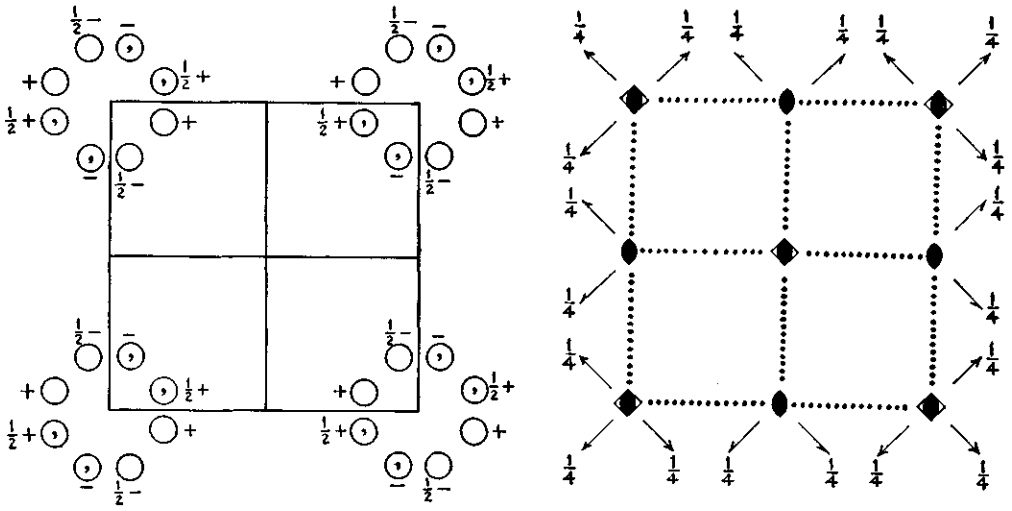


Origin at $\bar{4}m2$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	l	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,z$; $x,\bar{y},z$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; $y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$.	hkl: $0kl$: hhl: $h00$: $hh0$: No conditions
				Special: as above, plus
4	k	m	$x,\frac{1}{2},z$; $\bar{x},\frac{1}{2},z$; $\frac{1}{2},x,\bar{z}$; $\frac{1}{2},\bar{x},\bar{z}$.	no conditions
4	j	m	$x,0,z$; $\bar{x},0,z$; $0,x,\bar{z}$; $0,\bar{x},\bar{z}$.	
4	i	2	$x,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $x,\bar{x},\frac{1}{2}$; $\bar{x},x,\frac{1}{2}$.	
4	h	2	$x,x,0$; $\bar{x},\bar{x},0$; $x,\bar{x},0$; $\bar{x},x,0$.	
2	g	mm	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$.	$hk0$: $h+k=2n$
2	f	mm	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	no conditions
2	e	mm	$0,0,z$; $0,0,\bar{z}$.	
1	d	$\bar{4}2m$	$0,0,\frac{1}{2}$.	
1	c	$\bar{4}2m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
1	b	$\bar{4}2m$	$\frac{1}{2},\frac{1}{2},0$.	
1	a	$\bar{4}2m$	$0,0,0$.	

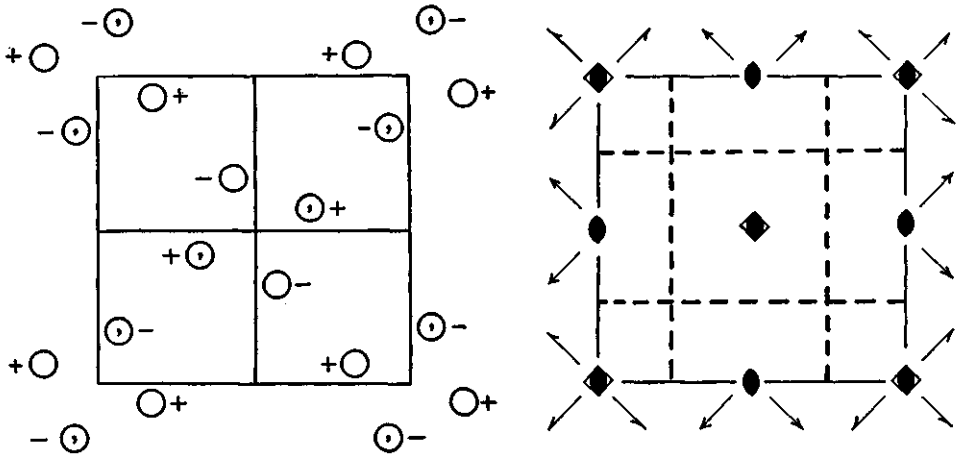
$P\bar{4}c2$ D_{2d}^{6}

No. 116 $P\bar{4}c2$ $\bar{4}m2$ Tetragonal



Origin at $\bar{4}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	j	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\frac{1}{2}+z$; $x,\bar{y},\frac{1}{2}+z$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; $y,x,\frac{1}{2}-z$; $\bar{y},\bar{x},\frac{1}{2}-z$.	hkl: No conditions $0kl$: $l=2n$ hhl: No conditions $h00$: No conditions $hh0$: No conditions
				Special: as above, plus
4	i	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$; $0,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $l=2n$ $hk0$: $h+k=2n$
4	h	2	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $l=2n$
4	g	2	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	
4	f	2	$x,x,\frac{3}{4}$; $\bar{x},\bar{x},\frac{3}{4}$; $x,\bar{x},\frac{1}{4}$; $\bar{x},x,\frac{1}{4}$.	no extra conditions
4	e	2	$x,x,\frac{1}{4}$; $\bar{x},\bar{x},\frac{1}{4}$; $x,\bar{x},\frac{3}{4}$; $\bar{x},x,\frac{3}{4}$.	
2	d	$\bar{4}$	$\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $l=2n$
2	c	$\bar{4}$	$0,0,0$; $0,0,\frac{1}{2}$.	
2	b	222	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},\frac{3}{4}$.	
2	a	222	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	

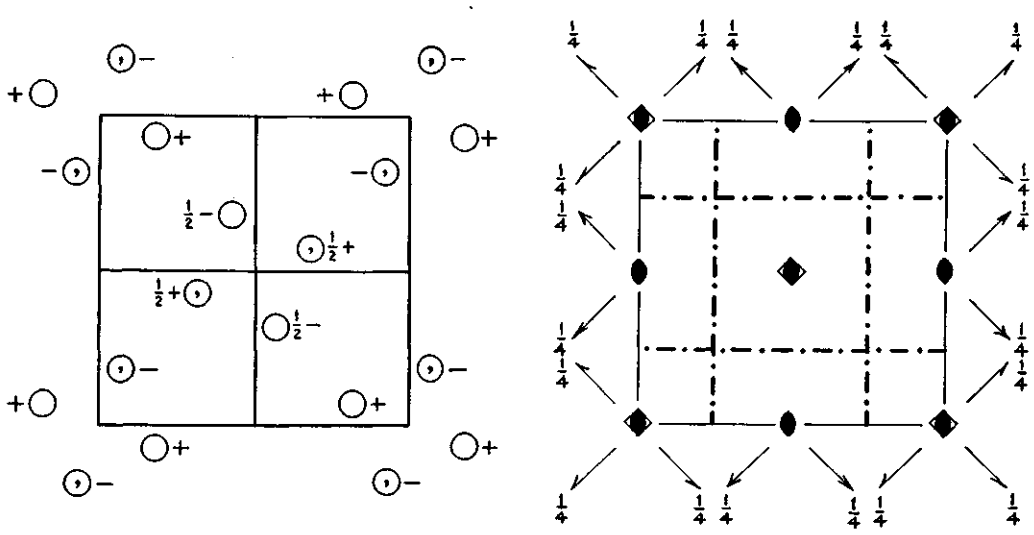


Origin at $\bar{4}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	i	1	x,y,z; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,z$; $\bar{y},x,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\bar{z}$; $y,\bar{x},\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}-x,\bar{z}$.	hkl: No conditions $0kl$: $k=2n$ hhl: No conditions $h00$: $(h=2n)$ $hh0$: No conditions
				Special: as above, plus
4	h	2	$x,\frac{1}{2}+x,\frac{1}{2}$; $\bar{x},\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2}+x,\bar{x},\frac{1}{2}$; $\frac{1}{2}-x,x,\frac{1}{2}$.	no extra conditions
4	g	2	$x,\frac{1}{2}+x,0$; $\bar{x},\frac{1}{2}-x,0$; $\frac{1}{2}+x,\bar{x},0$; $\frac{1}{2}-x,x,0$.	
4	f	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$.	hkl: $h+k=2n$
4	e	2	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	
2	d	222	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	
2	c	222	$0,\frac{1}{2},0$; $\frac{1}{2},0,0$.	
2	b	$\bar{4}$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
2	a	$\bar{4}$	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$.	

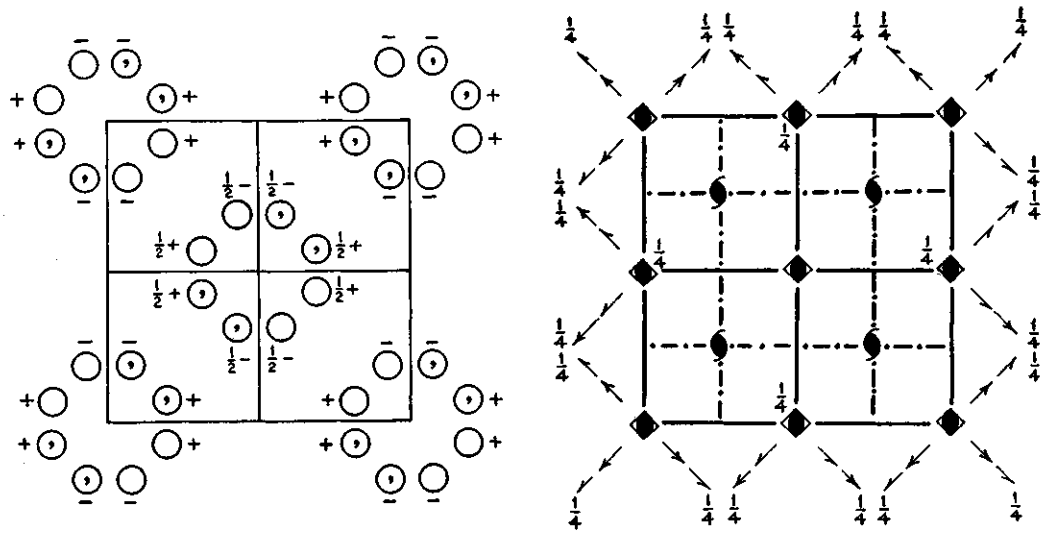
$P\bar{4}n2$ D_{2d}^{8}

No. 118 $P\bar{4}n2$ $\bar{4}m2$ Tetragonal



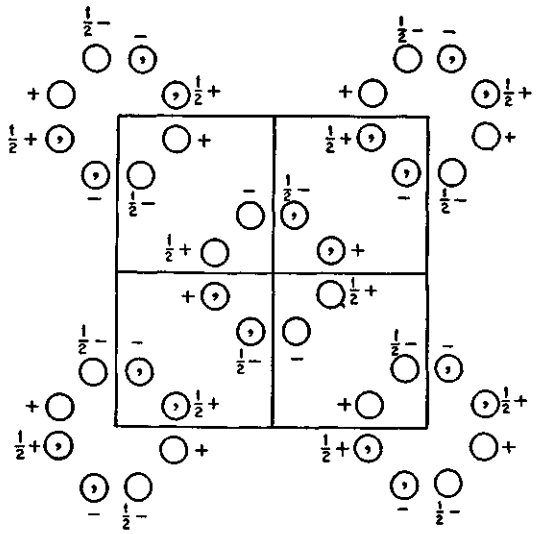
Origin at $\bar{4}$

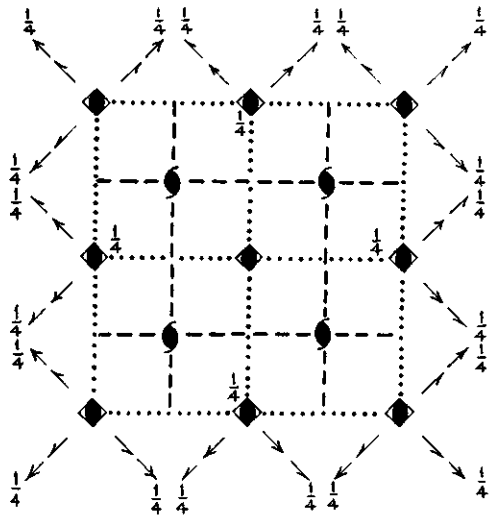
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	i	1	x,y,z; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$; $\bar{y},x,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}-z$; $y,\bar{x},\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$.	hkl: No conditions $0kl$: $k+l=2n$ hhl: No conditions $h00$: $(h=2n)$ $hh0$: No conditions
				Special: as above, plus
4	h	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$; $\frac{1}{2},0,\frac{1}{2}+z$; $0,\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
4	g	2	$x,\frac{1}{2}+x,\frac{1}{4}$; $\bar{x},\frac{1}{2}-x,\frac{1}{4}$; $\frac{1}{2}-x,x,\frac{3}{4}$; $\frac{1}{2}+x,\bar{x},\frac{3}{4}$.	no extra conditions
4	f	2	$x,\frac{1}{2}-x,\frac{1}{4}$; $\bar{x},\frac{1}{2}+x,\frac{1}{4}$; $\frac{1}{2}+x,x,\frac{3}{4}$; $\frac{1}{2}-x,\bar{x},\frac{3}{4}$.	
4	e	2	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
2	d	222	$0,\frac{1}{2},\frac{3}{4}$; $\frac{1}{2},0,\frac{1}{4}$.	
2	c	222	$0,\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},0,\frac{3}{4}$.	
2	b	$\bar{4}$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	
2	a	$\bar{4}$	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	



Origin at $\bar{4}m2$

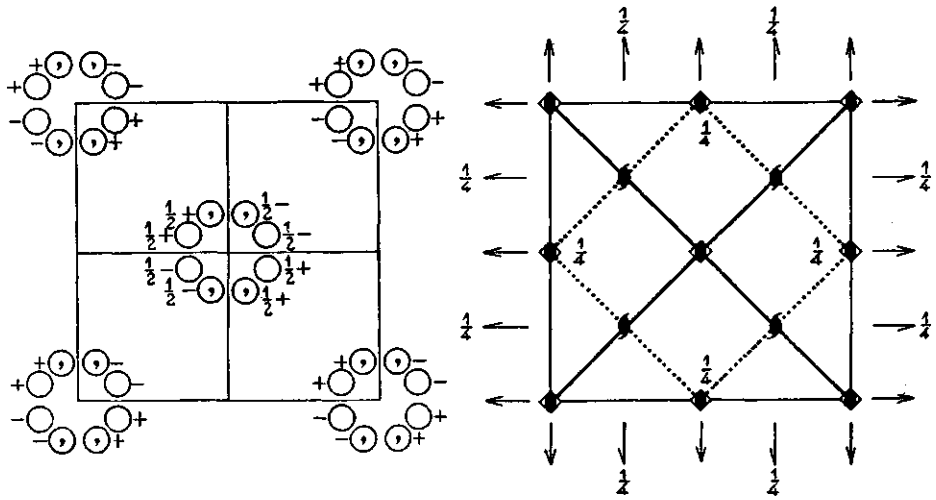
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
16	j	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z;$ $\bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ y,x,\bar{z};\ \bar{y},\bar{x},\bar{z}.$	General: hkl: $h+k+l=2n$ $0kl$: $(k+l=2n)$ hhl: $(l=2n)$ $h00$: $(h=2n)$ $hh0$: No conditions
				Special: as above only.
8	i	m	$x,0,z;\ \bar{x},0,z;\ 0,x,\bar{z};\ 0,\bar{x},\bar{z}.$	
8	h	2	$x,\frac{1}{2}+x,\frac{1}{4};\ \bar{x},\frac{1}{2}-x,\frac{1}{4};\ x,\frac{1}{2}-x,\frac{1}{4};\ \bar{x},\frac{1}{2}+x,\frac{1}{4}.$	
8	g	2	$x,x,0;\ \bar{x},\bar{x},0;\ x,\bar{x},0;\ \bar{x},x,0.$	
4	f	mm	$0,\frac{1}{2},z;\ \frac{1}{2},0,\bar{z}.$	
4	e	mm	$0,0,z;\ 0,0,\bar{z}.$	
2	d	$\bar{4}2m$	$0,\frac{1}{2},\frac{3}{4}.$	
2	c	$\bar{4}2m$	$0,\frac{1}{2},\frac{1}{4}.$	
2	b	$\bar{4}2m$	$0,0,\frac{1}{2}.$	
2	a	$\bar{4}2m$	$0,0,0.$	





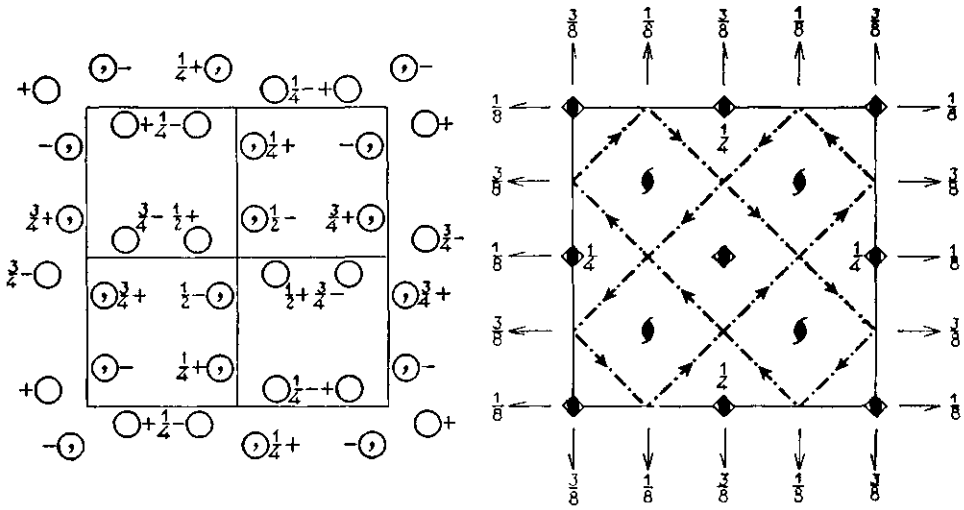
Origin at $\bar{4}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
16	i	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z;$ $\bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ y,x,\frac{1}{2}-z;\ \bar{y},\bar{x},\frac{1}{2}-z.$	hkl: $h+k+l=2n$ $0kl$: $l,(k)=2n$ hhl: $(l=2n)$ $h00$: $(h=2n)$ $hh0$: No conditions
				Special: as above, plus
8	h	2	$x,\frac{1}{2}+x,0;\ \bar{x},\frac{1}{2}-x,0;\ x,\frac{1}{2}-x,\frac{1}{2};\ \bar{x},\frac{1}{2}+x,\frac{1}{2}.$	no extra conditions
8	g	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\bar{z};\ 0,\frac{1}{2},\frac{1}{2}+z;\ 0,\frac{1}{2},\frac{1}{2}-z.$	hkl: $l=2n$; $(h+k=2n)$
8	f	2	$0,0,z;\ 0,0,\bar{z};\ 0,0,\frac{1}{2}+z;\ 0,0,\frac{1}{2}-z.$	
8	e	2	$x,x,\frac{1}{4};\ \bar{x},\bar{x},\frac{1}{4};\ x,\bar{x},\frac{3}{4};\ \bar{x},x,\frac{3}{4}.$	no extra conditions
4	d	222	$0,\frac{1}{2},0;\ 0,\frac{1}{2},\frac{1}{2}.$	hkl: $l=2n$; $(h+k=2n)$
4	c	$\bar{4}$	$0,\frac{1}{2},\frac{1}{4};\ 0,\frac{1}{2},\frac{3}{4}.$	
4	b	$\bar{4}$	$0,0,0;\ 0,0,\frac{1}{2}.$	
4	a	222	$0,0,\frac{1}{4};\ 0,0,\frac{3}{4}.$	



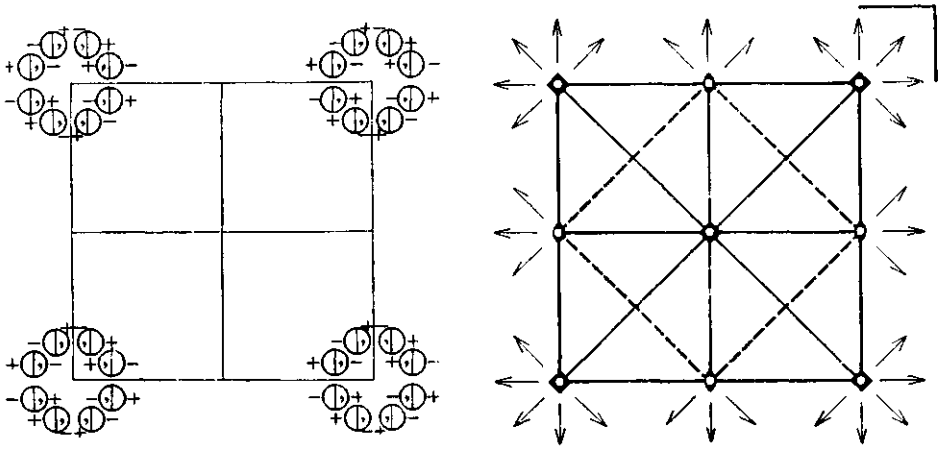
Origin at $\bar{4}2m$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
16	j	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\bar{z};\ x,\bar{y},\bar{z};$ $\bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ y,x,z;\ \bar{y},\bar{x},z.$	hkl: $h+k+l=2n$ $0kl$: $(k+l=2n)$ hhl: $(l=2n)$ $h00$: $(h=2n)$ $hh0$: No conditions
				Special: as above, plus
8	i	m	$x,x,z;\ \bar{x},\bar{x},z;\ x,\bar{x},\bar{z};\ \bar{x},x,\bar{z}.$	no extra conditions
8	h	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\bar{z};\ \frac{1}{2},0,z;\ \frac{1}{2},0,\bar{z}.$	hkl: $l=2n$; $(h+k=2n)$
8	g	2	$x,0,\frac{1}{2};\ \bar{x},0,\frac{1}{2};\ 0,x,\frac{1}{2};\ 0,\bar{x},\frac{1}{2}.$	no extra conditions
8	f	2	$x,0,0;\ \bar{x},0,0;\ 0,x,0;\ 0,\bar{x},0.$	
4	e	mm	$0,0,z;\ 0,0,\bar{z}.$	
4	d	$\bar{4}$	$0,\frac{1}{2},\frac{1}{4};\ \frac{1}{2},0,\frac{1}{4}.$	hkl: $l=2n$; $(h+k=2n)$
4	c	222	$0,\frac{1}{2},0;\ \frac{1}{2},0,0.$	
2	b	$\bar{4}2m$	$0,0,\frac{1}{2}.$	no extra conditions
2	a	$\bar{4}2m$	$0,0,0.$	



Origin at $\bar{4}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
16	e	1	$x,y,z;\ \bar{x},\frac{1}{2}+y,\frac{1}{4}-z;$ $\bar{x},\bar{y},z;\ x,\frac{1}{2}-y,\frac{1}{4}-z;$ $\bar{y},x,\bar{z};\ y,\frac{1}{2}+x,\frac{1}{4}+z;$ $y,\bar{x},\bar{z};\ \bar{y},\frac{1}{2}-x,\frac{1}{4}+z.$	hkl: $h+k+l=2n$ $0kl$: $(k+l=2n)$ hhl: $(l=2n)$; $2h+l=4n$ $h00$: $(h=2n)$ $hh0$: $(h=2n)$
				Special: as above, plus
8	d	2	$x,\frac{1}{4},\frac{1}{8};\ \bar{x},\frac{3}{4},\frac{1}{8};\ \frac{3}{4},x,\frac{7}{8};\ \frac{1}{4},\bar{x},\frac{7}{8}.$	no extra conditions
8	c	2	$0,0,z;\ 0,0,\bar{z};\ 0,\frac{1}{2},\frac{1}{4}+z;\ 0,\frac{1}{2},\frac{1}{4}-z.$	hkl: $2k+l=2n+1$ or $4n$
4	b	$\bar{4}$	$0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{3}{4}.$	
4	a	$\bar{4}$	$0,0,0;\ 0,\frac{1}{2},\frac{1}{4}$	



Origin at centre ($4/mmm$)

Number of positions,	Wyckoff notation,	and point symmetry	Co-ordinates of equivalent positions				Conditions limiting possible reflections
							General:
16	u	1	x,y,z;	$\bar{x},\bar{y},z$;	$x,y,\bar{z}$;	$\bar{x},\bar{y},\bar{z}$;	No conditions
			$\bar{x},y,z$;	$x,\bar{y},z$;	$\bar{x},y,\bar{z}$;	$x,\bar{y},\bar{z}$;	
			$\bar{y},x,z$;	$y,\bar{x},z$;	$\bar{y},x,\bar{z}$;	$y,\bar{x},\bar{z}$;	
			y,x,z;	$\bar{y},\bar{x},z$;	$y,x,\bar{z}$;	$\bar{y},\bar{x},\bar{z}$.	
							Special:
8	t	m	$x,\frac{1}{2},z$;	$\bar{x},\frac{1}{2},z$;	$x,\frac{1}{2},\bar{z}$;	$\bar{x},\frac{1}{2},\bar{z}$;	No conditions
			$\frac{1}{2},x,z$;	$\frac{1}{2},\bar{x},z$;	$\frac{1}{2},x,\bar{z}$;	$\frac{1}{2},\bar{x},\bar{z}$.	
8	s	m	$x,0,z$;	$\bar{x},0,z$;	$x,0,\bar{z}$;	$\bar{x},0,\bar{z}$;	
			$0,x,z$;	$0,\bar{x},z$;	$0,x,\bar{z}$;	$0,\bar{x},\bar{z}$.	
8	r	m	x,x,z;	$\bar{x},\bar{x},z$;	$x,x,\bar{z}$;	$\bar{x},\bar{x},\bar{z}$;	
			$\bar{x},x,z$;	$x,\bar{x},z$;	$\bar{x},x,\bar{z}$;	$x,\bar{x},\bar{z}$.	
8	q	m	$x,y,\frac{1}{2}$;	$\bar{x},\bar{y},\frac{1}{2}$;	$\bar{x},y,\frac{1}{2}$;	$x,\bar{y},\frac{1}{2}$;	
			$\bar{y},x,\frac{1}{2}$;	$y,\bar{x},\frac{1}{2}$;	$y,x,\frac{1}{2}$;	$\bar{y},\bar{x},\frac{1}{2}$.	
8	p	m	$x,y,0$;	$\bar{x},\bar{y},0$;	$\bar{x},y,0$;	$x,\bar{y},0$;	
			$\bar{y},x,0$;	$y,\bar{x},0$;	$y,x,0$;	$\bar{y},\bar{x},0$.	
4	o	mm	$x,\frac{1}{2},\frac{1}{2}$;	$\bar{x},\frac{1}{2},\frac{1}{2}$;	$\frac{1}{2},x,\frac{1}{2}$;	$\frac{1}{2},\bar{x},\frac{1}{2}$.	
4	n	mm	$x,\frac{1}{2},0$;	$\bar{x},\frac{1}{2},0$;	$\frac{1}{2},x,0$;	$\frac{1}{2},\bar{x},0$.	
4	m	mm	$x,0,\frac{1}{2}$;	$\bar{x},0,\frac{1}{2}$;	$0,x,\frac{1}{2}$;	$0,\bar{x},\frac{1}{2}$.	
4	l	mm	$x,0,0$;	$\bar{x},0,0$;	$0,x,0$;	$0,\bar{x},0$.	
4	k	mm	$x,x,\frac{1}{2}$;	$\bar{x},\bar{x},\frac{1}{2}$;	$x,\bar{x},\frac{1}{2}$;	$\bar{x},x,\frac{1}{2}$.	
4	j	mm	$x,x,0$;	$\bar{x},\bar{x},0$;	$x,\bar{x},0$;	$\bar{x},x,0$.	

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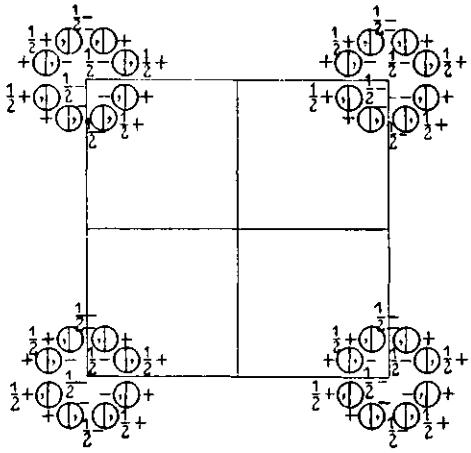
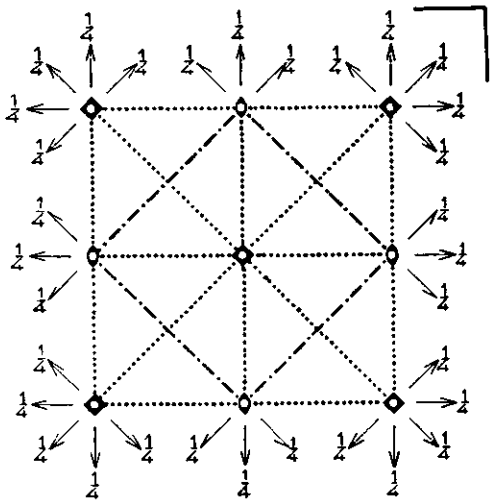
4	i mm	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$.		hkl: $h+k=2n$
2	h $4mm$	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.		No conditions
2	g $4mm$	$0,0,z$; $0,0,\bar{z}$.		
2	f mmm	$0,\frac{1}{2},0$; $\frac{1}{2},0,0$.		hkl: $h+k=2n$
2	e mmm	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.		
1	d $4/mmm$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.		No conditions
1	c $4/mmm$	$\frac{1}{2},\frac{1}{2},0$.		
1	b $4/mmm$	$0,0,\frac{1}{2}$.		
1	a $4/mmm$	$0,0,0$.		



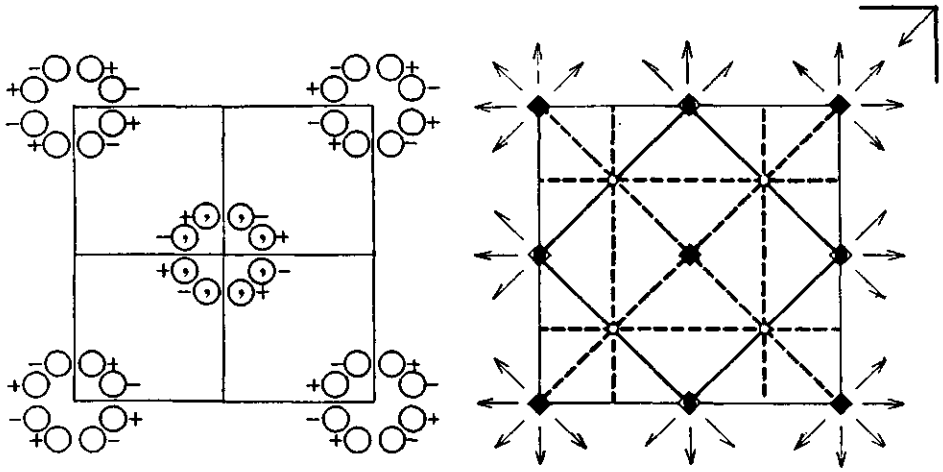


Origin at centre ($4/m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions				Conditions limiting possible reflections
							General:
16	n	1	x,y,z;	$\bar{x},\bar{y},z$;	$x,y,\bar{z}$;	$\bar{x},\bar{y},\bar{z}$;	hkl: No conditions
			$\bar{y},x,z$;	$y,\bar{x},z$;	$\bar{y},x,\bar{z}$;	$y,\bar{x},\bar{z}$;	$hk0$: No conditions
			$\bar{x},y,\frac{1}{2}+z$;	$x,\bar{y},\frac{1}{2}+z$;	$\bar{x},y,\frac{1}{2}-z$;	$x,\bar{y},\frac{1}{2}-z$;	$0kl$: $l=2n$
			$y,x,\frac{1}{2}+z$;	$\bar{y},\bar{x},\frac{1}{2}+z$;	$\bar{y},\bar{x},\frac{1}{2}-z$;	$y,x,\frac{1}{2}-z$.	hhl: $l=2n$
							Special: as above, plus
8	m	m	$x,y,0$;	$\bar{x},\bar{y},0$;	$\bar{y},x,0$;	$y,\bar{x},0$;	no extra conditions
			$\bar{x},y,\frac{1}{2}$;	$x,\bar{y},\frac{1}{2}$;	$y,x,\frac{1}{2}$;	$\bar{y},\bar{x},\frac{1}{2}$.	
8	l	2	$x,\frac{1}{2},\frac{1}{4}$;	$\bar{x},\frac{1}{2},\frac{1}{4}$;	$\frac{1}{2},x,\frac{1}{4}$;	$\frac{1}{2},\bar{x},\frac{1}{4}$;	hkl: $l=2n$
			$x,\frac{1}{2},\frac{3}{4}$;	$\bar{x},\frac{1}{2},\frac{3}{4}$;	$\frac{1}{2},x,\frac{3}{4}$;	$\frac{1}{2},\bar{x},\frac{3}{4}$.	
8	k	2	$x,0,\frac{1}{4}$;	$\bar{x},0,\frac{1}{4}$;	$0,x,\frac{1}{4}$;	$0,\bar{x},\frac{1}{4}$;	
			$x,0,\frac{3}{4}$;	$\bar{x},0,\frac{3}{4}$;	$0,x,\frac{3}{4}$;	$0,\bar{x},\frac{3}{4}$.	
8	j	2	$x,x,\frac{1}{4}$;	$\bar{x},\bar{x},\frac{1}{4}$;	$\bar{x},x,\frac{1}{4}$;	$x,\bar{x},\frac{1}{4}$;	
			$x,x,\frac{3}{4}$;	$\bar{x},\bar{x},\frac{3}{4}$;	$\bar{x},x,\frac{3}{4}$;	$x,\bar{x},\frac{3}{4}$.	
8	i	2	$0,\frac{1}{2},z$;	$0,\frac{1}{2},\bar{z}$;	$0,\frac{1}{2},\frac{1}{2}+z$;	$0,\frac{1}{2},\frac{1}{2}-z$;	hkl: $h+k=2n$; $l=2n$
			$\frac{1}{2},0,z$;	$\frac{1}{2},0,\bar{z}$;	$\frac{1}{2},0,\frac{1}{2}+z$;	$\frac{1}{2},0,\frac{1}{2}-z$.	
4	h	4	$\frac{1}{2},\frac{1}{2},z$;	$\frac{1}{2},\frac{1}{2},\bar{z}$;	$\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$;	$\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $l=2n$
4	g	4	$0,0,z$;	$0,0,\bar{z}$;	$0,0,\frac{1}{2}+z$;	$0,0,\frac{1}{2}-z$.	
4	f	222	$0,\frac{1}{2},\frac{1}{4}$;	$\frac{1}{2},0,\frac{1}{4}$;	$0,\frac{1}{2},\frac{3}{4}$;	$\frac{1}{2},0,\frac{3}{4}$.	hkl: $h+k=2n$; $l=2n$
4	e	$2/m$	$0,\frac{1}{2},0$;	$\frac{1}{2},0,0$;	$0,\frac{1}{2},\frac{1}{2}$;	$\frac{1}{2},0,\frac{1}{2}$.	

(*continued on next page*)

2	*d*	4/*m*	$\frac{1}{2},\frac{1}{2},0$;	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
2	*c*	42	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$;	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$.	*hkl*: $l=2n$
2	*b*	4/*m*	0,0,0;	$0,0,\frac{1}{2}$.	
2	*a*	42	$0,0,\frac{1}{4}$;	$0,0,\frac{3}{4}$.	



Origin at 422, at $\bar{\frac{1}{4}},\bar{\frac{1}{4}},0$ from centre ($2/m$) (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	n	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}-y,\bar{z}$; $\bar{x},y,\bar{z}$; $x,\bar{y},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-y,z$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $\bar{y},x,z$; $y,\bar{x},z$; $\frac{1}{2}-y,\frac{1}{2}+x,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}-x,\bar{z}$; $y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,z$; $\frac{1}{2}-y,\frac{1}{2}-x,z$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: $k=2n$ hhl: No conditions
				Special: as above, plus
8	m	m	$x,\frac{1}{2}+x,z$; $\bar{x},\frac{1}{2}-x,z$; $\frac{1}{2}+x,x,\bar{z}$; $\frac{1}{2}-x,\bar{x},\bar{z}$; $x,\frac{1}{2}-x,\bar{z}$; $\bar{x},\frac{1}{2}+x,\bar{z}$; $\frac{1}{2}+x,\bar{x},z$; $\frac{1}{2}-x,x,z$.	no extra conditions
8	l	2	$x,0,\frac{1}{2}$; $\bar{x},0,\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2},\frac{1}{2}$; $0,x,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}-x,\frac{1}{2}$.	
8	k	2	$x,0,0$; $\bar{x},0,0$; $\frac{1}{2}+x,\frac{1}{2},0$; $\frac{1}{2}-x,\frac{1}{2},0$; $0,x,0$; $0,\bar{x},0$; $\frac{1}{2},\frac{1}{2}+x,0$; $\frac{1}{2},\frac{1}{2}-x,0$.	
8	j	2	$x,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}$; $x,\bar{x},\frac{1}{2}$; $\bar{x},x,\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}$.	hkl: $h+k=2n$
8	i	2	$x,x,0$; $\bar{x},\bar{x},0$; $\frac{1}{2}+x,\frac{1}{2}+x,0$; $\frac{1}{2}-x,\frac{1}{2}-x,0$; $x,\bar{x},0$; $\bar{x},x,0$; $\frac{1}{2}+x,\frac{1}{2}-x,0$; $\frac{1}{2}-x,\frac{1}{2}+x,0$.	
4	h	mm	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$.	
4	g	4	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	
4	f	$2/m$	$\bar{\frac{1}{4}},\bar{\frac{1}{4}},\frac{1}{2}$; $\bar{\frac{3}{4}},\bar{\frac{3}{4}},\frac{1}{2}$; $\bar{\frac{1}{4}},\bar{\frac{3}{4}},\frac{1}{2}$; $\bar{\frac{3}{4}},\bar{\frac{1}{4}},\frac{1}{2}$.	hkl: $h,k=2n$
4	e	$2/m$	$\bar{\frac{1}{4}},\bar{\frac{1}{4}},0$; $\bar{\frac{3}{4}},\bar{\frac{3}{4}},0$; $\bar{\frac{1}{4}},\bar{\frac{3}{4}},0$; $\bar{\frac{3}{4}},\bar{\frac{1}{4}},0$.	

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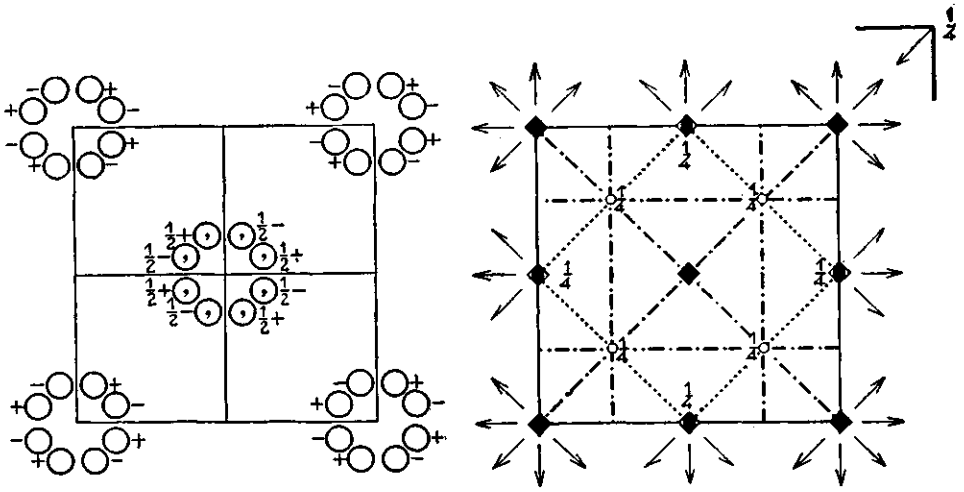
2	d	$\bar{4}2m$	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	2	b	42	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.			(*a*) to (*d*) inclusive
2	c	$\bar{4}2m$	$0,\frac{1}{2},0$; $\frac{1}{2},0,0$.	2	a	42	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$.			hkl: $h+k=2n$

Origin at centre ($2/m$), at $\frac{1}{4},\frac{1}{4},0$ from 422 (compare previous page for alternative origin)

										General:
16	n	1	x,y,z; $\bar{x},\frac{1}{2}+y,z$; $\frac{1}{2}+x,\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}-y,z$; $\bar{x},\bar{y},\bar{z}$; $x,\frac{1}{2}-y,\bar{z}$; $\frac{1}{2}-x,y,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $y,x,\bar{z}$; $\bar{y},\frac{1}{2}+x,\bar{z}$; $\frac{1}{2}+y,\bar{x},\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}-x,\bar{z}$; $\bar{y},\bar{x},z$; $y,\frac{1}{2}-x,z$; $\frac{1}{2}-y,x,z$; $\frac{1}{2}+y,\frac{1}{2}+x,z$.								hkl: No conditions $hk0$: $h+k=2n$ $0kl$: $k=2n$ hhl: No conditions
										Special: as above, plus
8	m	m	$\bar{x},x,z$; $\frac{1}{2}+x,\frac{1}{2}-x,z$; $x,\frac{1}{2}+x,z$; $\frac{1}{2}-x,\bar{x},z$; $x,\bar{x},\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+x,\bar{z}$; $\bar{x},\frac{1}{2}-x,\bar{z}$; $\frac{1}{2}+x,x,\bar{z}$.							no extra conditions
8	l	2	$x,\frac{1}{4},\frac{1}{2}$; $\frac{1}{4},x,\frac{1}{2}$; $\frac{1}{2}+x,\frac{3}{4},\frac{1}{2}$; $\frac{3}{4},\frac{1}{2}+x,\frac{1}{2}$; $\bar{x},\frac{3}{4},\frac{1}{2}$; $\frac{3}{4},\bar{x},\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{4},\frac{1}{2}$; $\frac{1}{4},\frac{1}{2}-x,\frac{1}{2}$.								
8	k	2	$x,\frac{1}{4},0$; $\frac{1}{4},x,0$; $\frac{1}{2}+x,\frac{3}{4},0$; $\frac{3}{4},\frac{1}{2}+x,0$; $\bar{x},\frac{3}{4},0$; $\frac{3}{4},\bar{x},0$; $\frac{1}{2}-x,\frac{1}{4},0$; $\frac{1}{4},\frac{1}{2}-x,0$.								
8	j	2	$x,x,\frac{1}{2}$; $x,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2}-x,x,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $\bar{x},\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}+x,\bar{x},\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}$.								hkl: $h+k=2n$
8	i	2	$x,x,0$; $x,\frac{1}{2}-x,0$; $\frac{1}{2}-x,x,0$; $\frac{1}{2}-x,\frac{1}{2}-x,0$; $\bar{x},\bar{x},0$; $\bar{x},\frac{1}{2}+x,0$; $\frac{1}{2}+x,\bar{x},0$; $\frac{1}{2}+x,\frac{1}{2}+x,0$.								
4	h	mm	$\frac{3}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{1}{4},\bar{z}$; $\frac{1}{4},\frac{3}{4},z$; $\frac{1}{4},\frac{3}{4},\bar{z}$.							
4	g	4	$\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},\bar{z}$; $\frac{3}{4},\frac{3}{4},z$; $\frac{3}{4},\frac{3}{4},\bar{z}$.							
4	f	$2/m$	$0,0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.							hkl: $h,k=2n$
4	e	$2/m$	$0,0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},0,0$; $\frac{1}{2},\frac{1}{2},0$.							
2	d	$\bar{4}2m$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}$.	2	b	42	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}$.			(*a*) to (*d*) inclusive
2	c	$\bar{4}2m$	$\frac{3}{4},\frac{1}{4},0$; $\frac{1}{4},\frac{3}{4},0$.	2	a	42	$\frac{1}{4},\frac{1}{4},0$; $\frac{3}{4},\frac{3}{4},0$.			hkl: $h+k=2n$



Origin at 422, at $\bar{\tfrac{1}{4}},\bar{\tfrac{1}{4}},\bar{\tfrac{1}{4}}$ from $\bar{1}$ (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	k	1	x,y,z; $\bar{x},\bar{y},z$; $\tfrac{1}{2}+x,\tfrac{1}{2}+y,\tfrac{1}{2}-z$; $\tfrac{1}{2}-x,\tfrac{1}{2}-y,\tfrac{1}{2}-z$; $\bar{x},y,\bar{z}$; $x,\bar{y},\bar{z}$; $\tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{2}+z$; $\tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{1}{2}+z$; $\bar{y},x,z$; $y,\bar{x},z$; $\tfrac{1}{2}-y,\tfrac{1}{2}+x,\tfrac{1}{2}-z$; $\tfrac{1}{2}+y,\tfrac{1}{2}-x,\tfrac{1}{2}-z$; $y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $\tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}+z$; $\tfrac{1}{2}-y,\tfrac{1}{2}-x,\tfrac{1}{2}+z$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$
				Special: as above, plus
8	j	2	$x,0,\tfrac{1}{2}$; $\bar{x},0,\tfrac{1}{2}$; $\tfrac{1}{2}+x,\tfrac{1}{2},0$; $\tfrac{1}{2}-x,\tfrac{1}{2},0$; $0,x,\tfrac{1}{2}$; $0,\bar{x},\tfrac{1}{2}$; $\tfrac{1}{2},\tfrac{1}{2}+x,0$; $\tfrac{1}{2},\tfrac{1}{2}-x,0$.	
8	i	2	$x,0,0$; $\bar{x},0,0$; $\tfrac{1}{2}+x,\tfrac{1}{2},\tfrac{1}{2}$; $\tfrac{1}{2}-x,\tfrac{1}{2},\tfrac{1}{2}$; $0,x,0$; $0,\bar{x},0$; $\tfrac{1}{2},\tfrac{1}{2}+x,\tfrac{1}{2}$; $\tfrac{1}{2},\tfrac{1}{2}-x,\tfrac{1}{2}$.	hkl: $h+k+l=2n$
8	h	2	$x,x,0$; $\bar{x},\bar{x},0$; $\tfrac{1}{2}+x,\tfrac{1}{2}+x,\tfrac{1}{2}$; $\tfrac{1}{2}-x,\tfrac{1}{2}-x,\tfrac{1}{2}$; $\bar{x},x,0$; $x,\bar{x},0$; $\tfrac{1}{2}-x,\tfrac{1}{2}+x,\tfrac{1}{2}$; $\tfrac{1}{2}+x,\tfrac{1}{2}-x,\tfrac{1}{2}$.	
8	g	2	$\tfrac{1}{2},0,z$; $\tfrac{1}{2},0,\bar{z}$; $\tfrac{1}{2},0,\tfrac{1}{2}+z$; $\tfrac{1}{2},0,\tfrac{1}{2}-z$; $0,\tfrac{1}{2},z$; $0,\tfrac{1}{2},\bar{z}$; $0,\tfrac{1}{2},\tfrac{1}{2}+z$; $0,\tfrac{1}{2},\tfrac{1}{2}-z$.	hkl: $h+k=2n$; $l=2n$
8	f	$\bar{1}$	$\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$; $\tfrac{3}{4},\tfrac{3}{4},\tfrac{1}{4}$; $\tfrac{1}{4},\tfrac{3}{4},\tfrac{1}{4}$; $\tfrac{3}{4},\tfrac{1}{4},\tfrac{1}{4}$; $\tfrac{1}{4},\tfrac{1}{4},\tfrac{3}{4}$; $\tfrac{3}{4},\tfrac{3}{4},\tfrac{3}{4}$; $\tfrac{1}{4},\tfrac{3}{4},\tfrac{3}{4}$; $\tfrac{3}{4},\tfrac{1}{4},\tfrac{3}{4}$.	hkl: $h,k,l=2n$
4	e	4	$0,0,z$; $0,0,\bar{z}$; $\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}+z$; $\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}-z$.	hkl: $h+k+l=2n$
4	d	$\bar{4}$	$\tfrac{1}{2},0,\tfrac{1}{4}$; $0,\tfrac{1}{2},\tfrac{1}{4}$; $\tfrac{1}{2},0,\tfrac{3}{4}$; $0,\tfrac{1}{2},\tfrac{3}{4}$.	hkl: $h+k=2n$; $l=2n$
4	c	222	$\tfrac{1}{2},0,0$; $0,\tfrac{1}{2},0$; $\tfrac{1}{2},0,\tfrac{1}{2}$; $0,\tfrac{1}{2},\tfrac{1}{2}$.	
2	b	42	$0,0,\tfrac{1}{2}$; $\tfrac{1}{2},\tfrac{1}{2},0$.	hkl: $h+k+l=2n$
2	a	42	$0,0,0$; $\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}$.	

$P4/nnc$ D_{4h}^{4}

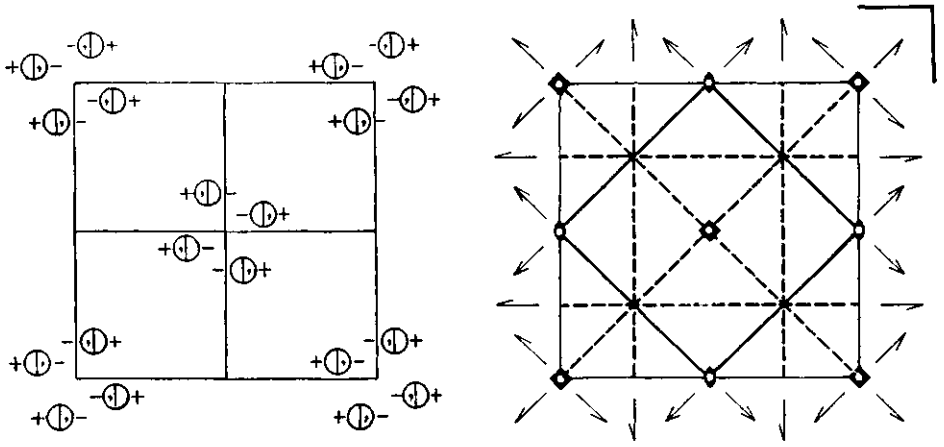
No. 126 $P\,4/n\,2/n\,2/c$ $4/m\,m\,m$ Tetragonal

Origin at $\bar{1}$, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 422 (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	k	1	x,y,z; $\frac{1}{2}-x,\frac{1}{2}-y,z$; $x,\frac{1}{2}-y,\frac{1}{2}-z$; $\frac{1}{2}-x,y,\frac{1}{2}-z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}+z$; $\frac{1}{2}+x,\bar{y},\frac{1}{2}+z$; $y,x,\frac{1}{2}-z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$; $y,\frac{1}{2}-x,z$; $\frac{1}{2}-y,x,z$; $\bar{y},\bar{x},\frac{1}{2}+z$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $\bar{y},\frac{1}{2}+x,\bar{z}$; $\frac{1}{2}+y,\bar{x},\bar{z}$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$
				Special: as above, plus
8	j	2	$x,\frac{3}{4},\frac{1}{4}$; $\frac{1}{2}-x,\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},x,\frac{1}{4}$; $\frac{3}{4},\frac{1}{2}-x,\frac{1}{4}$; $\bar{x},\frac{1}{4},\frac{3}{4}$; $\frac{1}{2}+x,\frac{1}{4},\frac{3}{4}$; $\frac{1}{4},\bar{x},\frac{3}{4}$; $\frac{1}{4},\frac{1}{2}+x,\frac{3}{4}$.	
8	i	2	$x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},x,\frac{1}{4}$; $\frac{1}{4},\frac{1}{2}-x,\frac{1}{4}$; $\bar{x},\frac{3}{4},\frac{3}{4}$; $\frac{1}{2}+x,\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\bar{x},\frac{3}{4}$; $\frac{3}{4},\frac{1}{2}+x,\frac{3}{4}$.	hkl: $h+k+l=2n$
8	h	2	$x,x,\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{4}$; $x,\frac{1}{2}-x,\frac{1}{4}$; $\frac{1}{2}-x,x,\frac{1}{4}$; $\bar{x},\bar{x},\frac{3}{4}$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{3}{4}$; $\bar{x},\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{2}+x,\bar{x},\frac{3}{4}$.	
8	g	2	$\frac{1}{4},\frac{3}{4},z$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}-z$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}-z$; $\frac{3}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{1}{4},\bar{z}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}+z$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}+z$; $\frac{1}{4},\frac{3}{4},\bar{z}$.	hkl: $h+k=2n$; $l=2n$
8	f	$\bar{1}$	$0,0,0$; $0,0,\frac{1}{2}$; $0,\frac{1}{2},0$; $\frac{1}{2},0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$.	hkl: $h,k,l=2n$
4	e	4	$\frac{1}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{3}{4},\bar{z}$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}-z$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}+z$.	hkl: $h+k+l=2n$
4	d	$\bar{4}$	$\frac{1}{4},\frac{3}{4},0$; $\frac{3}{4},\frac{1}{4},0$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}$.	hkl: $h+k=2n$; $l=2n$
4	c	222	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$.	
2	b	42	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$.	hkl: $h+k+l=2n$
2	a	42	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$.	

Tetragonal $4/m\,m\,m$ $P\,4/m\,2_1/b\,2/m$ No. 127

$P4/mbm$ D_{4h}^5

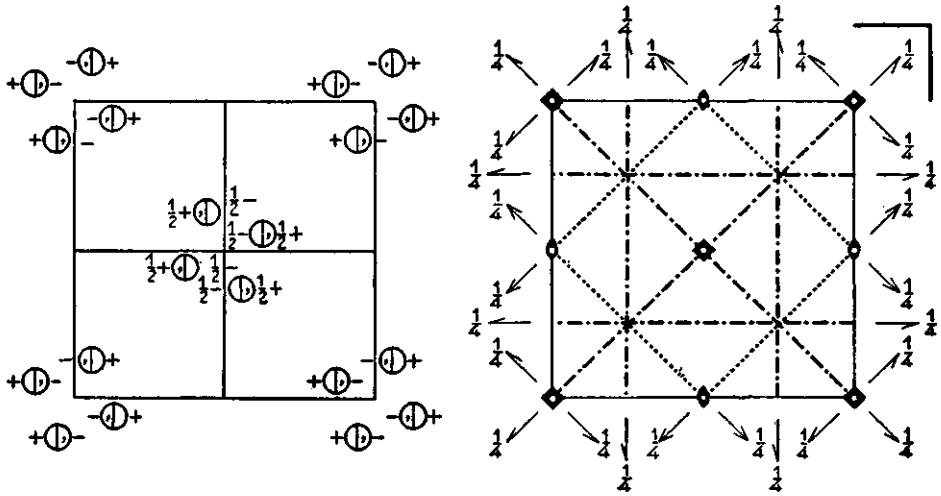


Origin at centre ($4/m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	l	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,z$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $x,y,\bar{z}$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$; $\bar{y},x,z$; $y,\bar{x},z$; $\frac{1}{2}+y,\frac{1}{2}+x,z$; $\frac{1}{2}-y,\frac{1}{2}-x,z$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}-x,\bar{z}$.	hkl: No conditions $hk0$: No conditions $0kl$: $k=2n$ hhl: No conditions
				Special: as above, plus
8	k	m	$x,\frac{1}{2}+x,z$; $\bar{x},\frac{1}{2}-x,z$; $\frac{1}{2}+x,\bar{x},z$; $\frac{1}{2}-x,x,z$; $x,\frac{1}{2}+x,\bar{z}$; $\bar{x},\frac{1}{2}-x,\bar{z}$; $\frac{1}{2}+x,\bar{x},\bar{z}$; $\frac{1}{2}-x,x,\bar{z}$.	no extra conditions
8	j	m	$x,y,\frac{1}{2}$; $\bar{x},\bar{y},\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}$; $\bar{y},x,\frac{1}{2}$; $y,\bar{x},\frac{1}{2}$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}$.	
8	i	m	$x,y,0$; $\bar{x},\bar{y},0$; $\frac{1}{2}+x,\frac{1}{2}-y,0$; $\frac{1}{2}-x,\frac{1}{2}+y,0$; $\bar{y},x,0$; $y,\bar{x},0$; $\frac{1}{2}+y,\frac{1}{2}+x,0$; $\frac{1}{2}-y,\frac{1}{2}-x,0$.	
4	h	mm	$x,\frac{1}{2}+x,\frac{1}{2}$; $\bar{x},\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2}+x,\bar{x},\frac{1}{2}$; $\frac{1}{2}-x,x,\frac{1}{2}$.	
4	g	mm	$x,\frac{1}{2}+x,0$; $\bar{x},\frac{1}{2}-x,0$; $\frac{1}{2}+x,\bar{x},0$; $\frac{1}{2}-x,x,0$.	
4	f	mm	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$.	hkl: $h+k=2n$
4	e	4	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	
2	d	mmm	$0,\frac{1}{2},0$; $\frac{1}{2},0,0$.	
2	c	mmm	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	
2	b	$4/m$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
2	a	$4/m$	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$.	

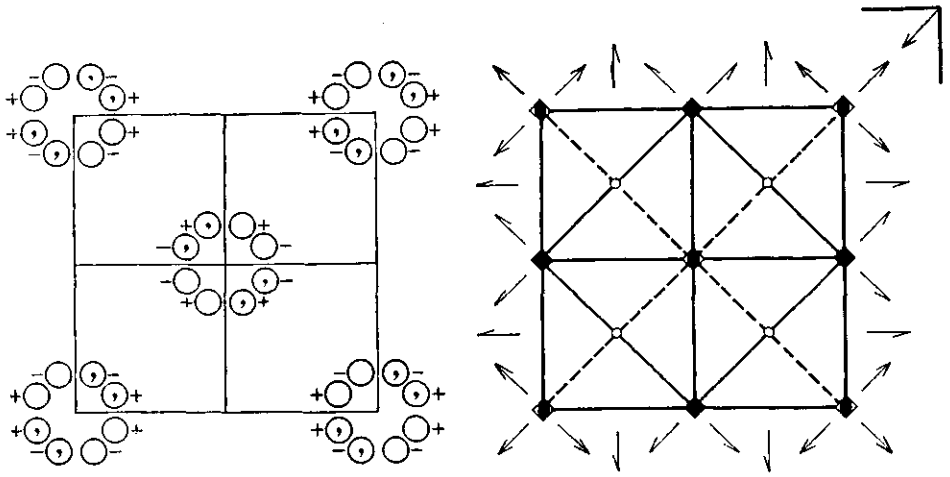
$P4/mnc$ D_{4h}^{6}

No. 128 $P\,4/m\,2_1/n\,2/c$ $4/m\,m\,m$ Tetragonal



Origin at centre (4/m)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	i	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $x,y,\bar{z}$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; $\bar{y},x,z$; $y,\bar{x},z$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}-z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$.	hkl: No conditions $hk0$: No conditions $0kl$: $k+l=2n$ hhl: $l=2n$
				Special: as above, plus
8	h	m	$x,y,0$; $\bar{x},\bar{y},0$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}$; $\bar{y},x,0$; $y,\bar{x},0$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}$.	no extra conditions
8	g	2	$x,\frac{1}{2}+x,\frac{1}{4}$; $\bar{x},\frac{1}{2}-x,\frac{1}{4}$; $\frac{1}{2}+x,\bar{x},\frac{1}{4}$; $\frac{1}{2}-x,x,\frac{1}{4}$; $x,\frac{1}{2}+x,\frac{3}{4}$; $\bar{x},\frac{1}{2}-x,\frac{3}{4}$; $\frac{1}{2}+x,\bar{x},\frac{3}{4}$; $\frac{1}{2}-x,x,\frac{3}{4}$.	hkl: $l=2n$
8	f	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $0,\frac{1}{2},\frac{1}{2}+z$; $0,\frac{1}{2},\frac{1}{2}-z$; $\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$; $\frac{1}{2},0,\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $h+k=2n$; $l=2n$
4	e	4	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
4	d	222	$0,\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},0,\frac{1}{4}$; $0,\frac{1}{2},\frac{3}{4}$; $\frac{1}{2},0,\frac{3}{4}$.	hkl: $h+k=2n$; $l=2n$
4	c	$2/m$	$0,\frac{1}{2},0$; $\frac{1}{2},0,0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	
2	b	$4/m$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	hkl: $h+k+l=2n$
2	a	$4/m$	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	



Origin at $\bar{4}m2$, at $\frac{1}{4},\frac{1}{4},0$ from centre $(2/m)$ (compare next page for alternative origin)

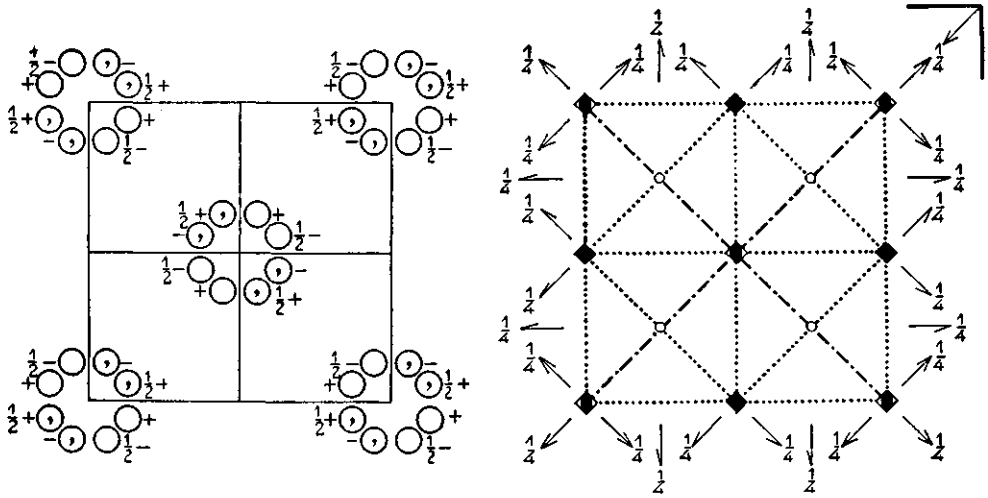
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	k	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}-y,\bar{z}$; $\bar{x},y,z$; $x,\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}+x,z$; $\frac{1}{2}+y,\frac{1}{2}-x,z$; $y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,z$; $\frac{1}{2}-y,\frac{1}{2}-x,z$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: No conditions hhl: No conditions
				Special: as above, plus
8	j	m	$x,\frac{1}{2}+x,z$; $\bar{x},\frac{1}{2}-x,z$; $\frac{1}{2}+x,x,\bar{z}$; $\frac{1}{2}-x,\bar{x},\bar{z}$; $\bar{x},\frac{1}{2}+x,z$; $x,\frac{1}{2}-x,z$; $\frac{1}{2}-x,x,\bar{z}$; $\frac{1}{2}+x,\bar{x},\bar{z}$.	no extra conditions
8	i	m	$0,x,z$; $x,0,\bar{z}$; $\frac{1}{2},\frac{1}{2}+x,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2},z$; $0,\bar{x},z$; $\bar{x},0,\bar{z}$; $\frac{1}{2},\frac{1}{2}-x,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2},z$.	
8	h	2	$x,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}$; $\bar{x},x,\frac{1}{2}$; $x,\bar{x},\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}$.	hkl: $h+k=2n$
8	g	2	$x,x,0$; $\bar{x},\bar{x},0$; $\frac{1}{2}+x,\frac{1}{2}+x,0$; $\frac{1}{2}-x,\frac{1}{2}-x,0$; $\bar{x},x,0$; $x,\bar{x},0$; $\frac{1}{2}-x,\frac{1}{2}+x,0$; $\frac{1}{2}+x,\frac{1}{2}-x,0$.	
4	f	mm	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	
4	e	$2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}$.	hkl: $h,k=2n$
4	d	$2/m$	$\frac{1}{4},\frac{1}{4},0$; $\frac{3}{4},\frac{3}{4},0$; $\frac{1}{4},\frac{3}{4},0$; $\frac{3}{4},\frac{1}{4},0$.	
2	c	$4mm$	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$.	no extra conditions
2	b	$\bar{4}2m$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h+k=2n$
2	a	$\bar{4}2m$	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$.	

$P4/nmm$ D_{4h}^{7}

No. 129 $P\,4/n\,2_1/m\,2/m$ $4/m\,m\,m$ Tetragonal

Origin at centre $(2/m)$, at $\frac{1}{4},\bar{\frac{1}{4}},0$ from $\bar{4}m2$ (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	k	1	x,y,z; $\frac{1}{2}-x,y,z$; $x,\frac{1}{2}-y,z$; $\frac{1}{2}-x,\frac{1}{2}-y,z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,\bar{y},\bar{z}$; $\bar{x},\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; y,x,z; $\frac{1}{2}-y,x,z$; $y,\frac{1}{2}-x,z$; $\frac{1}{2}-y,\frac{1}{2}-x,z$; $\bar{y},\bar{x},\bar{z}$; $\frac{1}{2}+y,\bar{x},\bar{z}$; $\bar{y},\frac{1}{2}+x,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\bar{z}$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: No conditions hhl: No conditions
				Special: as above, plus
8	j	m	x,x,z; $\frac{1}{2}-x,x,z$; $x,\frac{1}{2}-x,z$; $\frac{1}{2}-x,\frac{1}{2}-x,z$; $\bar{x},\bar{x},\bar{z}$; $\frac{1}{2}+x,\bar{x},\bar{z}$; $\bar{x},\frac{1}{2}+x,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}+x,\bar{z}$.	no extra conditions
8	i	m	$\frac{1}{4},x,z$; $\frac{1}{4},\frac{1}{2}-x,z$; $x,\frac{1}{4},z$; $\frac{1}{2}-x,\frac{1}{4},z$; $\frac{3}{4},\bar{x},\bar{z}$; $\frac{3}{4},\frac{1}{2}+x,\bar{z}$; $\bar{x},\frac{3}{4},\bar{z}$; $\frac{1}{2}+x,\frac{3}{4},\bar{z}$.	
8	h	2	$x,\bar{x},\frac{1}{2}$; $\frac{1}{2}-x,\bar{x},\frac{1}{2}$; $x,\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}$; $\bar{x},x,\frac{1}{2}$; $\frac{1}{2}+x,x,\frac{1}{2}$; $\bar{x},\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}$.	hkl: $h+k=2n$
8	g	2	$x,\bar{x},0$; $\frac{1}{2}-x,\bar{x},0$; $x,\frac{1}{2}+x,0$; $\frac{1}{2}-x,\frac{1}{2}+x,0$; $\bar{x},x,0$; $\frac{1}{2}+x,x,0$; $\bar{x},\frac{1}{2}-x,0$; $\frac{1}{2}+x,\frac{1}{2}-x,0$.	
4	f	mm	$\frac{3}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{3}{4},\bar{z}$; $\frac{1}{4},\frac{3}{4},z$; $\frac{3}{4},\frac{1}{4},\bar{z}$.	
4	e	$2/m$	$0,0,\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h,k=2n$
4	d	$2/m$	$0,0,0$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$.	
2	c	$4mm$	$\frac{1}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{3}{4},\bar{z}$.	no extra conditions
2	b	$\bar{4}2m$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}$.	hkl: $h+k=2n$
2	a	$\bar{4}2m$	$\frac{3}{4},\frac{1}{4},0$; $\frac{1}{4},\frac{3}{4},0$.	



Origin at $\bar{4}$, at $\bar{\frac{1}{4}},\frac{1}{4},0$ from $\bar{1}$ (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	g	1	x,y,z; $\bar{x},y,\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; $\bar{x},\bar{y},z$; $x,\bar{y},\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}-y,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z$; $\bar{y},x,\bar{z}$; $y,x,\frac{1}{2}-z$; $\frac{1}{2}-y,\frac{1}{2}+x,z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$; $y,\bar{x},\bar{z}$; $\bar{y},\bar{x},\frac{1}{2}-z$; $\frac{1}{2}+y,\frac{1}{2}-x,z$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: $l=2n$ hhl: $l=2n$
				Special: as above, plus
8	f	2	$x,x,\frac{1}{4}$; $\bar{x},\bar{x},\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{4}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{4}$; $\bar{x},x,\frac{3}{4}$; $x,\bar{x},\frac{3}{4}$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{3}{4}$.	hkl: $h+k+l=2n$
8	e	2	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k=2n$; $l=2n$
8	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}$; $\frac{3}{4},\frac{3}{4},0$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}$; $\frac{3}{4},\frac{1}{4},0$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}$; $\frac{1}{4},\frac{3}{4},0$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}$.	hkl: $h,k,l=2n$
4	c	4	$0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},0,\bar{z}$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $l=2n$
4	b	$\bar{4}$	$0,0,0$; $0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h+k=2n$; $l=2n$
4	a	222	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$; $\frac{1}{2},\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},\frac{3}{4}$.	

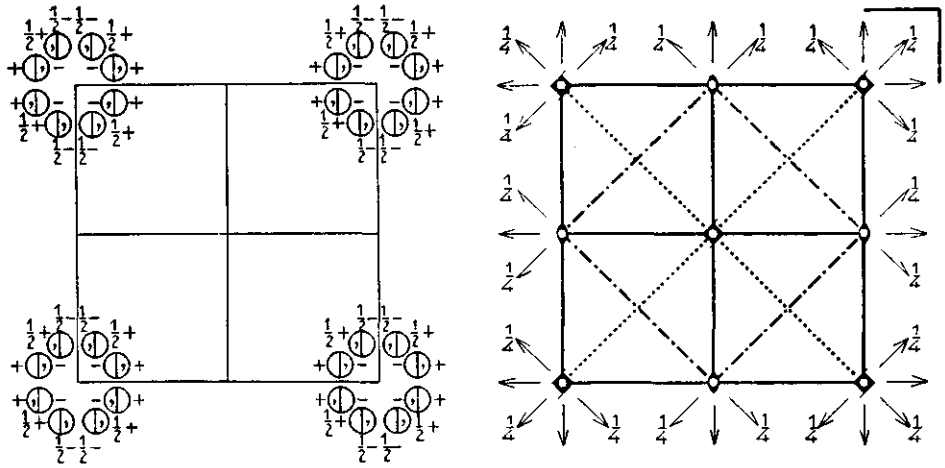
R

$P4/ncc$ D_{4h}^{8}

No. 130 $P\,4/n\,2_1/c\,2/c$ $4/m\,m\,m$ Tetragonal

Origin at $\bar{1}$, at $\frac{1}{4},\frac{\bar{1}}{4},0$ from $\bar{4}$ (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	g	1	x,y,z; $\frac{1}{2}-x,y,\frac{1}{2}+z$; $x,\frac{1}{2}-y,\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}-y,z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,\bar{y},\frac{1}{2}-z$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $y,x,\frac{1}{2}+z$; $\frac{1}{2}-y,x,z$; $y,\frac{1}{2}-x,z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}-z$; $\frac{1}{2}+y,\bar{x},\bar{z}$; $\bar{y},\frac{1}{2}+x,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}-z$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: $l=2n$ hhl: $l=2n$
				Special: as above, plus
8	f	2	$\bar{x},x,\frac{1}{4}$; $\frac{1}{2}-x,\bar{x},\frac{1}{4}$; $x,\frac{1}{2}+x,\frac{1}{4}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{4}$; $x,\bar{x},\frac{3}{4}$; $\frac{1}{2}+x,x,\frac{3}{4}$; $\bar{x},\frac{1}{2}-x,\frac{3}{4}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{3}{4}$.	hkl: $h+k+l=2n$
8	e	2	$\frac{3}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}+z$; $\frac{1}{4},\frac{3}{4},z$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}+z$; $\frac{1}{4},\frac{3}{4},\bar{z}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}-z$; $\frac{3}{4},\frac{1}{4},\bar{z}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}-z$.	hkl: $h+k=2n$; $l=2n$
8	d	$\bar{1}$	$0,0,0$; $0,0,\frac{1}{2}$; $\frac{1}{2},0,0$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h,k,l=2n$
4	c	4	$\frac{1}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{3}{4},\bar{z}$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}+z$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}-z$.	hkl: $l=2n$
4	b	$\bar{4}$	$\frac{3}{4},\frac{1}{4},0$; $\frac{1}{4},\frac{3}{4},0$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}$.	hkl: $h+k=2n$; $l=2n$
4	a	222	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$.	



Origin at centre (mmm) on 4_2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	r	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{y},x,\frac{1}{2}+z$; $y,\bar{x},\frac{1}{2}+z$; $\bar{x},y,\bar{z}$; $x,\bar{y},\bar{z}$; $y,x,\frac{1}{2}-z$; $\bar{y},\bar{x},\frac{1}{2}-z$; $\bar{x},\bar{y},\bar{z}$; $x,y,\bar{z}$; $y,\bar{x},\frac{1}{2}-z$; $\bar{y},x,\frac{1}{2}-z$; $x,\bar{y},z$; $\bar{x},y,z$; $\bar{y},\bar{x},\frac{1}{2}+z$; $y,x,\frac{1}{2}+z$.	hkl: No conditions $hk0$: No conditions $0kl$: No conditions hhl: $l=2n$
				Special: as above, plus
8	q	m	$x,y,0$; $\bar{x},\bar{y},0$; $\bar{x},y,0$; $x,\bar{y},0$; $y,\bar{x},\frac{1}{2}$; $\bar{y},x,\frac{1}{2}$; $y,x,\frac{1}{2}$; $\bar{y},\bar{x},\frac{1}{2}$.	no extra conditions
8	p	m	$\frac{1}{2},x,z$; $\frac{1}{2},\bar{x},z$; $\frac{1}{2},x,\bar{z}$; $\frac{1}{2},\bar{x},\bar{z}$; $x,\frac{1}{2},\frac{1}{2}+z$; $\bar{x},\frac{1}{2},\frac{1}{2}+z$; $x,\frac{1}{2},\frac{1}{2}-z$; $\bar{x},\frac{1}{2},\frac{1}{2}-z$.	
8	o	m	$0,x,z$; $0,\bar{x},z$; $0,x,\bar{z}$; $0,\bar{x},\bar{z}$; $x,0,\frac{1}{2}+z$; $\bar{x},0,\frac{1}{2}+z$; $x,0,\frac{1}{2}-z$; $\bar{x},0,\frac{1}{2}-z$.	
8	n	2	$x,x,\frac{1}{4}$; $\bar{x},\bar{x},\frac{1}{4}$; $\bar{x},x,\frac{1}{4}$; $x,\bar{x},\frac{1}{4}$; $x,x,\frac{3}{4}$; $\bar{x},\bar{x},\frac{3}{4}$; $\bar{x},x,\frac{3}{4}$; $x,\bar{x},\frac{3}{4}$.	hkl: $l=2n$
4	m	mm	$x,\frac{1}{2},0$; $\bar{x},\frac{1}{2},0$; $\frac{1}{2},x,\frac{1}{2}$; $\frac{1}{2},\bar{x},\frac{1}{2}$.	no extra conditions
4	l	mm	$x,0,\frac{1}{2}$; $\bar{x},0,\frac{1}{2}$; $0,x,0$; $0,\bar{x},0$.	
4	k	mm	$x,\frac{1}{2},\frac{1}{2}$; $\bar{x},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},x,0$; $\frac{1}{2},\bar{x},0$.	
4	j	mm	$x,0,0$; $\bar{x},0,0$; $0,x,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$.	
4	i	mm	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},0,\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $h+k+l=2n$

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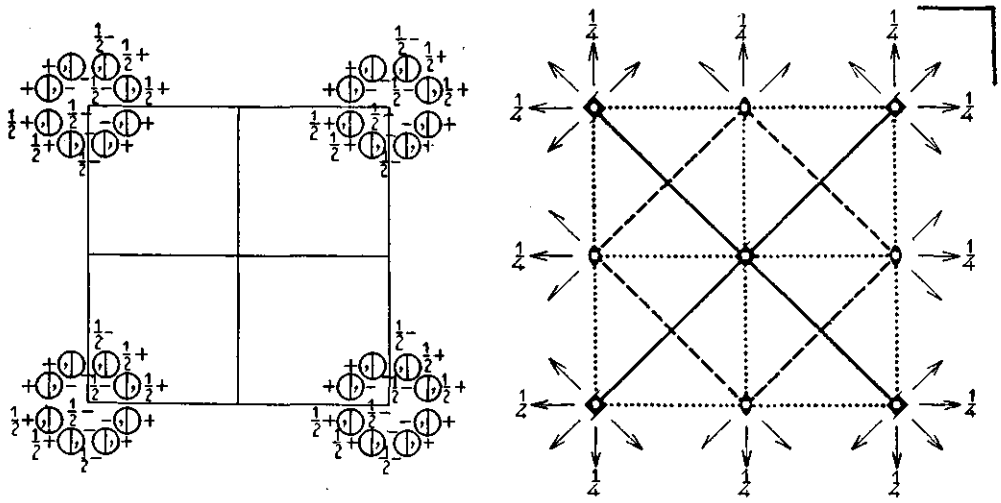
4	*h*	*mm*	$\frac{1}{2},\frac{1}{2},z$;	$\frac{1}{2},\frac{1}{2},\bar{z}$;	$\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$;	$\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	*hkl*: $l=2n$
4	*g*	*mm*	$0,0,z$;	$0,0,\bar{z}$;	$0,0,\frac{1}{2}+z$;	$0,0,\frac{1}{2}-z$.	
2	*f*	$\bar{4}2m$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$;	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$.			
2	*e*	$\bar{4}2m$	$0,0,\frac{1}{4}$;	$0,0,\frac{3}{4}$.			
2	*d*	*mmm*	$0,\frac{1}{2},\frac{1}{2}$;	$\frac{1}{2},0,0$.			*hkl*: $h+k+l=2n$
2	*c*	*mmm*	$0,\frac{1}{2},0$;	$\frac{1}{2},0,\frac{1}{2}$.			
2	*b*	*mmm*	$\frac{1}{2},\frac{1}{2},0$;	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.			*hkl*: $l=2n$
2	*a*	*mmm*	$0,0,0$;	$0,0,\frac{1}{2}$.			



Origin at centre (mmm) on 4_2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	p	1	x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\frac{1}{2}+z$; $x,\bar{y},\frac{1}{2}+z$; $x,y,\bar{z}$; $\bar{x},\bar{y},\bar{z}$; $\bar{x},y,\frac{1}{2}-z$; $x,\bar{y},\frac{1}{2}-z$; y,x,z; $\bar{y},\bar{x},z$; $\bar{y},x,\frac{1}{2}+z$; $y,\bar{x},\frac{1}{2}+z$; $y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $\bar{y},x,\frac{1}{2}-z$; $y,\bar{x},\frac{1}{2}-z$.	hkl: No conditions $hk0$: No conditions $0kl$: $l=2n$ hhl: No conditions
				Special: as above, plus
8	o	m	x,x,z; $\bar{x},\bar{x},z$; $x,\bar{x},\frac{1}{2}+z$; $\bar{x},x,\frac{1}{2}+z$; $x,x,\bar{z}$; $\bar{x},\bar{x},\bar{z}$; $x,\bar{x},\frac{1}{2}-z$; $\bar{x},x,\frac{1}{2}-z$.	no extra conditions
8	n	m	$x,y,0$; $\bar{x},\bar{y},0$; $x,\bar{y},\frac{1}{2}$; $\bar{x},y,\frac{1}{2}$; $y,x,0$; $\bar{y},\bar{x},0$; $\bar{y},x,\frac{1}{2}$; $y,\bar{x},\frac{1}{2}$.	
8	m	2	$x,\frac{1}{2},\frac{1}{4}$; $\bar{x},\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},x,\frac{1}{4}$; $\frac{1}{2},\bar{x},\frac{1}{4}$; $x,\frac{1}{2},\frac{3}{4}$; $\bar{x},\frac{1}{2},\frac{3}{4}$; $\frac{1}{2},x,\frac{3}{4}$; $\frac{1}{2},\bar{x},\frac{3}{4}$.	hkl: $l=2n$
8	l	2	$x,0,\frac{1}{4}$; $\bar{x},0,\frac{1}{4}$; $0,x,\frac{1}{4}$; $0,\bar{x},\frac{1}{4}$; $x,0,\frac{3}{4}$; $\bar{x},0,\frac{3}{4}$; $0,x,\frac{3}{4}$; $0,\bar{x},\frac{3}{4}$.	
8	k	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $0,\frac{1}{2},\frac{1}{2}+z$; $0,\frac{1}{2},\frac{1}{2}-z$; $\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$; $\frac{1}{2},0,\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $h+k=2n$; $l=2n$
4	j	mm	$x,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $\bar{x},x,0$; $x,\bar{x},0$.	no extra conditions
4	i	mm	$x,x,0$; $\bar{x},\bar{x},0$; $\bar{x},x,\frac{1}{2}$; $x,\bar{x},\frac{1}{2}$.	
4	h	mm	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $l=2n$
4	g	mm	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	

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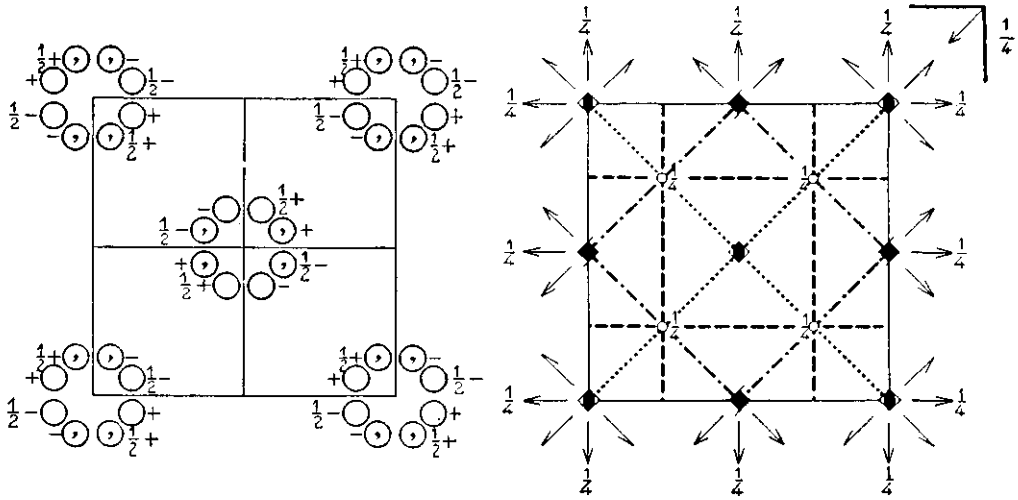
4	*f*	$2/m$	$0,\frac{1}{2},0$;	$0,\frac{1}{2},\frac{1}{2}$;	$\frac{1}{2},0,0$;	$\frac{1}{2},0,\frac{1}{2}$.	*hkl*: $h+k=2n$; $l=2n$
4	*e*	222	$0,\frac{1}{2},\frac{1}{4}$;	$0,\frac{1}{2},\frac{3}{4}$;	$\frac{1}{2},0,\frac{1}{4}$;	$\frac{1}{2},0,\frac{3}{4}$.	
2	*d*	$\bar{4}2m$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$;	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$.			*hkl*: $l=2n$
2	*c*	mmm	$\frac{1}{2},\frac{1}{2},0$;	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.			
2	*b*	$\bar{4}2m$	$0,0,\frac{1}{4}$;	$0,0,\frac{3}{4}$.			
2	*a*	mmm	$0,0,0$;	$0,0,\frac{1}{2}$.			



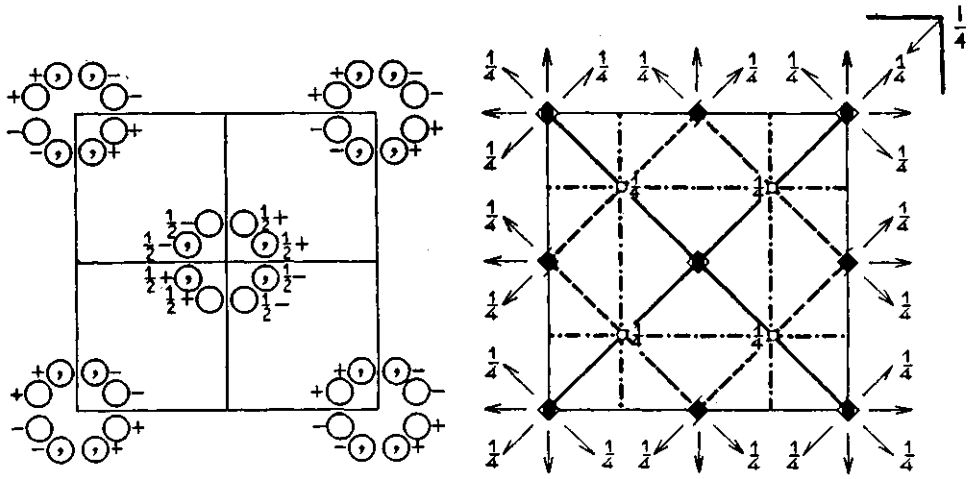
Origin at $\bar{4}$, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{1}$ (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	k	1	x,y,z; $\bar{x},y,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z$; $\bar{x},\bar{y},z$; $x,\bar{y},\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}-y,z$; $\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z$; $\bar{y},x,\bar{z}$; $y,x,\frac{1}{2}+z$; $\frac{1}{2}+y,\frac{1}{2}+x,\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$; $y,\bar{x},\bar{z}$; $\bar{y},\bar{x},\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}-x,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: $k=2n$ hhl: $l=2n$
				Special: as above, plus
8	j	2	$x,\frac{1}{2}+x,0$; $\bar{x},\frac{1}{2}-x,0$; $x,\frac{1}{2}-x,\frac{1}{2}$; $\bar{x},\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}+x,\bar{x},0$; $\frac{1}{2}-x,x,0$; $\frac{1}{2}+x,x,\frac{1}{2}$; $\frac{1}{2}-x,\bar{x},\frac{1}{2}$.	hkl: $h+k+l=2n$
8	i	2	$x,0,\frac{3}{4}$; $\bar{x},0,\frac{3}{4}$; $\frac{1}{2}+x,\frac{1}{2},\frac{3}{4}$; $\frac{1}{2}-x,\frac{1}{2},\frac{3}{4}$; $0,x,\frac{1}{4}$; $0,\bar{x},\frac{1}{4}$; $\frac{1}{2},\frac{1}{2}+x,\frac{1}{4}$; $\frac{1}{2},\frac{1}{2}-x,\frac{1}{4}$.	hkl: $h+k=2n$
8	h	2	$x,0,\frac{1}{4}$; $\bar{x},0,\frac{1}{4}$; $\frac{1}{2}+x,\frac{1}{2},\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{2},\frac{1}{4}$; $0,x,\frac{3}{4}$; $0,\bar{x},\frac{3}{4}$; $\frac{1}{2},\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{2},\frac{1}{2}-x,\frac{3}{4}$.	
8	g	2	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k=2n$; $l=2n$
8	f	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $0,\frac{1}{2},\frac{1}{2}+z$; $0,\frac{1}{2},\frac{1}{2}-z$; $\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$; $\frac{1}{2},0,\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	
8	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$.	hkl: $h,k,l=2n$
4	d	$\bar{4}$	$0,0,0$; $\frac{1}{2},\frac{1}{2},0$; $0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
4	c	222	$0,\frac{1}{2},0$; $\frac{1}{2},0,0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	hkl: $h+k=2n$; $l=2n$
4	b	222	$0,0,\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},\frac{1}{4}$; $0,0,\frac{3}{4}$; $\frac{1}{2},\frac{1}{2},\frac{3}{4}$.	
4	a	222	$0,\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},0,\frac{1}{4}$; $0,\frac{1}{2},\frac{3}{4}$; $\frac{1}{2},0,\frac{3}{4}$.	

$P4_2/nbc$ D_{4h}^{11} No. 133 $P\,4_2/n\,2/b\,2/c$ $4/m\,m\,m$ Tetragonal

Origin at $\bar{1}$, at $\frac{1}{4},\frac{\bar{1}}{4},\frac{1}{4}$ from $\bar{4}$ (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions				Conditions limiting possible reflections
							General:
16	k	1	x,y,z;	$\bar{x},\frac{1}{2}+y,z$;	$\frac{1}{2}+x,\bar{y},z$;	$\frac{1}{2}-x,\frac{1}{2}-y,z$;	hkl: No conditions
			$\bar{x},\bar{y},\bar{z}$;	$x,\frac{1}{2}-y,\bar{z}$;	$\frac{1}{2}-x,y,\bar{z}$;	$\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$;	$hk0$: $h+k=2n$
			$\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$;	$\frac{1}{2}-y,x,\frac{1}{2}+z$;	$y,\frac{1}{2}-x,\frac{1}{2}+z$;	$\bar{y},\bar{x},\frac{1}{2}+z$;	$0kl$: $k=2n$
			$\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$;	$\frac{1}{2}+y,\bar{x},\frac{1}{2}-z$;	$\bar{y},\frac{1}{2}+x,\frac{1}{2}-z$;	$y,x,\frac{1}{2}-z$.	hhl: $l=2n$
							Special: as above, plus
8	j	2	$x,x,\frac{1}{4}$;	$\bar{x},\frac{1}{2}+x,\frac{1}{4}$;	$\frac{1}{2}+x,\bar{x},\frac{1}{4}$;	$\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{4}$;	hkl: $h+k+l=2n$
			$\bar{x},\bar{x},\frac{3}{4}$;	$x,\frac{1}{2}-x,\frac{3}{4}$;	$\frac{1}{2}-x,x,\frac{3}{4}$;	$\frac{1}{2}+x,\frac{1}{2}+x,\frac{3}{4}$.	
8	i	2	$x,\frac{1}{4},\frac{1}{2}$;	$\frac{1}{2}-x,\frac{1}{4},\frac{1}{2}$;	$\frac{1}{4},\frac{1}{2}-x,0$;	$\frac{1}{4},x,0$;	hkl: $h+k=2n$
			$\bar{x},\frac{3}{4},\frac{1}{2}$;	$\frac{1}{2}+x,\frac{3}{4},\frac{1}{2}$;	$\frac{3}{4},\frac{1}{2}+x,0$;	$\frac{3}{4},\bar{x},0$.	
8	h	2	$x,\frac{1}{4},0$;	$\frac{1}{2}-x,\frac{1}{4},0$;	$\frac{1}{4},\frac{1}{2}-x,\frac{1}{2}$;	$\frac{1}{4},x,\frac{1}{2}$;	
			$\bar{x},\frac{3}{4},0$;	$\frac{1}{2}+x,\frac{3}{4},0$;	$\frac{3}{4},\frac{1}{2}+x,\frac{1}{2}$;	$\frac{3}{4},\bar{x},\frac{1}{2}$.	
8	g	2	$\frac{3}{4},\frac{1}{4},z$;	$\frac{3}{4},\frac{1}{4},\frac{1}{2}+z$;	$\frac{1}{4},\frac{3}{4},z$;	$\frac{1}{4},\frac{3}{4},\frac{1}{2}+z$;	hkl: $h+k=2n$; $l=2n$
			$\frac{1}{4},\frac{3}{4},\bar{z}$;	$\frac{1}{4},\frac{3}{4},\frac{1}{2}-z$;	$\frac{3}{4},\frac{1}{4},\bar{z}$;	$\frac{3}{4},\frac{1}{4},\frac{1}{2}-z$.	
8	f	2	$\frac{1}{4},\frac{1}{4},z$;	$\frac{3}{4},\frac{3}{4},z$;	$\frac{1}{4},\frac{1}{4},\frac{1}{2}+z$;	$\frac{3}{4},\frac{3}{4},\frac{1}{2}+z$;	
			$\frac{3}{4},\frac{3}{4},\bar{z}$;	$\frac{1}{4},\frac{1}{4},\bar{z}$;	$\frac{3}{4},\frac{3}{4},\frac{1}{2}-z$;	$\frac{1}{4},\frac{1}{4},\frac{1}{2}-z$.	
8	e	$\bar{1}$	$0,0,0$;	$0,\frac{1}{2},0$;	$\frac{1}{2},0,0$;	$\frac{1}{2},\frac{1}{2},0$;	hkl: $h,k,l=2n$
			$\frac{1}{2},\frac{1}{2},\frac{1}{2}$;	$\frac{1}{2},0,\frac{1}{2}$;	$0,\frac{1}{2},\frac{1}{2}$;	$0,0,\frac{1}{2}$.	
4	d	$\bar{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$;	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$;	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$;	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$.	hkl: $h+k=2n$; $l=2n$
4	c	222	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$;	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$;	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$;	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$.	
4	b	222	$\frac{3}{4},\frac{1}{4},0$;	$\frac{1}{4},\frac{3}{4},0$;	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$;	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$.	
4	a	222	$\frac{1}{4},\frac{1}{4},0$;	$\frac{3}{4},\frac{3}{4},0$;	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$;	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$.	



Origin at $\bar{4}2m$, at $\bar{\frac{1}{4}},\frac{1}{4},\bar{\frac{1}{4}}$ from centre $(2/m)$ (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	n	1	$x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z;\ \frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z;$ $\bar{x},y,\bar{z};\ x,\bar{y},\bar{z};\ \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z;$ $\bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ \frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z;\ \frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z;$ $y,x,z;\ \bar{y},\bar{x},z;\ \frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}-z;\ \frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z.$	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl: No conditions
				Special: as above, plus
8	m	m	$x,x,z;\ \bar{x},\bar{x},z;\ \frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}-z;\ \frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}-z;$ $\bar{x},x,\bar{z};\ x,\bar{x},\bar{z};\ \frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}+z.$	no extra conditions
8	l	2	$x,\frac{1}{2}+x,\frac{3}{4};\ \bar{x},\frac{1}{2}-x,\frac{3}{4};\ \frac{1}{2}+x,x,\frac{3}{4};\ \frac{1}{2}-x,\bar{x},\frac{3}{4};$ $x,\frac{1}{2}-x,\frac{1}{4};\ \bar{x},\frac{1}{2}+x,\frac{1}{4};\ \frac{1}{2}+x,\bar{x},\frac{1}{4};\ \frac{1}{2}-x,x,\frac{1}{4}.$	hkl: $h+k=2n$
8	k	2	$x,\frac{1}{2}+x,\frac{1}{4};\ \bar{x},\frac{1}{2}-x,\frac{1}{4};\ \frac{1}{2}+x,x,\frac{1}{4};\ \frac{1}{2}-x,\bar{x},\frac{1}{4};$ $x,\frac{1}{2}-x,\frac{3}{4};\ \bar{x},\frac{1}{2}+x,\frac{3}{4};\ \frac{1}{2}+x,\bar{x},\frac{3}{4};\ \frac{1}{2}-x,x,\frac{3}{4}.$	
8	j	2	$x,0,\frac{1}{2};\ \bar{x},0,\frac{1}{2};\ \frac{1}{2}+x,\frac{1}{2},0;\ \frac{1}{2}-x,\frac{1}{2},0;$ $0,x,\frac{1}{2};\ 0,\bar{x},\frac{1}{2};\ \frac{1}{2},\frac{1}{2}+x,0;\ \frac{1}{2},\frac{1}{2}-x,0.$	hkl: $h+k+l=2n$
8	i	2	$x,0,0;\ \bar{x},0,0;\ \frac{1}{2}+x,\frac{1}{2},\frac{1}{2};\ \frac{1}{2}-x,\frac{1}{2},\frac{1}{2};$ $0,x,0;\ 0,\bar{x},0;\ \frac{1}{2},\frac{1}{2}+x,\frac{1}{2};\ \frac{1}{2},\frac{1}{2}-x,\frac{1}{2}.$	
8	h	2	$0,\frac{1}{2},z;\ 0,\frac{1}{2},\bar{z};\ 0,\frac{1}{2},\frac{1}{2}+z;\ 0,\frac{1}{2},\frac{1}{2}-z;$ $\frac{1}{2},0,z;\ \frac{1}{2},0,\bar{z};\ \frac{1}{2},0,\frac{1}{2}+z;\ \frac{1}{2},0,\frac{1}{2}-z.$	hkl: $h+k=2n$; $l=2n$
4	g	mm	$0,0,z;\ 0,0,\bar{z};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}+z;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}-z.$	hkl: $h+k+l=2n$
4	f	$2/m$	$\frac{3}{4},\frac{3}{4},\frac{3}{4};\ \frac{1}{4},\frac{1}{4},\frac{3}{4};\ \frac{1}{4},\frac{3}{4},\frac{1}{4};\ \frac{3}{4},\frac{1}{4},\frac{1}{4}.$	hkl: $h+k,k+l,(l+h)=2n$
4	e	$2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{3}{4},\frac{3}{4},\frac{1}{4};\ \frac{3}{4},\frac{1}{4},\frac{3}{4};\ \frac{1}{4},\frac{3}{4},\frac{3}{4}.$	

(*continued on next page*)

4	d	222	$0,\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},0,\frac{1}{4}$; $0,\frac{1}{2},\frac{3}{4}$; $\frac{1}{2},0,\frac{3}{4}$.	hkl: $h+k+l=2n, l=2n$
4	c	222	$0,\frac{1}{2},0$; $\frac{1}{2},0,0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	
2	b	$\bar{4}2m$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	hkl: $h+k+l=2n$
2	a	$\bar{4}2m$	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	

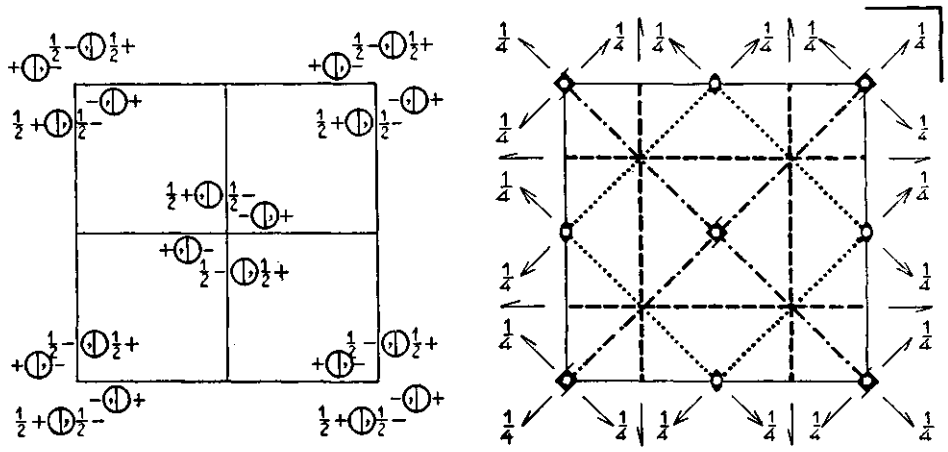
Origin at centre (2/m), at $\frac{1}{4},\bar{\frac{1}{4}},\frac{1}{4}$ from $\bar{4}2m$ (compare previous page for alternative origin)

General:

16	n	1	x,y,z; $\bar{x},\frac{1}{2}+y,\frac{1}{2}+z$; $\frac{1}{2}+x,\bar{y},\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}-y,z$; $\bar{x},\bar{y},\bar{z}$; $x,\frac{1}{2}-y,\frac{1}{2}-z$; $\frac{1}{2}-x,y,\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,z$; $\frac{1}{2}-y,x,\frac{1}{2}+z$; $y,\frac{1}{2}-x,\frac{1}{2}+z$; $\bar{y},\bar{x},z$; $\frac{1}{2}-y,\frac{1}{2}-x,\bar{z}$; $\frac{1}{2}+y,\bar{x},\frac{1}{2}-z$; $\bar{y},\frac{1}{2}+x,\frac{1}{2}-z$; $y,x,\bar{z}$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl: No conditions

Special: as above, plus

8	m	m	$x,\bar{x},z$; $\bar{x},\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}+x,x,\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}+x,z$; $\bar{x},x,\bar{z}$; $x,\frac{1}{2}+x,\frac{1}{2}-z$; $\frac{1}{2}-x,\bar{x},\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}-x,\bar{z}$.	no extra conditions
8	l	2	$x,x,\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}$; $\bar{x},\frac{1}{2}+x,0$; $\frac{1}{2}-x,x,0$; $\bar{x},\bar{x},\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}$; $x,\frac{1}{2}-x,0$; $\frac{1}{2}+x,\bar{x},0$.	hkl: $h+k=2n$
8	k	2	$x,x,0$; $\frac{1}{2}+x,\frac{1}{2}+x,0$; $\bar{x},\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}-x,x,\frac{1}{2}$; $\bar{x},\bar{x},0$; $\frac{1}{2}-x,\frac{1}{2}-x,0$; $x,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2}+x,\bar{x},\frac{1}{2}$.	
8	j	2	$x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{2}+x,\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{2}+x,\frac{1}{4}$; $\frac{1}{4},x,\frac{3}{4}$; $\bar{x},\frac{3}{4},\frac{3}{4}$; $\frac{1}{2}-x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{2}-x,\frac{3}{4}$; $\frac{3}{4},\bar{x},\frac{1}{4}$.	hkl: $h+k+l=2n$
8	i	2	$x,\frac{1}{4},\frac{3}{4}$; $\frac{1}{2}+x,\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{4},x,\frac{1}{4}$; $\bar{x},\frac{3}{4},\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{4},\frac{3}{4}$; $\frac{1}{4},\frac{1}{2}-x,\frac{1}{4}$; $\frac{3}{4},\bar{x},\frac{3}{4}$.	
8	h	2	$\frac{1}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}+z$; $\frac{3}{4},\frac{3}{4},z$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}+z$; $\frac{3}{4},\frac{3}{4},\bar{z}$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}-z$; $\frac{1}{4},\frac{1}{4},\bar{z}$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}-z$.	hkl: $h+k=2n$; $l=2n$
4	g	mm	$\frac{3}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{3}{4},\bar{z}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}+z$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
4	f	$2/m$	$0,0,0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	hkl: $h+k, k+l, (l+h)=2n$
4	e	$2/m$	$0,0,\frac{1}{2}$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
4	d	222	$\frac{1}{4},\frac{1}{4},0$; $\frac{3}{4},\frac{3}{4},0$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}$.	hkl: $h+k=2n$; $l=2n$
4	c	222	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{3}{4}$.	
2	b	$\bar{4}2m$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$.	hkl: $h+k+l=2n$
2	a	$\bar{4}2m$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$.	

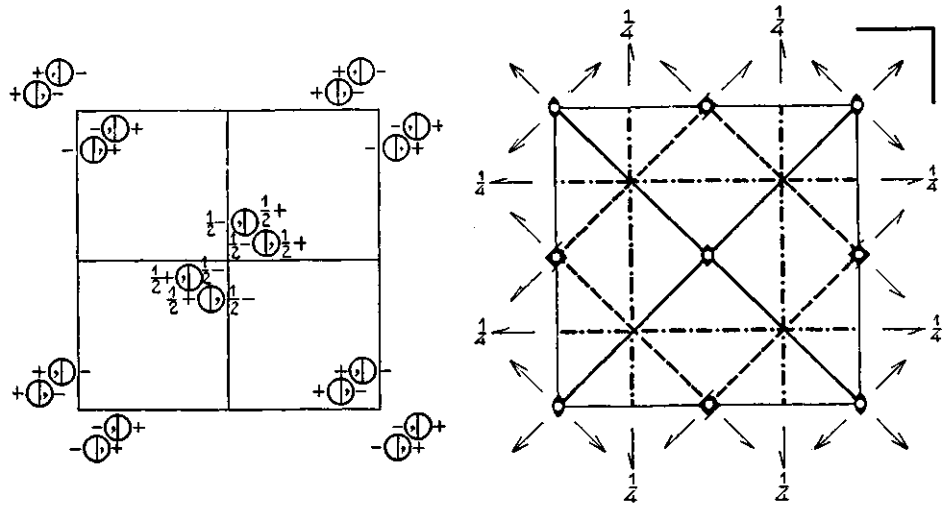


Origin at centre $(2/m)$ on 4_2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	i	1	x,y,z; $\bar{y},x,\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}-y,z$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $x,y,\bar{z}$; $\bar{y},x,\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}-z$; $\bar{x},\bar{y},z$; $y,\bar{x},\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$; $\bar{x},\bar{y},\bar{z}$; $y,\bar{x},\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$.	hkl: No conditions $hk0$: No conditions $0kl$: $k=2n$ hhl: $l=2n$
				Special: as above, plus
8	h	m	$x,y,0$; $\bar{x},\bar{y},0$; $\frac{1}{2}+x,\frac{1}{2}-y,0$; $\frac{1}{2}-x,\frac{1}{2}+y,0$; $\bar{y},x,\frac{1}{2}$; $y,\bar{x},\frac{1}{2}$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}$.	no extra conditions
8	g	2	$x,\frac{1}{2}+x,\frac{1}{4}$; $\bar{x},\frac{1}{2}-x,\frac{1}{4}$; $\frac{1}{2}+x,\bar{x},\frac{1}{4}$; $\frac{1}{2}-x,x,\frac{1}{4}$; $x,\frac{1}{2}+x,\frac{3}{4}$; $\bar{x},\frac{1}{2}-x,\frac{3}{4}$; $\frac{1}{2}+x,\bar{x},\frac{3}{4}$; $\frac{1}{2}-x,x,\frac{3}{4}$.	hkl: $l=2n$
8	f	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $0,\frac{1}{2},\frac{1}{2}+z$; $0,\frac{1}{2},\frac{1}{2}-z$; $\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$; $\frac{1}{2},0,\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	
8	e	2	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	
4	d	222	$0,\frac{1}{2},\frac{1}{4}$; $0,\frac{1}{2},\frac{3}{4}$; $\frac{1}{2},0,\frac{1}{4}$; $\frac{1}{2},0,\frac{3}{4}$.	hkl: $h+k=2n$; $l=2n$
4	c	$2/m$	$0,\frac{1}{2},0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$; $\frac{1}{2},0,\frac{1}{2}$.	
4	b	$\bar{4}$	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$; $\frac{1}{2},\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},\frac{3}{4}$.	
4	a	$2/m$	$0,0,0$; $0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	

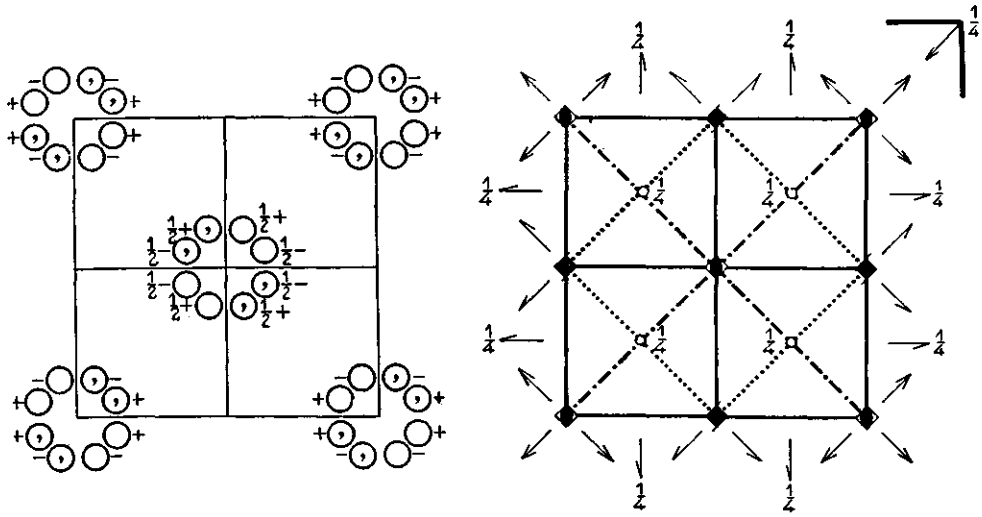
$P4_2/mnm$ D_{4h}^{14}

No. 136 $P\,4_2/m\,2_1/n\,2/m$ $4/m\,m\,m$ Tetragonal



Origin at centre (mmm)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	k	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $x,y,\bar{z}$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; y,x,z; $\bar{y},\bar{x},z$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$; $y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}-z$.	hkl: No conditions $hk0$: No conditions $0kl$: $k+l=2n$ hhl: No conditions
				Special: as above, plus
8	j	m	x,x,z; $\bar{x},\bar{x},z$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}+z$; $x,x,\bar{z}$; $\bar{x},\bar{x},\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}-z$.	no extra conditions
8	i	m	$x,y,0$; $\bar{x},\bar{y},0$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}$; $y,x,0$; $\bar{y},\bar{x},0$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}$.	
8	h	2	$0,\frac{1}{2},z$; $0,\frac{1}{2},\bar{z}$; $0,\frac{1}{2},\frac{1}{2}+z$; $0,\frac{1}{2},\frac{1}{2}-z$; $\frac{1}{2},0,z$; $\frac{1}{2},0,\bar{z}$; $\frac{1}{2},0,\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $h+k=2n$; $l=2n$
4	g	mm	$x,\bar{x},0$; $\bar{x},x,0$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}$.	no extra conditions
4	f	mm	$x,x,0$; $\bar{x},\bar{x},0$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}$.	
4	e	mm	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
4	d	$\bar{4}$	$0,\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},0,\frac{1}{4}$; $0,\frac{1}{2},\frac{3}{4}$; $\frac{1}{2},0,\frac{3}{4}$.	hkl: $h+k=2n$; $l=2n$
4	c	$2/m$	$0,\frac{1}{2},0$; $\frac{1}{2},0,0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$.	
2	b	mmm	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	hkl: $h+k+l=2n$
2	a	mmm	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	



Origin at $\bar{4}m2$, at $\bar{1}\frac{1}{4},\frac{1}{4},\bar{1}\frac{1}{4}$ from $\bar{1}$ (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	h	1	x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z$; $\bar{x},y,z$; $x,\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$; $y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: No conditions hhl: $l=2n$
				Special: as above, plus
8	g	m	$0,x,z$; $x,0,\bar{z}$; $\frac{1}{2},\frac{1}{2}+x,\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2},\frac{1}{2}+z$; $0,\bar{x},z$; $\bar{x},0,\bar{z}$; $\frac{1}{2},\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2},\frac{1}{2}+z$.	no extra conditions
8	f	2	$x,x,0$; $\bar{x},\bar{x},0$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}$; $x,\bar{x},0$; $\bar{x},x,0$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}$.	hkl: $h+k+l=2n$
8	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$.	hkl: $h,k,l=2n$
4	d	mm	$0,\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$; $0,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $l=2n$
4	c	mm	$0,0,z$; $0,0,\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
2	b	$\bar{4}2m$	$0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	hkl: $h+k+l=2n$
2	a	$\bar{4}2m$	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h+k+l=2n$

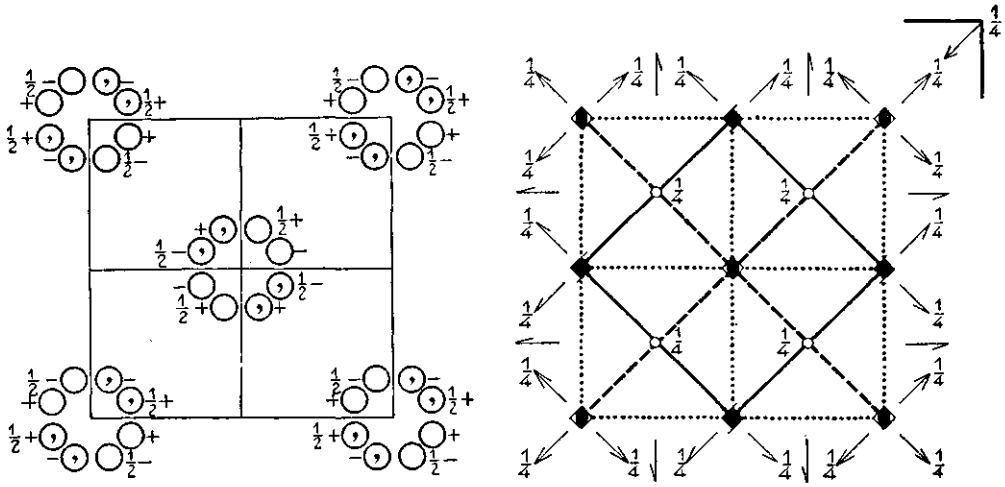
$P4_2/nmc$ D_{4h}^{15} No. 137 $P\,4_2/n\,2_1/m\,2/c$ $4/m\,m\,m$ Tetragonal

Origin at $\bar{1}$, at $\frac{1}{4},\frac{\bar{1}}{4},\frac{1}{4}$ from $\bar{4}m2$ (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	h	1	x,y,z; $\frac{1}{2}-x,y,z$; $x,\frac{1}{2}-y,z$; $\frac{1}{2}-x,\frac{1}{2}-y,z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,\bar{y},\bar{z}$; $\bar{x},\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $y,x,\frac{1}{2}+z$; $\frac{1}{2}-y,x,\frac{1}{2}+z$; $y,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}-z$; $\frac{1}{2}+y,\bar{x},\frac{1}{2}-z$; $\bar{y},\frac{1}{2}+x,\frac{1}{2}-z$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}-z$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: No conditions hhl: $l=2n$
				Special: as above, plus
8	g	m	$\frac{1}{4},x,z$; $\frac{1}{4},\frac{1}{2}-x,z$; $x,\frac{1}{4},\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{4},\frac{1}{2}+z$; $\frac{3}{4},\bar{x},\bar{z}$; $\frac{3}{4},\frac{1}{2}+x,\bar{z}$; $\bar{x},\frac{3}{4},\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{3}{4},\frac{1}{2}-z$.	no extra conditions
8	f	2	$\bar{x},x,\frac{1}{4}$; $\frac{1}{2}+x,x,\frac{1}{4}$; $\bar{x},\frac{1}{2}-x,\frac{1}{4}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{4}$; $x,\bar{x},\frac{3}{4}$; $\frac{1}{2}-x,\bar{x},\frac{3}{4}$; $x,\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{3}{4}$.	hkl: $h+k+l=2n$
8	e	$\bar{1}$	$0,0,0$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$; $0,0,\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h,k,l=2n$
4	d	mm	$\frac{1}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{3}{4},\bar{z}$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}+z$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}-z$.	hkl: $l=2n$
4	c	mm	$\frac{3}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{3}{4},\bar{z}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}+z$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}-z$.	hkl: $h+k+l=2n$
2	b	$\bar{4}2m$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$.	
2	a	$\bar{4}2m$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$.	

Tetragonal $4/m\,m\,m$ $P\,4_2/n\,2_1/c\,2/m$ No. 138

$P\,4_2/n\,c\,m$ D_{4h}^{16}

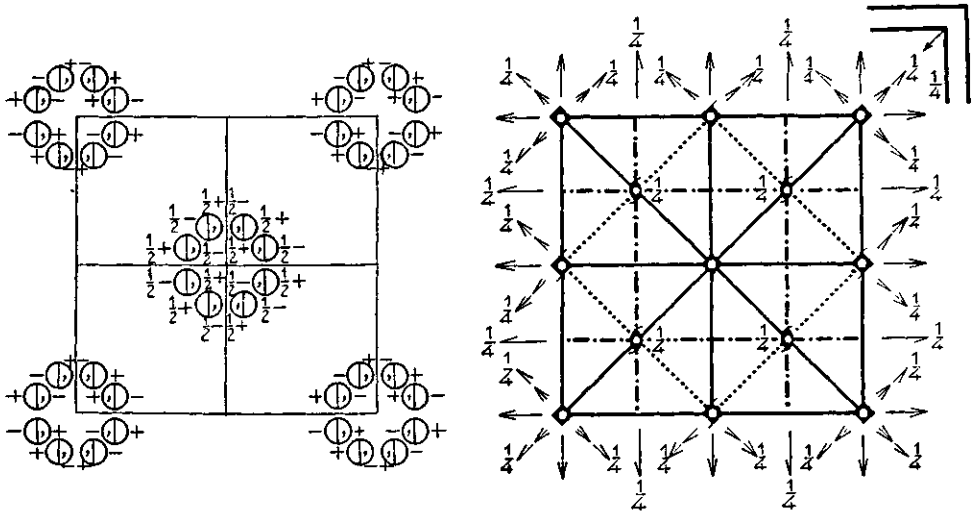


Origin at $\bar{4}$, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from centre $(2/m)$ (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	j	1	x,y,z; $\bar{x},y,\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z$; $\bar{x},\bar{y},z$; $x,\bar{y},\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z$; $\bar{y},x,\bar{z}$; $y,x,\frac{1}{2}-z$; $\frac{1}{2}+y,\frac{1}{2}+x,z$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$; $y,\bar{x},\bar{z}$; $\bar{y},\bar{x},\frac{1}{2}-z$; $\frac{1}{2}-y,\frac{1}{2}-x,z$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: $l=2n$ hhl: No conditions
				Special: as above, plus
8	i	m	$x,\frac{1}{2}+x,z$; $\frac{1}{2}+x,x,\frac{1}{2}-z$; $x,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}+x,\bar{x},\bar{z}$; $\bar{x},\frac{1}{2}-x,z$; $\frac{1}{2}-x,\bar{x},\frac{1}{2}-z$; $\bar{x},\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}-x,x,\bar{z}$.	no extra conditions
8	h	2	$x,x,\frac{3}{4}$; $\bar{x},\bar{x},\frac{3}{4}$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{3}{4}$; $x,\bar{x},\frac{1}{4}$; $\bar{x},x,\frac{1}{4}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{4}$.	hkl: $h+k=2n$
8	g	2	$x,x,\frac{1}{4}$; $\bar{x},\bar{x},\frac{1}{4}$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{4}$; $x,\bar{x},\frac{3}{4}$; $\bar{x},x,\frac{3}{4}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{3}{4}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{3}{4}$.	
8	f	2	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	hkl: $h+k=2n$; $l=2n$
4	e	mm	$0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},0,\bar{z}$; $\frac{1}{2},0,\frac{1}{2}-z$.	hkl: $l=2n$
4	d	$2/m$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{4}$.	hkl: $h+k,k+l,(l+h)=2n$
4	c	$2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$.	
4	b	$\bar{4}$	$0,0,0$; $0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h+k=2n$; $l=2n$
4	a	222	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$; $\frac{1}{2},\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},\frac{3}{4}$.	

Origin at centre ($2/m$), at $\frac{1}{4},\bar{\frac{1}{4}},\frac{1}{4}$ from $\bar{4}$ (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
16	j	1	x,y,z; $\frac{1}{2}-x,y,\frac{1}{2}+z$; $x,\frac{1}{2}-y,\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}-y,z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}+x,\bar{y},\frac{1}{2}-z$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; y,x,z; $\frac{1}{2}+y,\bar{x},\frac{1}{2}-z$; $\bar{y},\frac{1}{2}+x,\frac{1}{2}-z$; $\frac{1}{2}+y,\frac{1}{2}+x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $\frac{1}{2}-y,x,\frac{1}{2}+z$; $y,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}-x,z$.	hkl: No conditions $hk0$: $h+k=2n$ $0kl$: $l=2n$ hhl: No conditions
				Special: as above, plus
8	i	m	x,x,z; $\frac{1}{2}-x,x,\frac{1}{2}+z$; $x,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}-x,\frac{1}{2}-x,z$; $\bar{x},\bar{x},\bar{z}$; $\frac{1}{2}+x,\bar{x},\frac{1}{2}-z$; $\bar{x},\frac{1}{2}+x,\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}+x,\bar{z}$.	no extra conditions
8	h	2	$x,\bar{x},0$; $\frac{1}{2}-x,\bar{x},\frac{1}{2}$; $x,\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2}+x,0$; $\bar{x},x,0$; $\frac{1}{2}+x,x,\frac{1}{2}$; $\bar{x},\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2}-x,0$.	hkl: $h+k=2n$
8	g	2	$x,\bar{x},\frac{1}{2}$; $\frac{1}{2}-x,\bar{x},0$; $x,\frac{1}{2}+x,0$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}$; $\bar{x},x,\frac{1}{2}$; $\frac{1}{2}+x,x,0$; $\bar{x},\frac{1}{2}-x,0$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}$.	
8	f	2	$\frac{3}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}+z$; $\frac{1}{4},\frac{3}{4},z$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}+z$; $\frac{1}{4},\frac{3}{4},\bar{z}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}-z$; $\frac{3}{4},\frac{1}{4},\bar{z}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}-z$.	hkl: $h+k=2n$; $l=2n$
4	e	mm	$\frac{1}{4},\frac{1}{4},z$; $\frac{3}{4},\frac{3}{4},\bar{z}$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}+z$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}-z$.	hkl: $l=2n$
4	d	$2/m$	$0,0,0$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	hkl: $h+k,k+l,(l+h)=2n$
4	c	$2/m$	$0,0,\frac{1}{2}$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
4	b	$\bar{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{4}$.	hkl: $h+k=2n$; $l=2n$
4	a	222	$\frac{3}{4},\frac{1}{4},0$; $\frac{1}{4},\frac{3}{4},0$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}$.	



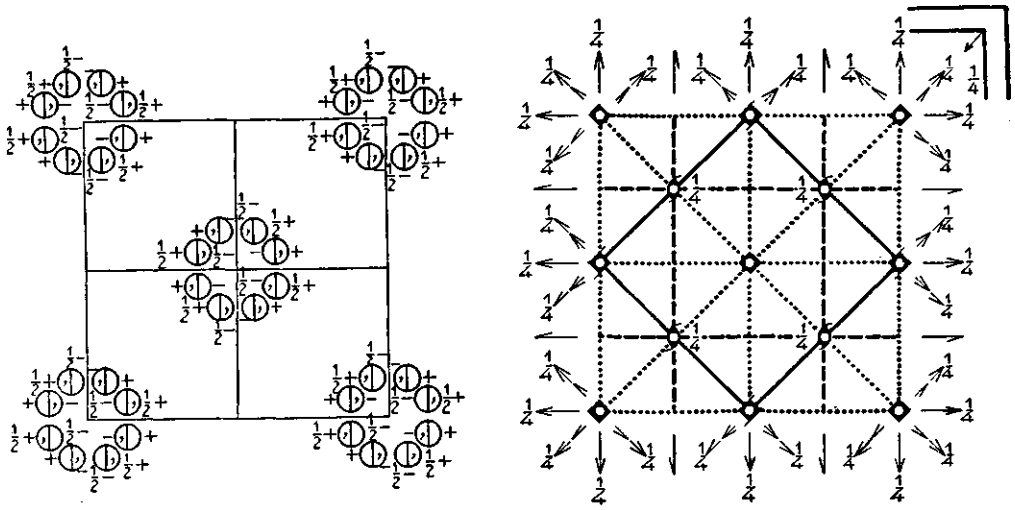
Origin at centre ($4/mmm$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+$	Conditions limiting possible reflections
				General:
32	o	1	$x,y,z;\ \bar{x},\bar{y},z;\ x,y,\bar{z};\ \bar{x},\bar{y},\bar{z};$ $\bar{x},y,z;\ x,\bar{y},z;\ \bar{x},y,\bar{z};\ x,\bar{y},\bar{z};$ $\bar{y},x,z;\ y,\bar{x},z;\ \bar{y},x,\bar{z};\ y,\bar{x},\bar{z};$ $y,x,z;\ \bar{y},\bar{x},z;\ y,x,\bar{z};\ \bar{y},\bar{x},\bar{z}.$	hkl: $h+k+l=2n$ $hk0$: $(h+k=2n)$ $0kl$: $(k+l=2n)$ hhl: $(l=2n)$
				Special: as above, plus
16	n	m	$0,x,z;\ 0,\bar{x},z;\ 0,x,\bar{z};\ 0,\bar{x},\bar{z};$ $x,0,z;\ \bar{x},0,z;\ x,0,\bar{z};\ \bar{x},0,\bar{z}.$	no extra conditions
16	m	m	$x,x,z;\ \bar{x},\bar{x},z;\ \bar{x},x,z;\ x,\bar{x},z;$ $x,x,\bar{z};\ \bar{x},\bar{x},\bar{z};\ \bar{x},x,\bar{z};\ x,\bar{x},\bar{z}.$	no extra conditions
16	l	m	$x,y,0;\ \bar{x},\bar{y},0;\ \bar{x},y,0;\ x,\bar{y},0;$ $\bar{y},x,0;\ y,\bar{x},0;\ y,x,0;\ \bar{y},\bar{x},0.$	no extra conditions
16	k	2	$x,\tfrac{1}{2}+x,\tfrac{1}{4};\ \bar{x},\tfrac{1}{2}-x,\tfrac{1}{4};\ \tfrac{1}{2}+x,x,\tfrac{1}{4};\ \tfrac{1}{2}-x,\bar{x},\tfrac{1}{4};$ $x,\tfrac{1}{2}-x,\tfrac{1}{4};\ \bar{x},\tfrac{1}{2}+x,\tfrac{1}{4};\ \tfrac{1}{2}+x,\bar{x},\tfrac{1}{4};\ \tfrac{1}{2}-x,x,\tfrac{1}{4}.$	hkl: $l=2n$; $(h+k=2n)$
8	j	mm	$x,\tfrac{1}{2},0;\ \bar{x},\tfrac{1}{2},0;\ \tfrac{1}{2},x,0;\ \tfrac{1}{2},\bar{x},0.$	no extra conditions
8	i	mm	$x,0,0;\ \bar{x},0,0;\ 0,x,0;\ 0,\bar{x},0.$	no extra conditions
8	h	mm	$x,x,0;\ \bar{x},\bar{x},0;\ x,\bar{x},0;\ \bar{x},x,0.$	no extra conditions
8	g	mm	$0,\tfrac{1}{2},z;\ 0,\tfrac{1}{2},\bar{z};\ \tfrac{1}{2},0,z;\ \tfrac{1}{2},0,\bar{z}.$	hkl: $l=2n$; $(h+k=2n)$
8	f	$2/m$	$\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{3}{4},\tfrac{3}{4},\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{3}{4},\tfrac{1}{4};\ \tfrac{3}{4},\tfrac{1}{4},\tfrac{1}{4}.$	hkl: $h,k,(l)=2n$

(*continued on next page*)

(*continued*)

4	*e*	$4mm$	$0,0,z$; $0,0,\bar{z}$.	no extra conditions
4	*d*	$\bar{4}m2$	$0,\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},0,\frac{1}{4}$.	*hkl*: $l=2n$; $(h+k=2n)$
4	*c*	mmm	$0,\frac{1}{2},0$; $\frac{1}{2},0,0$.	*hkl*: $l=2n$; $(h+k=2n)$
2	*b*	$4/mmm$	$0,0,\frac{1}{2}$.	no extra conditions
2	*a*	$4/mmm$	$0,0,0$.	no extra conditions



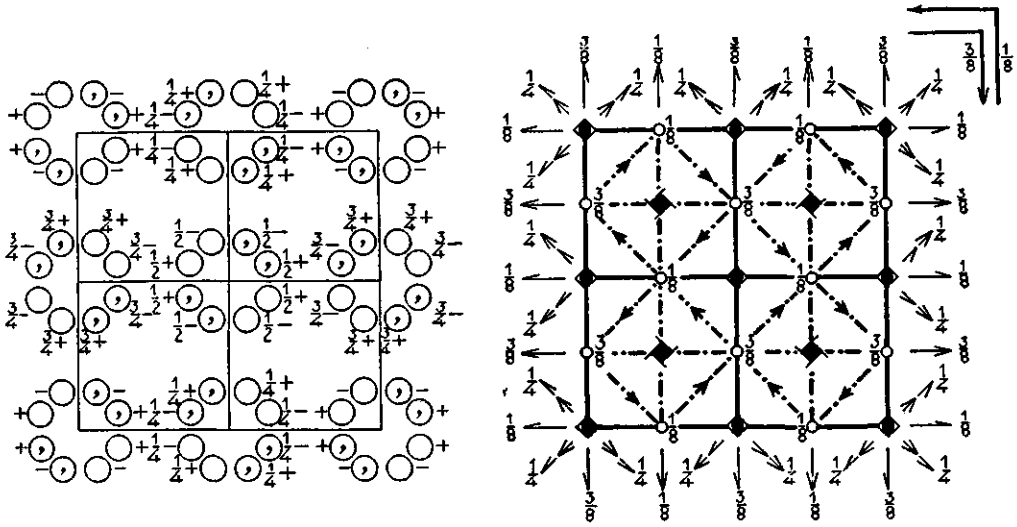
Origin at centre ($4/m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+$	Conditions limiting possible reflections
				General:
32	m	1	$x,y,z;\ \bar{x},\bar{y},z;\ x,\bar{y},\tfrac{1}{2}+z;\ \bar{x},y,\tfrac{1}{2}+z;$ $x,y,\bar{z};\ \bar{x},\bar{y},\bar{z};\ x,\bar{y},\tfrac{1}{2}-z;\ \bar{x},y,\tfrac{1}{2}-z;$ $\bar{y},x,z;\ y,\bar{x},z;\ y,x,\tfrac{1}{2}+z;\ \bar{y},\bar{x},\tfrac{1}{2}+z;$ $\bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ y,x,\tfrac{1}{2}-z;\ \bar{y},\bar{x},\tfrac{1}{2}-z.$	hkl: $h+k+l=2n$ $hk0$: $(h+k=2n)$ $0kl$: $l,(k)=2n$ hhl: $(l=2n)$
				Special: as above, plus
16	l	m	$x,\tfrac{1}{2}+x,z;\ \bar{x},\tfrac{1}{2}-x,z;\ \tfrac{1}{2}+x,\bar{x},z;\ \tfrac{1}{2}-x,x,z;$ $x,\tfrac{1}{2}+x,\bar{z};\ \bar{x},\tfrac{1}{2}-x,\bar{z};\ \tfrac{1}{2}+x,\bar{x},\bar{z};\ \tfrac{1}{2}-x,x,\bar{z}.$	no extra conditions
16	k	m	$x,y,0;\ \bar{x},\bar{y},0;\ \bar{y},x,0;\ y,\bar{x},0;$ $x,\bar{y},\tfrac{1}{2};\ \bar{x},y,\tfrac{1}{2};\ y,x,\tfrac{1}{2};\ \bar{y},\bar{x},\tfrac{1}{2}.$	
16	j	2	$x,0,\tfrac{1}{4};\ \bar{x},0,\tfrac{1}{4};\ 0,x,\tfrac{1}{4};\ 0,\bar{x},\tfrac{1}{4};$ $x,0,\tfrac{3}{4};\ \bar{x},0,\tfrac{3}{4};\ 0,x,\tfrac{3}{4};\ 0,\bar{x},\tfrac{3}{4}.$	hkl: $l=2n$; $(h+k=2n)$
16	i	2	$x,x,\tfrac{1}{4};\ \bar{x},\bar{x},\tfrac{1}{4};\ x,\bar{x},\tfrac{1}{4};\ \bar{x},x,\tfrac{1}{4};$ $x,x,\tfrac{3}{4};\ \bar{x},\bar{x},\tfrac{3}{4};\ x,\bar{x},\tfrac{3}{4};\ \bar{x},x,\tfrac{3}{4}.$	
8	h	mm	$x,\tfrac{1}{2}+x,0;\ \bar{x},\tfrac{1}{2}-x,0;\ \tfrac{1}{2}+x,\bar{x},0;\ \tfrac{1}{2}-x,x,0.$	no extra conditions
8	g	mm	$0,\tfrac{1}{2},z;\ 0,\tfrac{1}{2},\bar{z};\ \tfrac{1}{2},0,z;\ \tfrac{1}{2},0,\bar{z}.$	hkl: $l=2n$; $(h+k=2n)$
8	f	4	$0,0,z;\ 0,0,\bar{z};\ \tfrac{1}{2},\tfrac{1}{2},z;\ \tfrac{1}{2},\tfrac{1}{2},\bar{z}.$	
8	e	$2/m$	$\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{3}{4},\tfrac{3}{4},\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{3}{4},\tfrac{1}{4};\ \tfrac{3}{4},\tfrac{1}{4},\tfrac{1}{4}.$	hkl: $h,k,(l)=2n$

(*continued on next page*)

(*continued*)

4	*d*	*mmm*	$0,\frac{1}{2},0;$	$\frac{1}{2},0,0.$	
4	*c*	$4/m$	$0,0,0;$	$0,0,\frac{1}{2}.$	hkl: $l=2n$; $(h+k=2n)$
4	*b*	$\bar{4}2m$	$0,\frac{1}{2},\frac{1}{4};$	$\frac{1}{2},0,\frac{1}{4}.$	
4	*a*	42	$0,0,\frac{1}{4};$	$0,0,\frac{3}{4}.$	



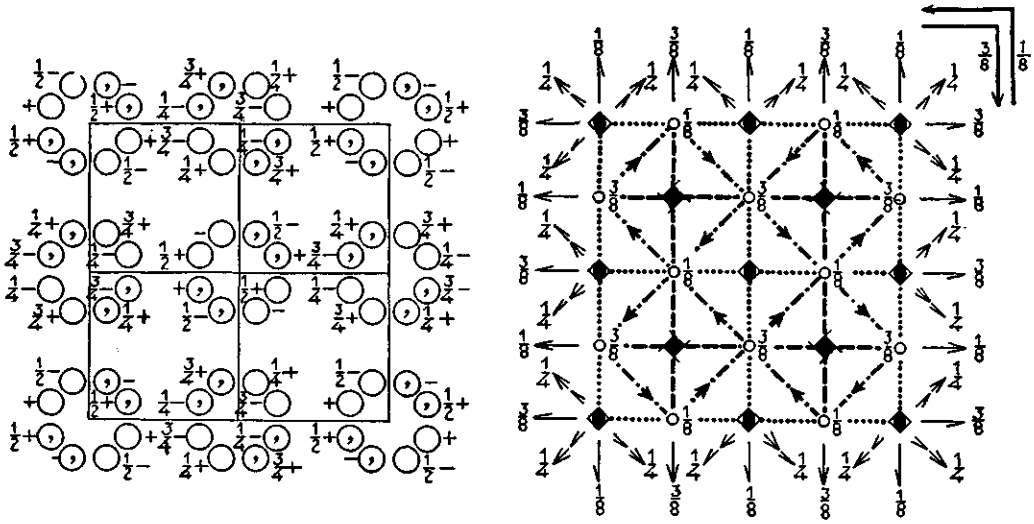
Origin at $\bar{4}m2$, at $0,\frac{1}{4},\frac{\bar{1}}{8}$ from centre $(2/m)$ (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
				General:
32	i	1	$x,y,z;\ \bar{x},\bar{y},z;\ x,\frac{1}{2}+y,\frac{1}{4}-z;\ \bar{x},\frac{1}{2}-y,\frac{1}{4}-z;$ $\bar{x},y,z;\ x,\bar{y},z;\ \bar{x},\frac{1}{2}+y,\frac{1}{4}-z;\ x,\frac{1}{2}-y,\frac{1}{4}-z;$ $y,x,\bar{z};\ \bar{y},\bar{x},\bar{z};\ y,\frac{1}{2}+x,\frac{1}{4}+z;\ \bar{y},\frac{1}{2}-x,\frac{1}{4}+z;$ $\bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ \bar{y},\frac{1}{2}+x,\frac{1}{4}+z;\ y,\frac{1}{2}-x,\frac{1}{4}+z.$	hkl: $h+k+l=2n$ $hk0$: $h,(k)=2n$ $0kl$: $(k+l=2n)$ hhl: $(l=2n)$; $2h+l=4n$
				Special: as above, plus
16	h	m	$0,x,z;\ 0,\bar{x},z;\ 0,\frac{1}{2}+x,\frac{1}{4}-z;\ 0,\frac{1}{2}-x,\frac{1}{4}-z;$ $x,0,\bar{z};\ \bar{x},0,\bar{z};\ x,\frac{1}{2},\frac{1}{4}+z;\ \bar{x},\frac{1}{2},\frac{1}{4}+z.$	no extra conditions
16	g	2	$x,x,0;\ \bar{x},\bar{x},0;\ x,\frac{1}{2}+x,\frac{1}{4};\ \bar{x},\frac{1}{2}-x,\frac{1}{4};$ $x,\bar{x},0;\ \bar{x},x,0;\ x,\frac{1}{2}-x,\frac{1}{4};\ \bar{x},\frac{1}{2}+x,\frac{1}{4}.$	hkl: $2k+l=2n+1$ or $4n$
16	f	2	$x,\frac{1}{4},\frac{1}{8};\ \bar{x},\frac{1}{4},\frac{1}{8};\ x,\frac{3}{4},\frac{1}{8};\ \bar{x},\frac{3}{4},\frac{1}{8};$ $\frac{1}{4},x,\frac{7}{8};\ \frac{1}{4},\bar{x},\frac{7}{8};\ \frac{3}{4},x,\frac{7}{8};\ \frac{3}{4},\bar{x},\frac{7}{8}.$	hkl: $l,(h+k)=2n+1$, or $h,k,(l)=2n$
8	e	mm	$0,0,z;\ 0,0,\bar{z};\ 0,\frac{1}{2},\frac{1}{4}+z;\ 0,\frac{1}{2},\frac{1}{4}-z.$	hkl: $2k+l=2n+1$ or $4n$
8	d	$2/m$	$0,\frac{1}{4},\frac{5}{8};\ 0,\frac{3}{4},\frac{5}{8};\ \frac{1}{4},0,\frac{3}{8};\ \frac{3}{4},0,\frac{3}{8}.$	hkl: $l,(h+k)=2n+1$, or $[h,k,(l)=2n;$ $h+k+l=4n]$
8	c	$2/m$	$0,\frac{1}{4},\frac{1}{8};\ 0,\frac{3}{4},\frac{1}{8};\ \frac{1}{4},0,\frac{7}{8};\ \frac{3}{4},0,\frac{7}{8}.$	
4	b	$\bar{4}2m$	$0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{3}{4}.$	hkl: $2k+l=2n+1$ or $4n$
4	a	$\bar{4}2m$	$0,0,0;\ 0,\frac{1}{2},\frac{1}{4}.$	

$I4_1/amd$ D_{4h}^{19} No. 141 $I\,4_1/a\,2/m\,2/d$ $4/m\,m\,m$ Tetragonal

Origin at centre ($2/m$), at $0,\frac{1}{4},\frac{1}{8}$ from $\bar{4}m2$ (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
32	i	1	$x,y,z;\ x,\frac{1}{2}-y,z;\ \frac{1}{4}+y,\frac{1}{4}+x,\frac{3}{4}+z;\ \frac{1}{4}+y,\frac{1}{4}-x,\frac{3}{4}+z;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},\frac{1}{2}+y,\bar{z};\ \frac{3}{4}-y,\frac{3}{4}-x,\frac{1}{4}-z;\ \frac{3}{4}-y,\frac{3}{4}+x,\frac{1}{4}-z;$ $\bar{x},y,z;\ \bar{x},\frac{1}{2}-y,z;\ \frac{3}{4}-y,\frac{1}{4}+x,\frac{3}{4}+z;\ \frac{3}{4}-y,\frac{1}{4}-x,\frac{3}{4}+z;$ $x,\bar{y},\bar{z};\ x,\frac{1}{2}+y,\bar{z};\ \frac{1}{4}+y,\frac{3}{4}-x,\frac{1}{4}-z;\ \frac{1}{4}+y,\frac{3}{4}+x,\frac{1}{4}-z.$	hkl: $h+k+l=2n$ $hk0$: $h,(k)=2n$ $0kl$: $(k+l=2n)$ hhl: $(l=2n)$; $2h+l=4n$
				Special: as above, plus
16	h	m	$0,x,z;\ 0,\frac{1}{2}-x,z;\ \frac{1}{4}+x,\frac{1}{4},\frac{3}{4}+z;\ \frac{3}{4}-x,\frac{1}{4},\frac{3}{4}+z;$ $0,\bar{x},\bar{z};\ 0,\frac{1}{2}+x,\bar{z};\ \frac{3}{4}-x,\frac{3}{4},\frac{1}{4}-z;\ \frac{1}{4}+x,\frac{3}{4},\frac{1}{4}-z.$	no extra conditions
16	g	2	$x,\frac{1}{4}+x,\frac{7}{8};\ \bar{x},\frac{1}{4}+x,\frac{7}{8};\ x,\frac{1}{4}-x,\frac{7}{8};\ \bar{x},\frac{1}{4}-x,\frac{7}{8};$ $\bar{x},\frac{3}{4}-x,\frac{1}{8};\ x,\frac{3}{4}-x,\frac{1}{8};\ \bar{x},\frac{3}{4}+x,\frac{1}{8};\ x,\frac{3}{4}+x,\frac{1}{8}.$	hkl: $2k+l=2n+1$ or $4n$
16	f	2	$x,0,0;\ x,\frac{1}{2},0;\ \frac{1}{4},\frac{1}{4}+x,\frac{3}{4};\ \frac{3}{4},\frac{3}{4}+x,\frac{3}{4};$ $\bar{x},0,0;\ \bar{x},\frac{1}{2},0;\ \frac{3}{4},\frac{3}{4}-x,\frac{1}{4};\ \frac{1}{4},\frac{3}{4}-x,\frac{1}{4}.$	hkl: $l,(h+k)=2n+1$, or $h,k,(l)=2n$
8	e	mm	$0,\frac{1}{4},z;\ 0,\frac{3}{4},\frac{1}{4}+z;\ 0,\frac{3}{4},\bar{z};\ 0,\frac{1}{4},\frac{3}{4}-z.$	hkl: $2k+l=2n+1$ or $4n$
8	d	$2/m$	$0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{3}{4}.$	hkl: $l,(h+k)=2n+1$, or $[h,k,(l)=2n$; $h+k+l=4n]$
8	c	$2/m$	$0,0,0;\ 0,\frac{1}{2},0;\ \frac{1}{4},\frac{1}{4},\frac{3}{4};\ \frac{1}{4},\frac{3}{4},\frac{1}{4}.$	
4	b	$\bar{4}2m$	$0,\frac{1}{4},\frac{3}{8};\ 0,\frac{3}{4},\frac{5}{8}.$	hkl: $2k+l=2n+1$ or $4n$
4	a	$\bar{4}2m$	$0,\frac{3}{4},\frac{1}{8};\ 0,\frac{1}{4},\frac{7}{8}.$	

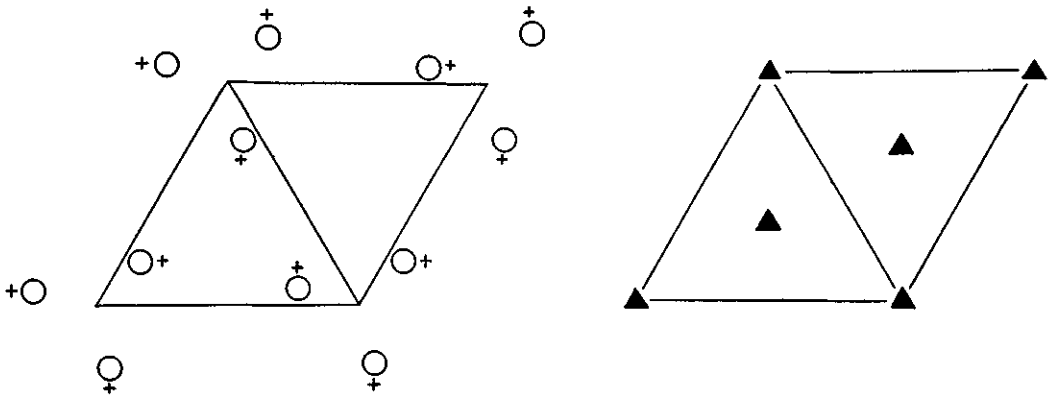


Origin at $\bar{4}$, at $0,\frac{1}{4},\frac{\bar{1}}{8}$ from $\bar{1}$ (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
32	g	1	$x,y,z;\ x,\bar{y},\frac{1}{2}+z;\ x,\frac{1}{2}+y,\frac{1}{4}-z;\ x,\frac{1}{2}-y,\frac{3}{4}-z;$ $\bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}+z;\ \bar{x},\frac{1}{2}-y,\frac{1}{4}-z;\ \bar{x},\frac{1}{2}+y,\frac{3}{4}-z;$ $\bar{y},x,\bar{z};\ y,x,\frac{1}{2}-z;\ \bar{y},\frac{1}{2}+x,\frac{1}{4}+z;\ y,\frac{1}{2}+x,\frac{3}{4}+z;$ $y,\bar{x},\bar{z};\ \bar{y},\bar{x},\frac{1}{2}-z;\ y,\frac{1}{2}-x,\frac{1}{4}+z;\ \bar{y},\frac{1}{2}-x,\frac{3}{4}+z.$	hkl: $h+k+l=2n$ $hk0$: $h,(k)=2n$ $0kl$: $l,(k)=2n$ hhl: $(l=2n)$; $2h+l=4n$
				Special: as above, plus
16	f	2	$x,x,\frac{1}{4};\ \bar{x},\bar{x},\frac{1}{4};\ x,\frac{1}{2}+x,0;\ \bar{x},\frac{1}{2}-x,0;$ $x,\bar{x},\frac{3}{4};\ \bar{x},x,\frac{3}{4};\ x,\frac{1}{2}-x,\frac{1}{2};\ \bar{x},\frac{1}{2}+x,\frac{1}{2}.$	hkl: $2k+l=2n+1$ or $4n$
16	e	2	$\frac{1}{4},x,\frac{1}{8};\ \frac{3}{4},\bar{x},\frac{1}{8};\ \frac{3}{4},x,\frac{5}{8};\ \frac{1}{4},\bar{x},\frac{5}{8};$ $x,\frac{1}{4},\frac{3}{8};\ \bar{x},\frac{3}{4},\frac{3}{8};\ x,\frac{3}{4},\frac{7}{8};\ \bar{x},\frac{1}{4},\frac{7}{8}.$	hkl: $l,(h+k)=2n+1$, or $h,k,(l)=2n$
16	d	2	$0,0,z;\ 0,0,\bar{z};\ 0,\frac{1}{2},\frac{1}{4}+z;\ 0,\frac{1}{2},\frac{1}{4}-z;$ $\frac{1}{2},\frac{1}{2},z;\ \frac{1}{2},\frac{1}{2},\bar{z};\ \frac{1}{2},0,\frac{1}{4}+z;\ \frac{1}{2},0,\frac{1}{4}-z.$	hkl: $l=2n$; $2k+l=4n$
16	c	$\bar{1}$	$0,\frac{1}{4},\frac{1}{8};\ 0,\frac{3}{4},\frac{1}{8};\ 0,\frac{1}{4},\frac{5}{8};\ 0,\frac{3}{4},\frac{5}{8};$ $\frac{1}{4},0,\frac{3}{8};\ \frac{3}{4},0,\frac{3}{8};\ \frac{1}{4},0,\frac{7}{8};\ \frac{3}{4},0,\frac{7}{8}.$	hkl: $h,k,(l)=2n$; $h+k+l=4n$
8	b	222	$0,0,\frac{1}{4};\ 0,0,\frac{3}{4};\ 0,\frac{1}{2},0;\ 0,\frac{1}{2},\frac{1}{2}.$	hkl: $l=2n$; $2k+l=4n$
8	a	$\bar{4}$	$0,0,0;\ 0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{4};\ 0,\frac{1}{2},\frac{3}{4}.$	

Origin at $\bar{1}$, at $0,\frac{\bar{1}}{4},\frac{1}{8}$ from $\bar{4}$ (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	
				General:
32	g	1	$x,y,z;\ \bar{x},y,\frac{1}{2}+z;\ \frac{1}{4}+y,\frac{1}{4}+x,\frac{1}{4}+z;\ \frac{3}{4}-y,\frac{1}{4}+x,\frac{3}{4}+z;$ $\bar{x},\bar{y},\bar{z};\ x,\bar{y},\frac{1}{2}-z;\ \frac{3}{4}-y,\frac{3}{4}-x,\frac{3}{4}-z;\ \frac{1}{4}+y,\frac{3}{4}-x,\frac{1}{4}-z;$ $x,\frac{1}{2}-y,\frac{1}{2}+z;\ \bar{x},\frac{1}{2}-y,z;\ \frac{1}{4}+y,\frac{1}{4}-x,\frac{3}{4}+z;\ \frac{3}{4}-y,\frac{1}{4}-x,\frac{1}{4}+z;$ $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z;\ x,\frac{1}{2}+y,\bar{z};\ \frac{3}{4}-y,\frac{3}{4}+x,\frac{1}{4}-z;\ \frac{1}{4}+y,\frac{3}{4}+x,\frac{3}{4}-z.$	hkl: $h+k+l=2n$ $hk0$: $h,(k)=2n$ $0kl$: $k,(l)=2n$ hhl: $(l=2n)$; $2h+l=4n$
				Special: as above, plus
16	f	2	$x,\frac{1}{4}+x,\frac{1}{8};\ \bar{x},\frac{1}{4}+x,\frac{5}{8};\ \bar{x},\frac{1}{4}-x,\frac{1}{8};\ x,\frac{1}{4}-x,\frac{5}{8};$ $\bar{x},\frac{3}{4}-x,\frac{7}{8};\ x,\frac{3}{4}-x,\frac{3}{8};\ x,\frac{3}{4}+x,\frac{7}{8};\ \bar{x},\frac{3}{4}+x,\frac{3}{8}.$	hkl: $2k+l=2n+1$ or $4n$
16	e	2	$x,0,\frac{1}{4};\ x,\frac{1}{2},\frac{3}{4};\ \frac{1}{4},\frac{1}{4}-x,0;\ \frac{1}{4},\frac{3}{4}-x,0;$ $\bar{x},0,\frac{3}{4};\ \bar{x},\frac{1}{2},\frac{1}{4};\ \frac{3}{4},\frac{3}{4}+x,0;\ \frac{3}{4},\frac{1}{4}+x,0.$	hkl: $l,(h+k)=2n+1$, or $h,k,(l)=2n$
16	d	2	$0,\frac{1}{4},z;\ 0,\frac{1}{4},\frac{1}{2}+z;\ 0,\frac{1}{4},\frac{1}{4}-z;\ 0,\frac{1}{4},\frac{3}{4}-z;$ $0,\frac{3}{4},\bar{z};\ 0,\frac{3}{4},\frac{1}{2}-z;\ 0,\frac{3}{4},\frac{3}{4}+z;\ 0,\frac{3}{4},\frac{1}{4}+z.$	hkl: $l=2n$; $2k+l=4n$
16	c	$\bar{1}$	$0,0,0;\ \frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2};$ $\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{3}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{3}{4}.$	hkl: $h,k,(l)=2n$; $h+k+l=4n$
8	b	222	$0,\frac{1}{4},\frac{1}{8};\ 0,\frac{3}{4},\frac{7}{8};\ 0,\frac{1}{4},\frac{5}{8};\ 0,\frac{3}{4},\frac{3}{8}.$	hkl: $l=2n$; $2k+l=4n$
8	a	$\bar{4}$	$0,\frac{1}{4},\frac{3}{8};\ 0,\frac{3}{4},\frac{5}{8};\ 0,\frac{1}{4},\frac{7}{8};\ 0,\frac{3}{4},\frac{1}{8}.$	

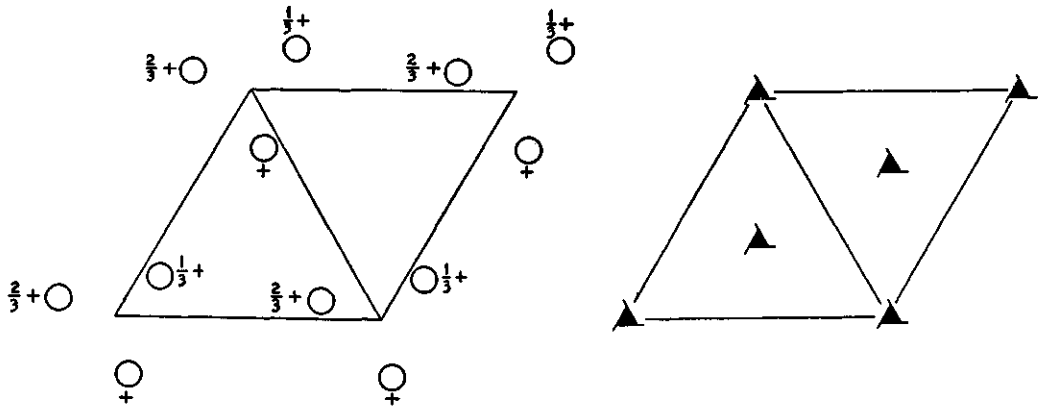


Origin on 3

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
3	d	1	$x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z.$	No conditions
				Special:
1	c	3	$\frac{2}{3},\frac{1}{3},z.$	No conditions
1	b	3	$\frac{1}{3},\frac{2}{3},z.$	
1	a	3	$0,0,z.$	

$P3_1$ C_3^2

No. 144 $P\,3_1$ 3 Trigonal

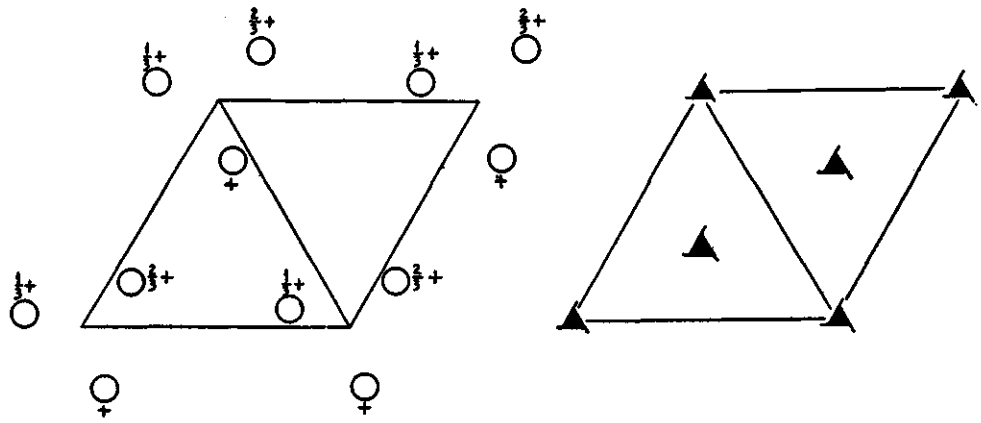


Origin on 3_1

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
3	a	1	$x,y,z;\quad \bar{y},x-y,\frac{1}{3}+z;\quad y-x,\bar{x},\frac{2}{3}+z.$	$hkil$: No conditions $000l$: $l=3n$

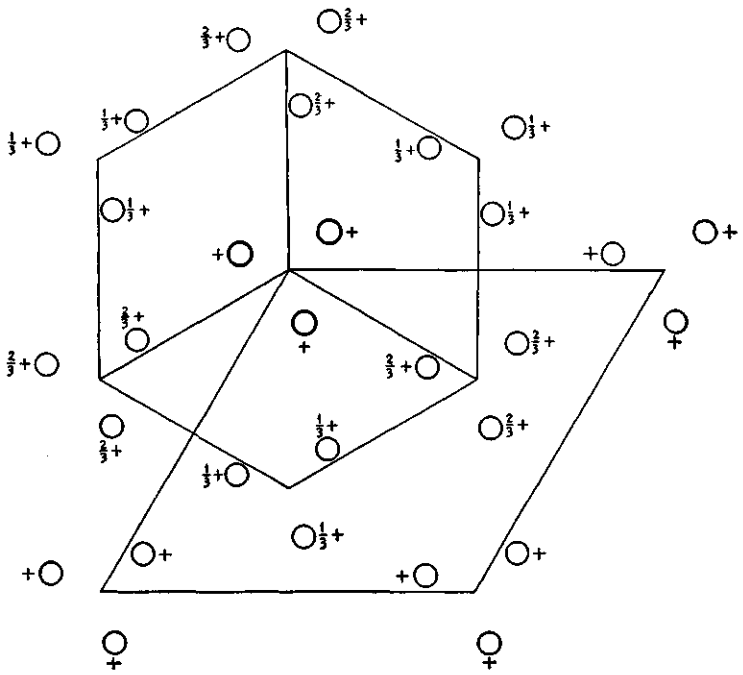
$P3_2$ C_3^3

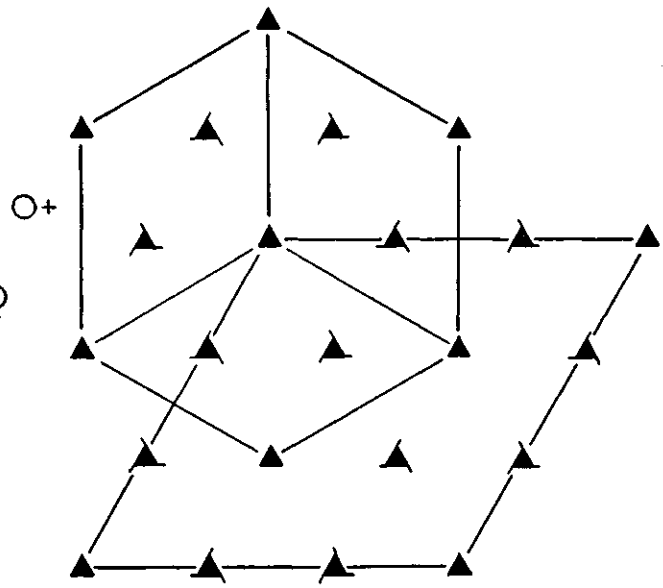
No. 145 $P\,3_2$ 3 Trigonal



Origin on 3_2

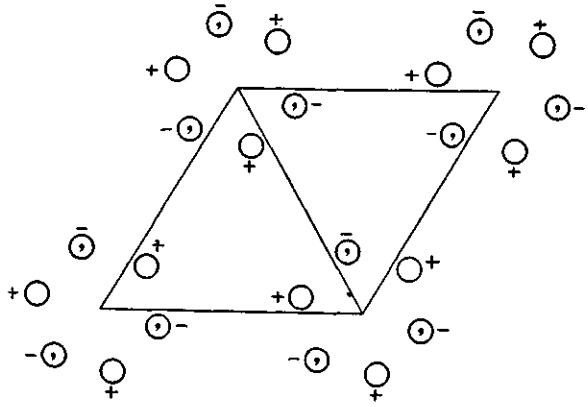
				General:
3	a	1	$x,y,z;\quad \bar{y},x-y,\frac{2}{3}+z;\quad y-x,\bar{x},\frac{1}{3}+z.$	$hkil$: No conditions $000l$: $l=3n$

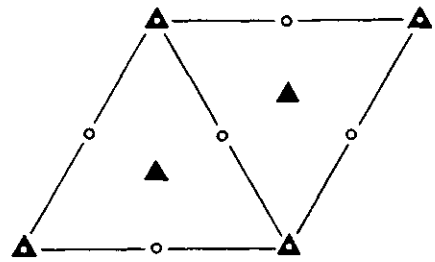




Origin on 3

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(1) RHOMBOHEDRAL AXES:	
				General:
3	*b*	1	x,y,z; z,x,y; y,z,x.	No conditions
				Special:
1	*a*	3	x,x,x.	No conditions
			(2) HEXAGONAL AXES:	
			$(0,0,0;\ \frac{1}{3},\frac{2}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3},\frac{1}{3})+$	
				General:
9	*b*	1	$x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z.$	$hkil$: $-h+k+l=3n$ $000l$: $(l=3n)$
				Special:
3	*a*	3	0,0,z.	No extra conditions





Origin at centre ($\bar{3}$)

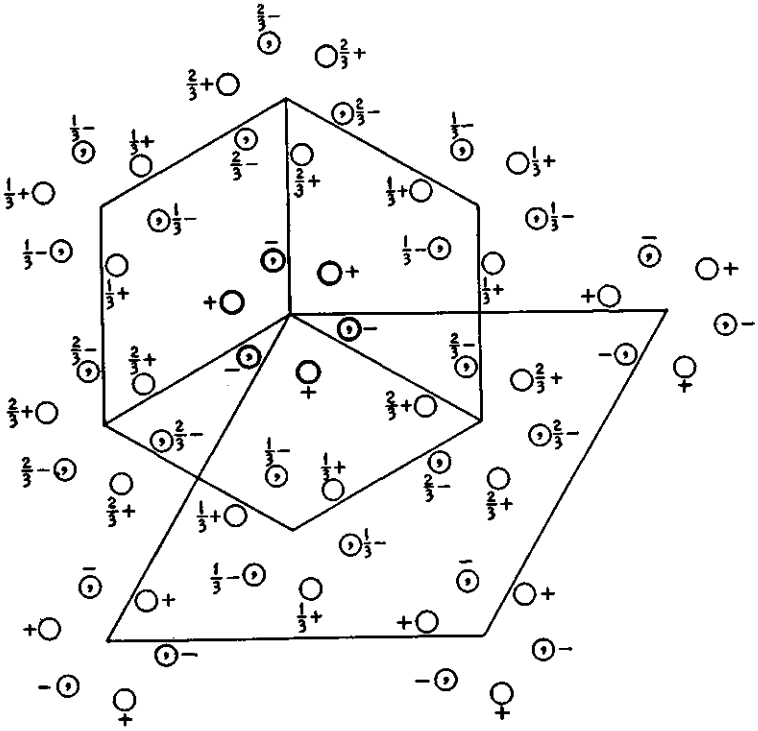
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions						Conditions limiting possible reflections
									General:
6	g	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$.						No conditions
									Special:
3	f	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.						No conditions
3	e	$\bar{1}$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$.						
2	d	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$.	1	b	$\bar{3}$	$0,0,\frac{1}{2}$.		
2	c	3	$0,0,z$; $0,0,\bar{z}$.	1	a	$\bar{3}$	$0,0,0$.		

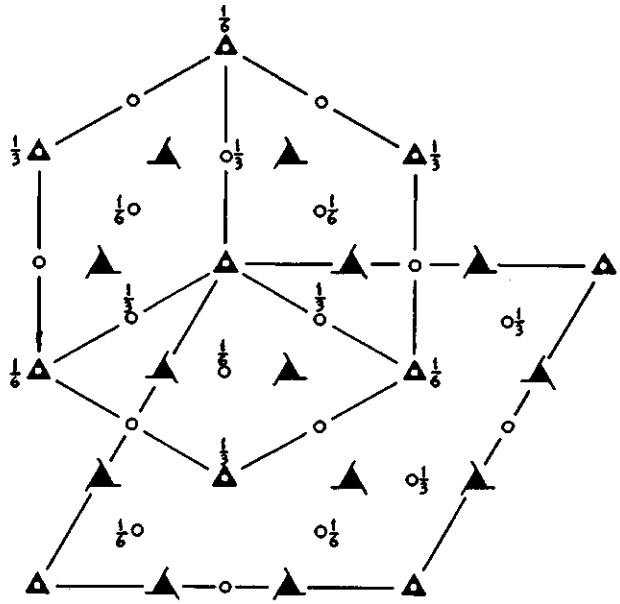
---

(2) HEXAGONAL AXES (No. 148. Continuation of p. 253):

$(0,0,0;\ \frac{1}{3},\frac{2}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3},\frac{1}{3})+$

									General:
18	f	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$.						$hkil$: $-h+k+l=3n$
									Special:
9	e	$\bar{1}$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$.						No extra conditions
9	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	3	b	$\bar{3}$	$0,0,\frac{1}{2}$.		
6	c	3	$0,0,z$; $0,0,\bar{z}$.	3	a	$\bar{3}$	$0,0,0$.		

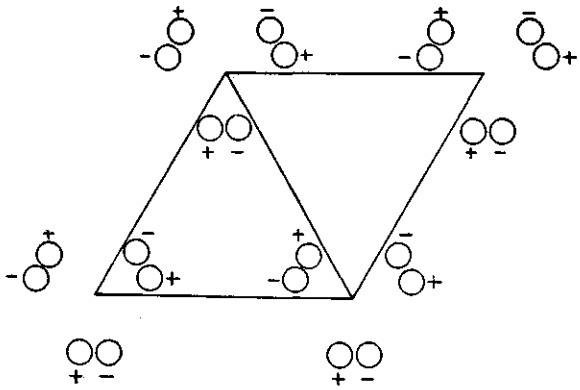


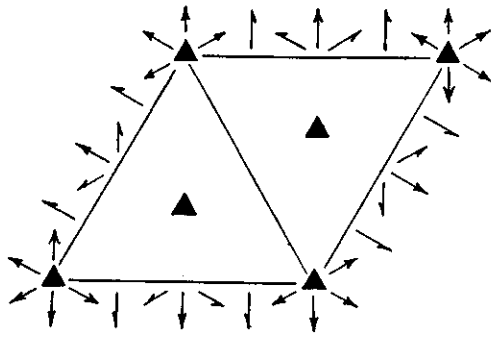


Origin at centre ($\bar{3}$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(1) RHOMBOHEDRAL AXES:	
				General:
6	*f*	1	x,y,z; z,x,y; y,z,x; $\bar{x},\bar{y},\bar{z}$; $\bar{z},\bar{x},\bar{y}$; $\bar{y},\bar{z},\bar{x}$.	No conditions
				Special:
3	*e*	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	No conditions
3	*d*	$\bar{1}$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	
2	*c*	3	x,x,x; $\bar{x},\bar{x},\bar{x}$.	
1	*b*	$\bar{3}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
1	*a*	$\bar{3}$	0,0,0.	

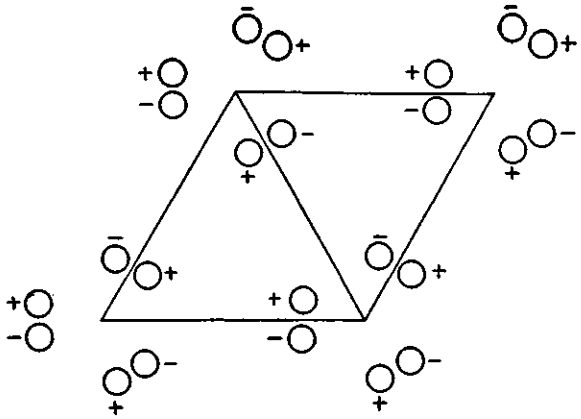
(continued on p. 252)

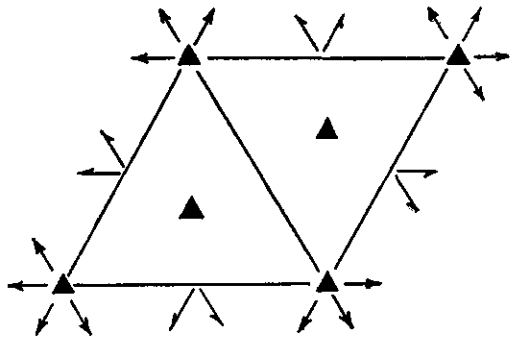




Origin at 312

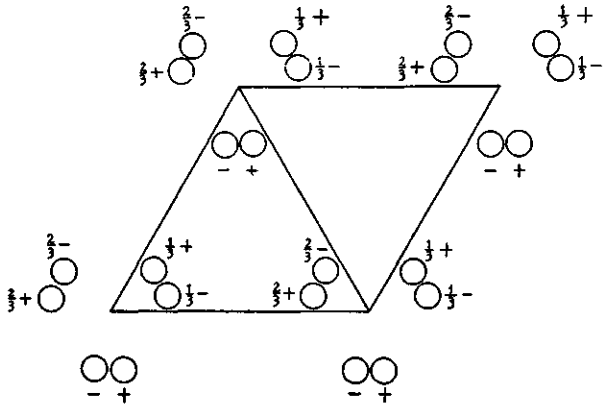
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	l	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{y},\bar{x},\bar{z}$; $x,x-y,\bar{z}$; $y-x,y,\bar{z}$.	No conditions
				Special:
3	k	2	$x,\bar{x},\frac{1}{2}$; $x,2x,\frac{1}{2}$; $2\bar{x},\bar{x},\frac{1}{2}$.	No conditions
3	j	2	$x,\bar{x},0$; $x,2x,0$; $2\bar{x},\bar{x},0$.	
2	i	3	$\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$.	
2	h	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\bar{z}$.	
2	g	3	$0,0,z$; $0,0,\bar{z}$.	
1	f	32	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$.	
1	e	32	$\frac{2}{3},\frac{1}{3},0$.	
1	d	32	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$.	
1	c	32	$\frac{1}{3},\frac{2}{3},0$.	
1	b	32	$0,0,\frac{1}{2}$.	
1	a	32	$0,0,0$.	

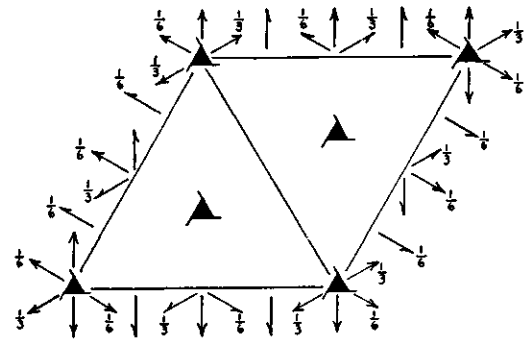




Origin at 321

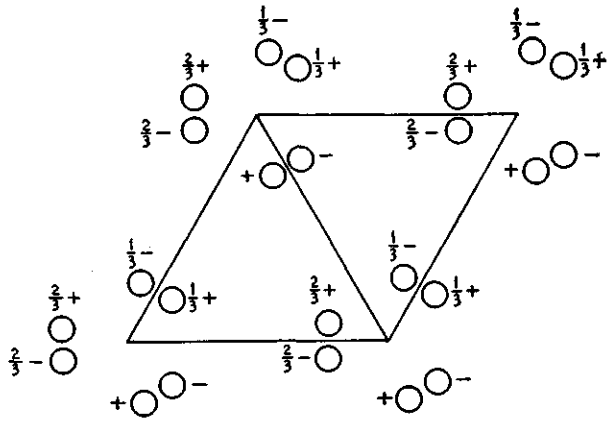
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	g	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $y,x,\bar{z}$; $\bar{x},y-x,\bar{z}$; $x-y,\bar{y},\bar{z}$.	No conditions
				Special:
3	f	2	$x,0,\frac{1}{2}$; $0,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$.	No conditions
3	e	2	$x,0,0$; $0,x,0$; $\bar{x},\bar{x},0$.	
2	d	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$.	
2	c	3	$0,0,z$; $0,0,\bar{z}$.	
1	b	32	$0,0,\frac{1}{2}$.	
1	a	32	$0,0,0$.	

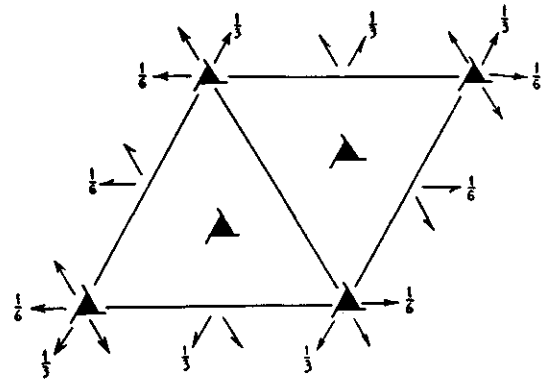




Origin at 3_112 [2-axis normal to $(10\bar{1}0)$]

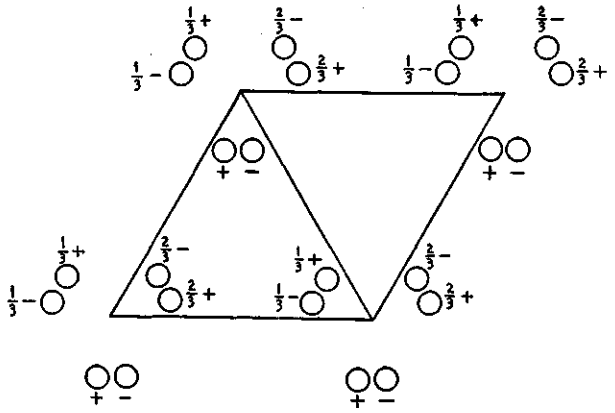
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	c	1	x,y,z; $\bar{y},x-y,\frac{1}{3}+z$; $y-x,\bar{x},\frac{2}{3}+z$; $x,x-y,\bar{z}$; $y-x,y,\frac{1}{3}-z$; $\bar{y},\bar{x},\frac{2}{3}-z$.	$hkil$: No conditions $000l$: $l=3n$
				Special: as above only
3	b	2	$x,\bar{x},\frac{5}{6}$; $x,2x,\frac{1}{6}$; $2\bar{x},\bar{x},\frac{1}{2}$.	
3	a	2	$x,\bar{x},\frac{1}{3}$; $x,2x,\frac{2}{3}$; $2\bar{x},\bar{x},0$.	

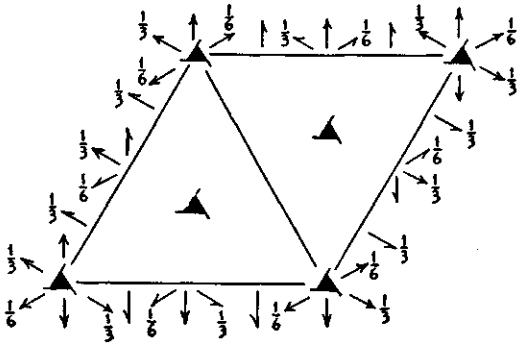




Origin at 3_121 [2-axis normal to $(11\bar{2}0)$]

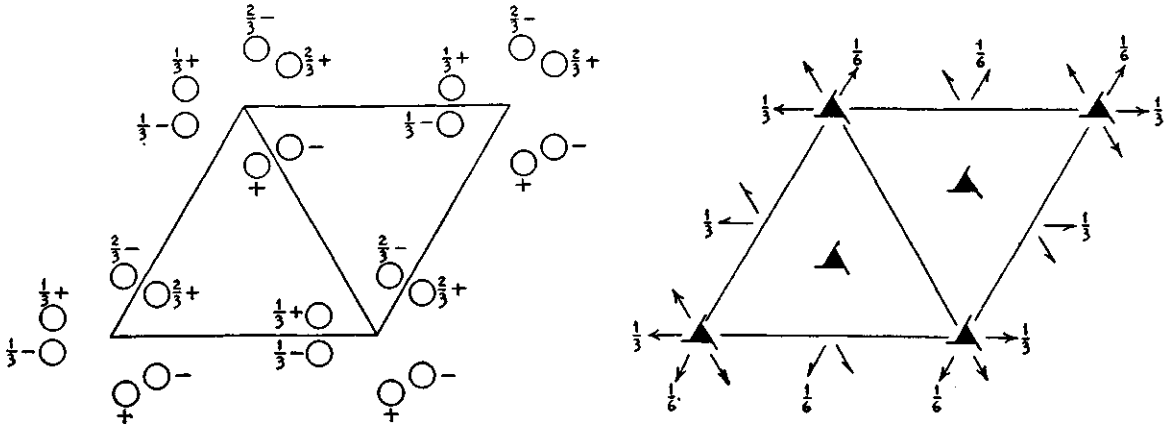
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	c	1	x,y,z; $\bar{y},x-y,\frac{1}{3}+z$; $y-x,\bar{x},\frac{2}{3}+z$; $y,x,\bar{z}$; $\bar{x},y-x,\frac{1}{3}-z$; $x-y,\bar{y},\frac{2}{3}-z$.	$hkil$: No conditions $000l$: $l=3n$
				Special: as above only
3	b	2	$x,0,\frac{5}{6}$; $0,x,\frac{1}{6}$; $\bar{x},\bar{x},\frac{1}{2}$.	
3	a	2	$x,0,\frac{1}{3}$; $0,x,\frac{2}{3}$; $\bar{x},\bar{x},0$.	





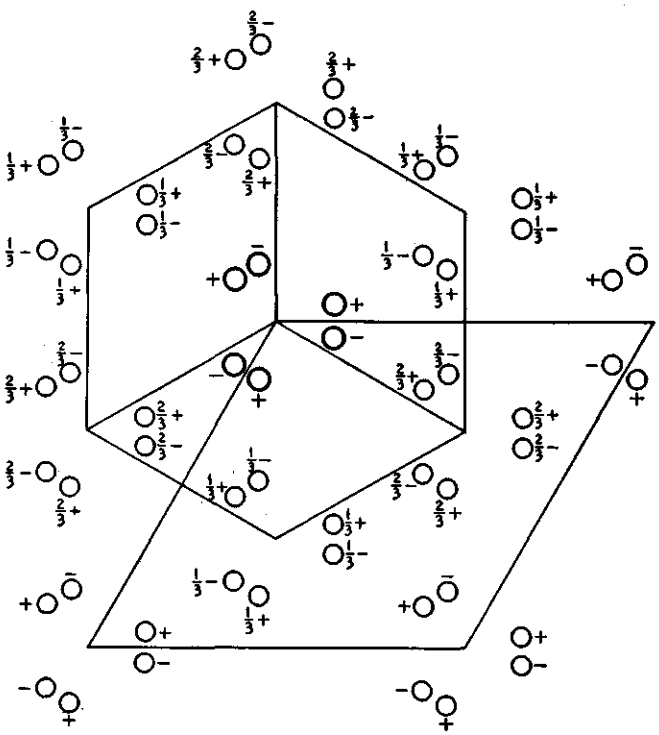
Origin at 3_212 [2-axis normal to $(10\bar{1}0)$]

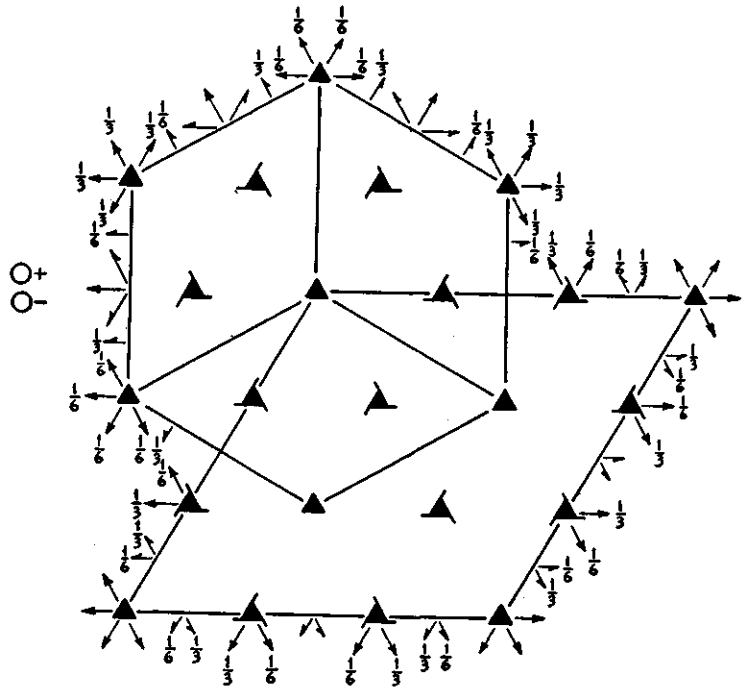
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	c	1	x,y,z; $\bar{y},x-y,\frac{2}{3}+z$; $y-x,\bar{x},\frac{1}{3}+z$; $x,x-y,\bar{z}$; $y-x,y,\frac{2}{3}-z$; $\bar{y},\bar{x},\frac{1}{3}-z$.	$hkil$: No conditions $000l$: $l=3n$
				Special: as above only
3	b	2	$x,\bar{x},\frac{1}{6}$; $x,2x,\frac{5}{6}$; $2\bar{x},\bar{x},\frac{1}{2}$.	
3	a	2	$x,\bar{x},\frac{2}{3}$; $x,2x,\frac{1}{3}$; $2\bar{x},\bar{x},0$.	



Origin at 3_221 [2-axis normal to $(11\bar{2}0)$]

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	c	1	x,y,z; $\bar{y},x-y,\frac{2}{3}+z$; $y-x,\bar{x},\frac{1}{3}+z$; $y,x,\bar{z}$; $\bar{x},y-x,\frac{2}{3}-z$; $x-y,\bar{y},\frac{1}{3}-z$.	$hkil$: No conditions $000l$: $l=3n$
				Special: as above only
3	b	2	$x,0,\frac{1}{6}$; $0,x,\frac{5}{6}$; $\bar{x},\bar{x},\frac{1}{2}$.	
3	a	2	$x,0,\frac{2}{3}$; $0,x,\frac{1}{3}$; $\bar{x},\bar{x},0$.	





Origin at 32

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(1) RHOMBOHEDRAL AXES:	
				General:
6	*f*	1	x,y,z; z,x,y; y,z,x; $\bar{y},\bar{x},\bar{z}$; $\bar{z},\bar{y},\bar{x}$; $\bar{x},\bar{z},\bar{y}$.	No conditions
				Special:
3	*e*	2	$\frac{1}{2}$,x,$\bar{x}$; $\bar{x}$,$\frac{1}{2}$,x; x,$\bar{x}$,$\frac{1}{2}$.	No conditions
3	*d*	2	0,x,$\bar{x}$; $\bar{x}$,0,x; x,$\bar{x}$,0.	
2	*c*	3	x,x,x; $\bar{x},\bar{x},\bar{x}$.	
1	*b*	32	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
1	*a*	32	0,0,0.	

(*continued on next page*)

(2) HEXAGONAL AXES:

$(0,0,0;\ \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3};\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3})+$

18	*f*	1	$x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;$ $y,x,\bar{z};\ \bar{x},y-x,\bar{z};\ x-y,\bar{y},\bar{z}.$
9	*e*	2	$x,0,\tfrac{1}{2};\ 0,x,\tfrac{1}{2};\ \bar{x},\bar{x},\tfrac{1}{2}.$
9	*d*	2	$x,0,0;\ 0,x,0;\ \bar{x},\bar{x},0.$
6	*c*	3	$0,0,z;\ 0,0,\bar{z}.$
3	*b*	32	$0,0,\tfrac{1}{2}.$
3	*a*	32	$0,0,0.$

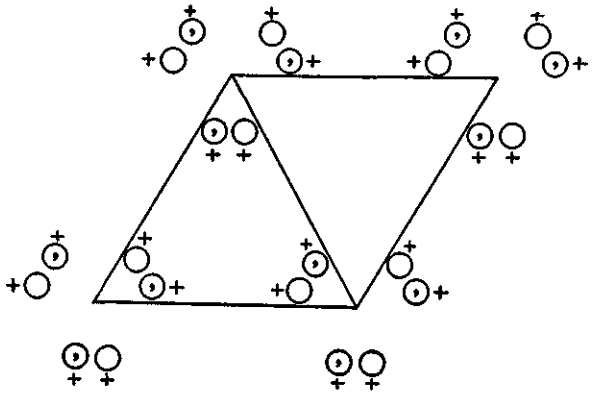
General:

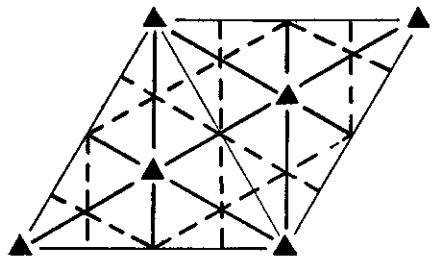
$hkil$: $-h+k+l=3n$
$000l$: $(l=3n)$

Special: as above only

$P3m1$ C_{3v}^{1}

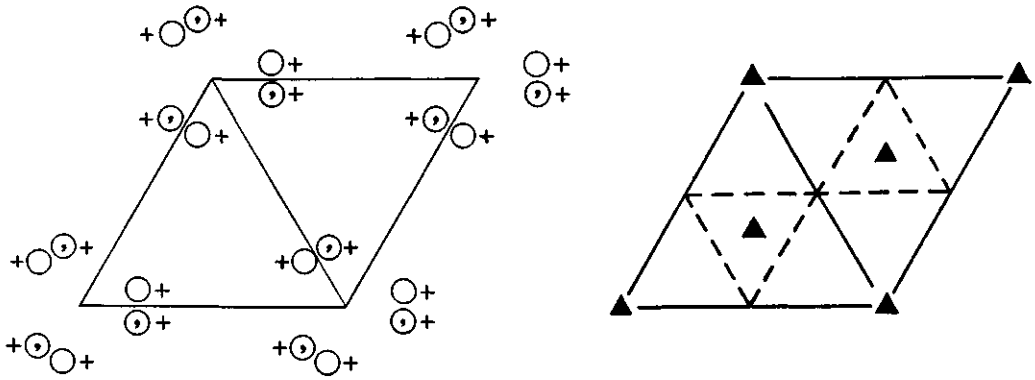
No. 156 $P\,3\,m\,1$ $3\,m\,1$ Trigonal





Origin on $3m1$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	e	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{y},\bar{x},z$; $x,x-y,z$; $y-x,y,z$.	No conditions
				Special:
3	d	m	$x,\bar{x},z$; $x,2x,z$; $2\bar{x},\bar{x},z$.	No conditions
1	c	$3m$	$\frac{2}{3},\frac{1}{3},z$.	
1	b	$3m$	$\frac{1}{3},\frac{2}{3},z$.	
1	a	$3m$	$0,0,z$.	

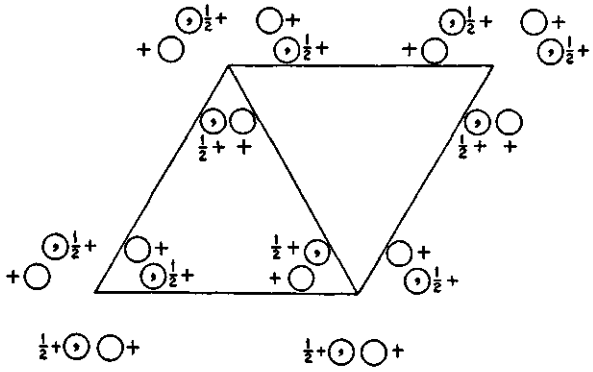


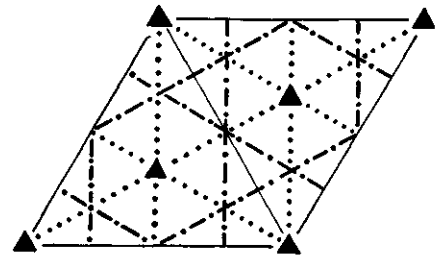
Origin on 31*m*

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	*d*	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; y,x,z; $\bar{x},y-x,z$; $x-y,\bar{y},z$.	No conditions
				Special:
3	*c*	*m*	$x,0,z$; $0,x,z$; $\bar{x},\bar{x},z$.	No conditions
2	*b*	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},z$.	
1	*a*	3*m*	$0,0,z$.	

$P3c1$ C_{3v}^{3}

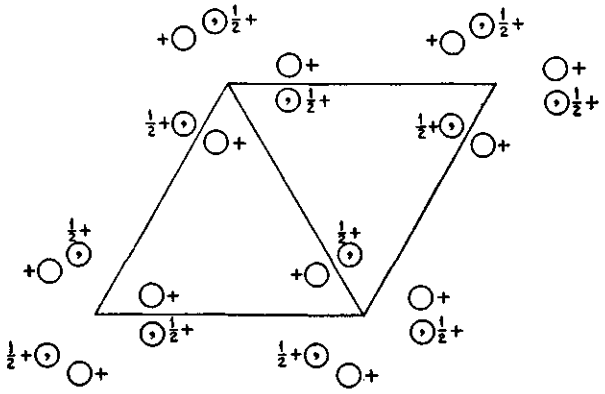
No. 158 $P\,3\,c\,1$ $3\,m\,1$ Trigonal

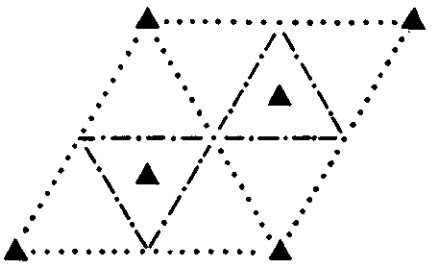




Origin on 3

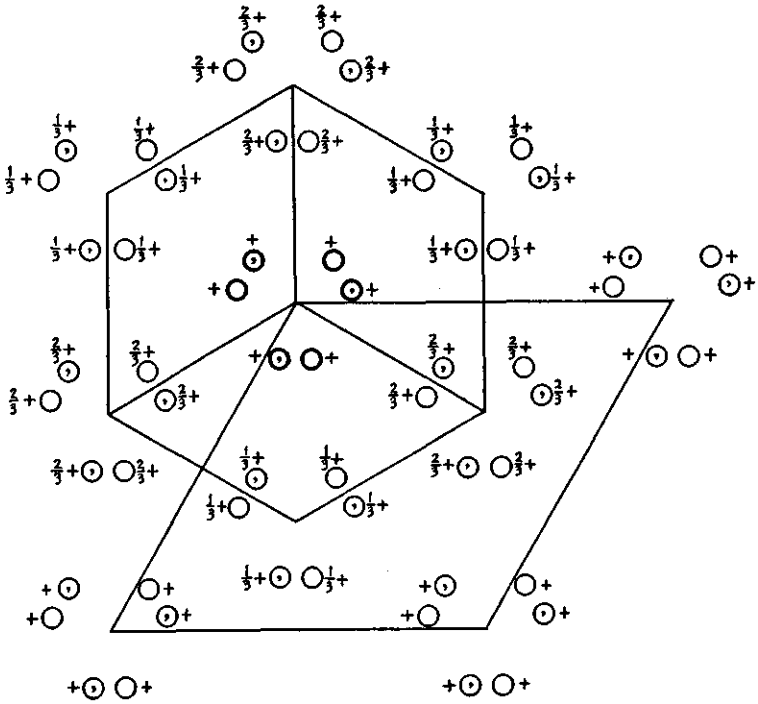
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	d	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{y},\bar{x},\frac{1}{2}+z$; $x,x-y,\frac{1}{2}+z$; $y-x,y,\frac{1}{2}+z$.	$hkil$: No conditions $hh2\bar{h}l$: No conditions $h\bar{h}0l$: $l=2n$
				Special: as above, plus
2	c	3	$\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$.	$hkil$: $l=2n$
2	b	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}+z$.	
2	a	3	$0,0,z$; $0,0,\frac{1}{2}+z$.	

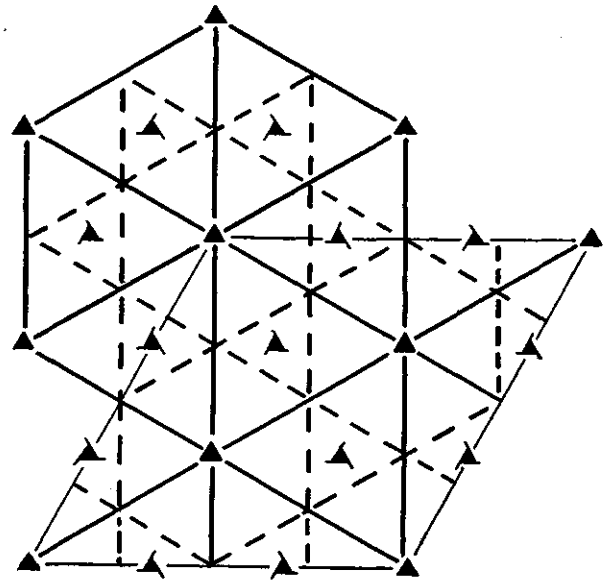




Origin on 3

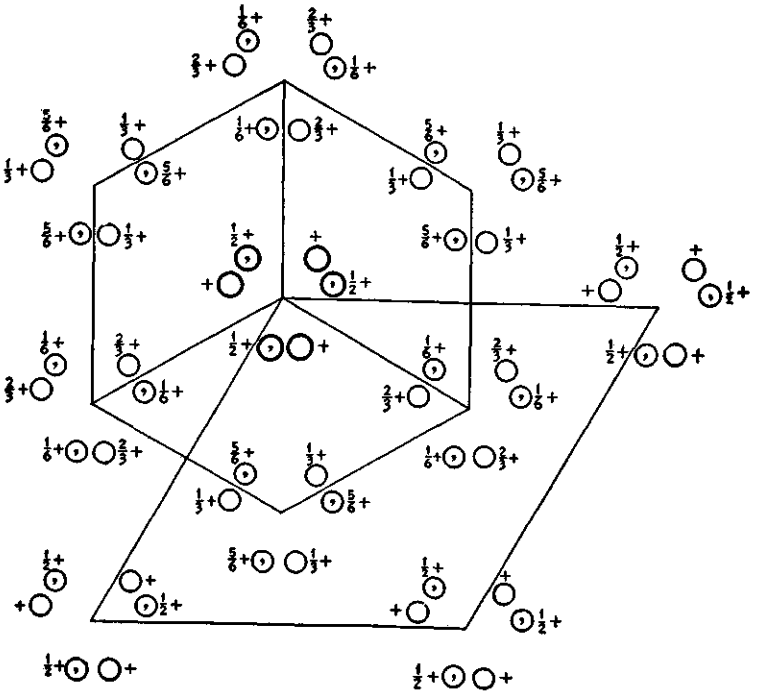
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	*c*	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $y,x,\frac{1}{2}+z$; $\bar{x},y-x,\frac{1}{2}+z$; $x-y,\bar{y},\frac{1}{2}+z$.	*hkil*: No conditions *hh*2$\bar{h}$*l*: $l=2n$ *h*$\bar{h}$0*l*: No conditions
				Special: as above, plus
2	*b*	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$.	*hkil*: If $h-k=3n$, then $l=2n$
2	*a*	3	$0,0,z$; $0,0,\frac{1}{2}+z$.	*hkil*: $l=2n$

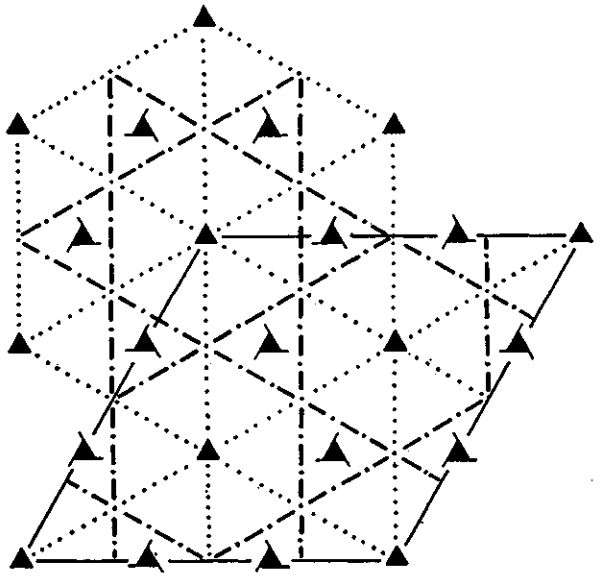




Origin on $3m$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(1) RHOMBOHEDRAL AXES:	
				General:
6	c	1	x,y,z; z,x,y; y,z,x; y,x,z; z,y,x; x,z,y.	No conditions
				Special:
3	b	m	x,x,z; x,z,x; z,x,x.	No conditions
1	a	$3m$	x,x,x.	
			(2) HEXAGONAL AXES:	
			$(0,0,0;\ \frac{1}{3},\frac{2}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3},\frac{1}{3})+$	
				General:
18	c	1	$x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;$ $\bar{y},\bar{x},z;\ x,x-y,z;\ y-x,y,z.$	$hkil$: $-h+k+l=3n$ $hh2\bar{h}l$: $(l=3n)$ $h\bar{h}0l$: $(h+l=3n)$
				Special: as above only
9	b	m	$x,\bar{x},z;\ x,2x,z;\ 2\bar{x},\bar{x},z.$	
3	a	$3m$	$0,0,z.$	



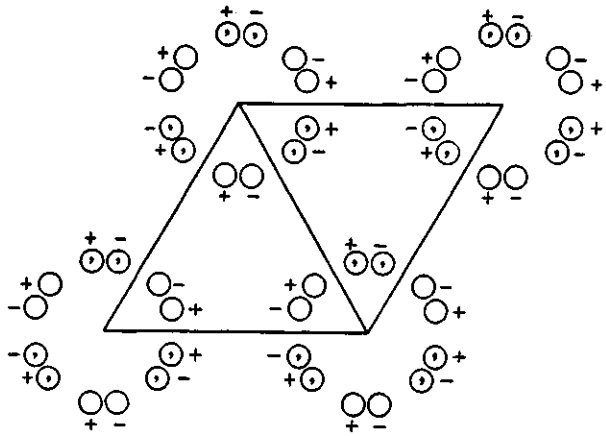


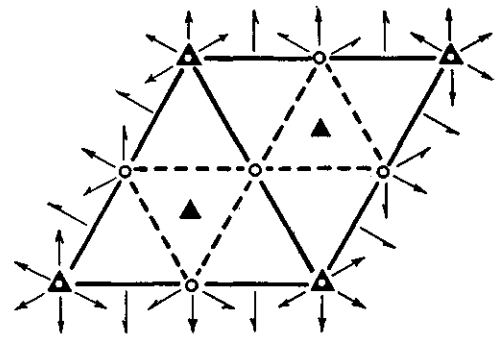
Origin on 3

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(1) RHOMBOHEDRAL AXES:	
				General:
6	*b*	1	x,y,z; z,x,y; y,z,x; $\frac{1}{2}$+y,$\frac{1}{2}$+x,$\frac{1}{2}$+z; $\frac{1}{2}$+z,$\frac{1}{2}$+y,$\frac{1}{2}$+x; $\frac{1}{2}$+x,$\frac{1}{2}$+z,$\frac{1}{2}$+y.	hkl: No conditions hhl: $l=2n$
				Special: as above, plus
2	*a*	3	x,x,x; $\frac{1}{2}$+x,$\frac{1}{2}$+x,$\frac{1}{2}$+x.	hkl: $h+k+l=2n$
			(2) HEXAGONAL AXES:	
			(0,0,0; $\frac{1}{3}$,$\frac{2}{3}$,$\frac{2}{3}$; $\frac{2}{3}$,$\frac{1}{3}$,$\frac{1}{3}$)+	
				General:
18	*b*	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{y},\bar{x},\frac{1}{2}+z$; $x,x-y,\frac{1}{2}+z$; $y-x,y,\frac{1}{2}+z$.	$hkil$: $-h+k+l=3n$ $hh2\bar{h}l$: $(l=3n)$ $h\bar{h}0l$: $(h+l=3n)$; $l=2n$
				Special: as above, plus
6	*a*	3	$0,0,z$; $0,0,\frac{1}{2}+z$.	$hkil$: $l=2n$

$P\bar{3}1m$ D_{3d}^{1}

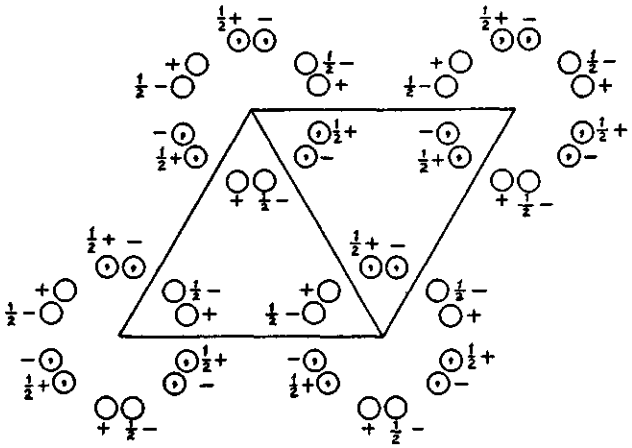
No. 162 $P\bar{3}12/m$ $\bar{3}1m$ Trigonal

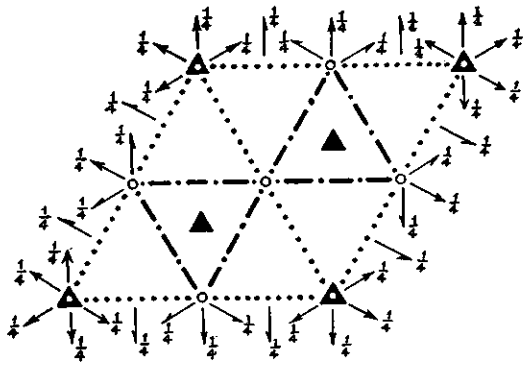




Origin at centre ($\bar{3}1m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	l	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$; y,x,z; $\bar{x},y-x,z$; $x-y,\bar{y},z$; $\bar{y},\bar{x},\bar{z}$; $x,x-y,\bar{z}$; $y-x,y,\bar{z}$.	No conditions
				Special:
6	k	m	$x,0,z$; $0,x,z$; $\bar{x},\bar{x},z$; $\bar{x},0,\bar{z}$; $0,\bar{x},\bar{z}$; $x,x,\bar{z}$.	No conditions
6	j	2	$x,\bar{x},\frac{1}{2}$; $x,2x,\frac{1}{2}$; $2\bar{x},\bar{x},\frac{1}{2}$; $\bar{x},x,\frac{1}{2}$; $\bar{x},2\bar{x},\frac{1}{2}$; $2x,x,\frac{1}{2}$.	
6	i	2	$x,\bar{x},0$; $x,2x,0$; $2\bar{x},\bar{x},0$; $\bar{x},x,0$; $\bar{x},2\bar{x},0$; $2x,x,0$.	
4	h	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\bar{z}$; $\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$.	
3	g	$2/m$	$\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
3	f	$2/m$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$.	
2	e	$3m$	$0,0,z$; $0,0,\bar{z}$.	
2	d	32	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}$.	
2	c	32	$\frac{1}{3},\frac{2}{3},0$; $\frac{2}{3},\frac{1}{3},0$.	
1	b	$\bar{3}m$	$0,0,\frac{1}{2}$.	
1	a	$\bar{3}m$	$0,0,0$.	



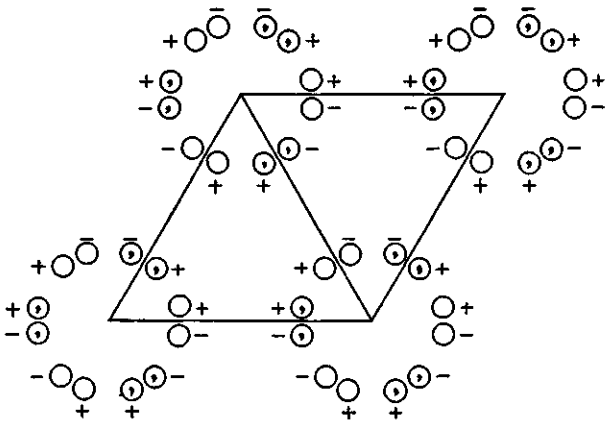


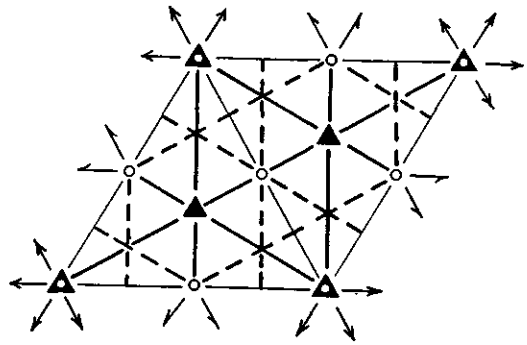
Origin at centre ($\bar{3}$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	i	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$; $y,x,\frac{1}{2}+z$; $\bar{x},y-x,\frac{1}{2}+z$; $x-y,\bar{y},\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}-z$; $x,x-y,\frac{1}{2}-z$; $y-x,y,\frac{1}{2}-z$.	$hkil$: No conditions $hh2\bar{h}l$: $l=2n$ $h\bar{h}0l$: No conditions
				Special: as above, plus
6	h	2	$x,\bar{x},\frac{1}{4}$; $x,2x,\frac{1}{4}$; $2\bar{x},\bar{x},\frac{1}{4}$; $\bar{x},x,\frac{3}{4}$; $\bar{x},2\bar{x},\frac{3}{4}$; $2x,x,\frac{3}{4}$.	no extra conditions
6	g	$\bar{1}$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	$hkil$: $l=2n$
4	f	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}-z$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$.	$hkil$: If $h-k=3n$, then $l=2n$
4	e	3	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	$hkil$: $l=2n$
2	d	32	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$; $\frac{1}{3},\frac{2}{3},\frac{3}{4}$.	$hkil$: If $h-k=3n$, then $l=2n$
2	c	32	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$; $\frac{2}{3},\frac{1}{3},\frac{3}{4}$.	
2	b	$\bar{3}$	$0,0,0$; $0,0,\frac{1}{2}$.	$hkil$: $l=2n$
2	a	32	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	

$P\bar{3}m1$ D_{3d}^{3}

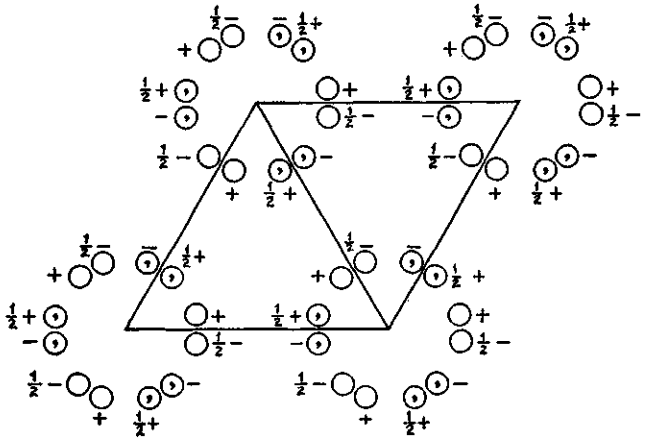
No. 164 $P\,\bar{3}\,2/m\,1$ $\bar{3}\,m\,1$ Trigonal

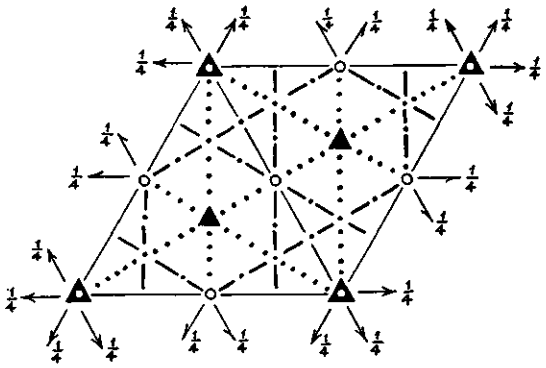




Origin at centre ($\bar{3}m1$)

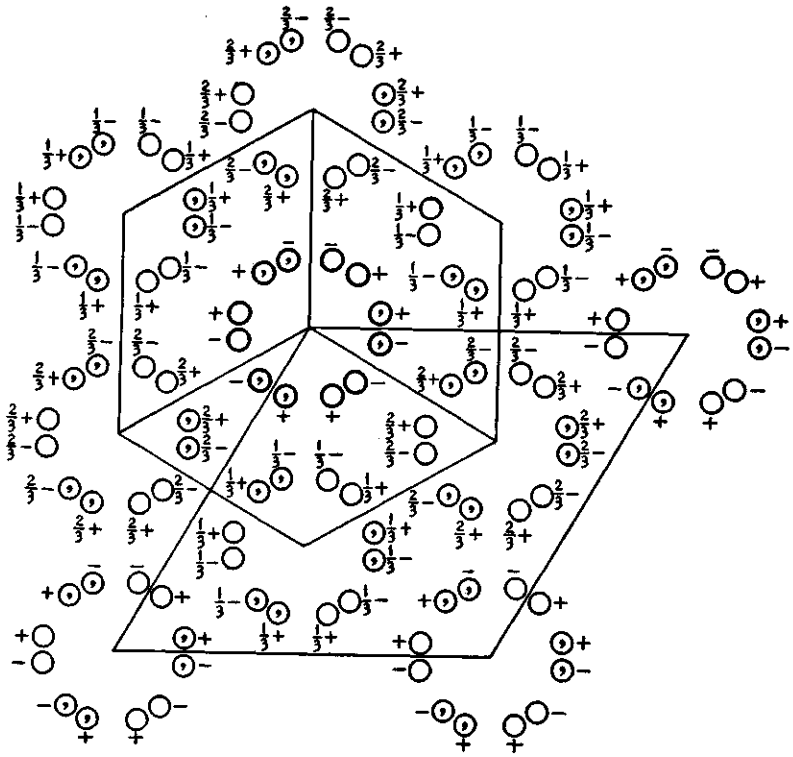
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	j	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$; $\bar{y},\bar{x},z$; $x,x-y,z$; $y-x,y,z$; $y,x,\bar{z}$; $\bar{x},y-x,\bar{z}$; $x-y,\bar{y},\bar{z}$.	No conditions
				Special:
6	i	m	$x,\bar{x},z$; $x,2x,z$; $2\bar{x},\bar{x},z$; $\bar{x},x,\bar{z}$; $\bar{x},2\bar{x},\bar{z}$; $2x,x,\bar{z}$.	No conditions
6	h	2	$x,0,\frac{1}{2}$; $0,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $\bar{x},0,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$; $x,x,\frac{1}{2}$.	
6	g	2	$x,0,0$; $0,x,0$; $\bar{x},\bar{x},0$; $\bar{x},0,0$; $0,\bar{x},0$; $x,x,0$.	
3	f	$2/m$	$\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
3	e	$2/m$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$.	
2	d	$3m$	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$.	
2	c	$3m$	$0,0,z$; $0,0,\bar{z}$.	
1	b	$\bar{3}m$	$0,0,\frac{1}{2}$.	
1	a	$\bar{3}m$	$0,0,0$.	





Origin at centre ($\bar{3}$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	g	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$; $\bar{y},\bar{x},\frac{1}{2}+z$; $x,x-y,\frac{1}{2}+z$; $y-x,y,\frac{1}{2}+z$; $y,x,\frac{1}{2}-z$; $\bar{x},y-x,\frac{1}{2}-z$; $x-y,\bar{y},\frac{1}{2}-z$.	$hkil$: No conditions $hh2\bar{h}l$: No conditions $h\bar{h}0l$: $l=2n$
				Special: as above, plus
6	f	2	$x,0,\frac{1}{4}$; $0,x,\frac{1}{4}$; $\bar{x},\bar{x},\frac{1}{4}$; $\bar{x},0,\frac{3}{4}$; $0,\bar{x},\frac{3}{4}$; $x,x,\frac{3}{4}$.	No extra conditions
6	e	$\bar{1}$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	$hkil$: $l=2n$
4	d	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}+z$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}-z$.	
4	c	3	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	
2	b	$\bar{3}$	$0,0,0$; $0,0,\frac{1}{2}$.	
2	a	32	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	



Origin at centre ($\bar{3}m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(1) RHOMBOHEDRAL AXES:	
				General:
12	i	1	x,y,z; z,x,y; y,z,x; y,x,z; z,y,x; x,z,y; $\bar{x},\bar{y},\bar{z}$; $\bar{z},\bar{x},\bar{y}$; $\bar{y},\bar{z},\bar{x}$; $\bar{y},\bar{x},\bar{z}$; $\bar{z},\bar{y},\bar{x}$; $\bar{x},\bar{z},\bar{y}$.	No conditions
				Special:
6	h	m	x,x,z; x,z,x; z,x,x; $\bar{x},\bar{x},\bar{z}$; $\bar{x},\bar{z},\bar{x}$; $\bar{z},\bar{x},\bar{x}$.	No conditions
6	g	2	$x,\bar{x},\frac{1}{2}$; $\bar{x},\frac{1}{2},x$; $\frac{1}{2},x,\bar{x}$; $\bar{x},x,\frac{1}{2}$; $x,\frac{1}{2},\bar{x}$; $\frac{1}{2},\bar{x},x$.	
6	f	2	$x,\bar{x},0$; $\bar{x},0,x$; $0,x,\bar{x}$; $\bar{x},x,0$; $x,0,\bar{x}$; $0,\bar{x},x$.	
3	e	$2/m$	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	
3	d	$2/m$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	
2	c	$3m$	x,x,x; $\bar{x},\bar{x},\bar{x}$.	
1	b	$\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
1	a	$\bar{3}m$	0,0,0.	

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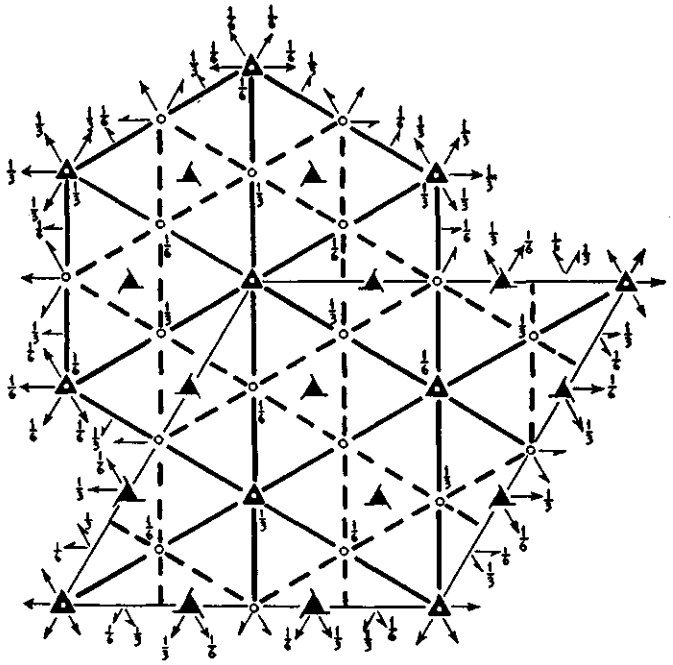
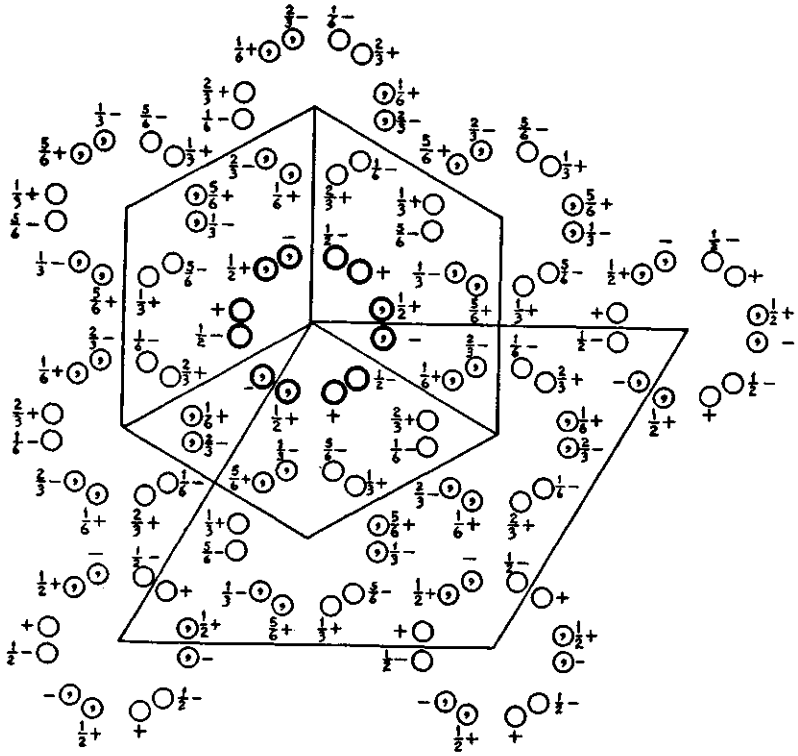


Origin at centre ($\bar{3}$m)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(2) HEXAGONAL AXES: $(0,0,0;\ \frac{1}{3},\frac{2}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3},\frac{1}{3})+$	
				General:
36	*i*	1	$x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;$ $\bar{x},\bar{y},\bar{z};\ y,y-x,\bar{z};\ x-y,x,\bar{z};$ $\bar{y},\bar{x},z;\ x,x-y,z;\ y-x,y,z;$ $y,x,\bar{z};\ \bar{x},y-x,\bar{z};\ x-y,\bar{y},\bar{z}.$	*hkil*: $-h+k+l=3n$ *hh*2*hl*: $(l=3n)$ *hh*0*l*: $(h+l=3n)$
				Special: as above only
18	*h*	*m*	$x,\bar{x},z;\ x,2x,z;\ 2\bar{x},\bar{x},z;$ $\bar{x},x,\bar{z};\ \bar{x},2\bar{x},\bar{z};\ 2x,x,\bar{z}.$	
18	*g*	2	$x,0,\frac{1}{2};\ 0,x,\frac{1}{2};\ \bar{x},\bar{x},\frac{1}{2};\ \bar{x},0,\frac{1}{2};\ 0,\bar{x},\frac{1}{2};\ x,x,\frac{1}{2}.$	
18	*f*	2	$x,0,0;\ 0,x,0;\ \bar{x},\bar{x},0;\ \bar{x},0,0;\ 0,\bar{x},0;\ x,x,0.$	
9	*e*	2/*m*	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ \frac{1}{2},\frac{1}{2},0.$	
9	*d*	2/*m*	$\frac{1}{2},0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	
6	*c*	3*m*	$0,0,z;\ 0,0,\bar{z}.$	
3	*b*	$\bar{3}m$	$0,0,\frac{1}{2}.$	
3	*a*	$\bar{3}m$	$0,0,0.$	



Origin at centre ($\bar{3}$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(1) RHOMBOHEDRAL AXES:	
				General:
12	f	1	x,y,z; z,x,y; y,z,x; $\bar{x},\bar{y},\bar{z}$; $\bar{z},\bar{x},\bar{y}$; $\bar{y},\bar{z},\bar{x}$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+z,\frac{1}{2}+y,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+z,\frac{1}{2}+y$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}-z,\frac{1}{2}-y,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}-z,\frac{1}{2}-y$.	hkl: No conditions hhl: $l=2n$
				Special: as above, plus
6	e	2	$x,\frac{1}{2}-x,\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{4},x$; $\frac{1}{4},x,\frac{1}{2}-x$; $\bar{x},\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{2}+x,\frac{3}{4},\bar{x}$; $\frac{3}{4},\bar{x},\frac{1}{2}+x$.	no extra conditions
6	d	$\bar{1}$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	hkl: $h+k+l=2n$
4	c	3	x,x,x; $\bar{x},\bar{x},\bar{x}$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}+x$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}-x$.	
2	b	$\bar{3}$	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
2	a	32	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$.	

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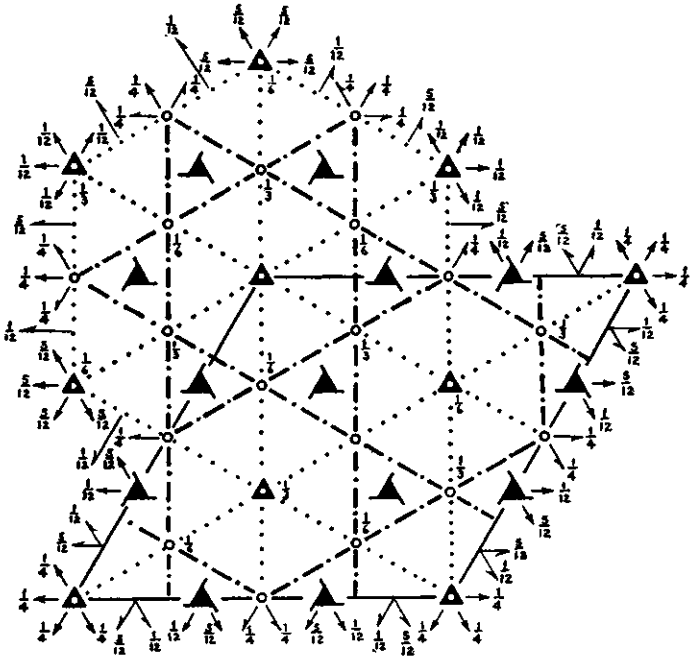
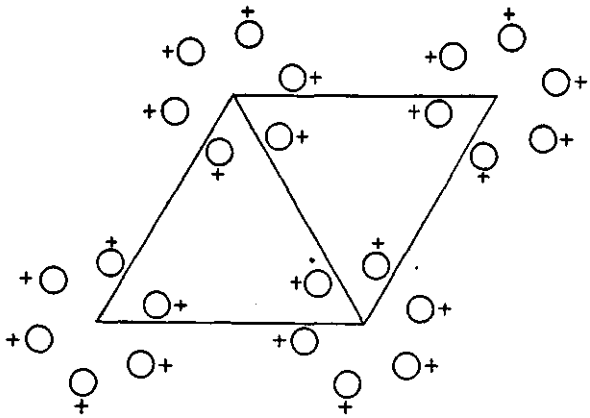
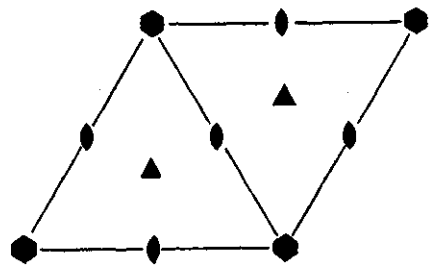


Origin at centre ($\bar{3}$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(2) HEXAGONAL AXES:	
			$(0,0,0;\ \frac{1}{3},\frac{2}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3},\frac{1}{3})+$	
				General:
36	f	1	$x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;$ $\bar{x},\bar{y},\bar{z};\ y,y-x,\bar{z};\ x-y,x,\bar{z};$ $\bar{y},\bar{x},\frac{1}{2}+z;\ x,x-y,\frac{1}{2}+z;\ y-x,y,\frac{1}{2}+z;$ $y,x,\frac{1}{2}-z;\ \bar{x},y-x,\frac{1}{2}-z;\ x-y,\bar{y},\frac{1}{2}-z.$	$hkil$: $-h+k+l=3n$ $hh2\bar{h}l$: $(l=3n)$ $h\bar{h}0l$: $(h+l=3n)$; $l=2n$
				Special: as above, plus
18	e	2	$x,0,\frac{1}{4};\ 0,x,\frac{1}{4};\ \bar{x},\bar{x},\frac{1}{4};\ \bar{x},0,\frac{3}{4};\ 0,\bar{x},\frac{3}{4};\ x,x,\frac{3}{4}.$	no extra conditions
18	d	$\bar{1}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ \frac{1}{2},\frac{1}{2},0;\ \frac{1}{2},0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	$hkil$: $l=2n$
12	c	3	$0,0,z;\ 0,0,\bar{z};\ 0,0,\frac{1}{2}+z;\ 0,0,\frac{1}{2}-z.$	
6	b	$\bar{3}$	$0,0,0;\ 0,0,\frac{1}{2}.$	
6	a	32	$0,0,\frac{1}{4};\ 0,0,\frac{3}{4}.$	

No. 168 $P\,6$ 6 Hexagonal

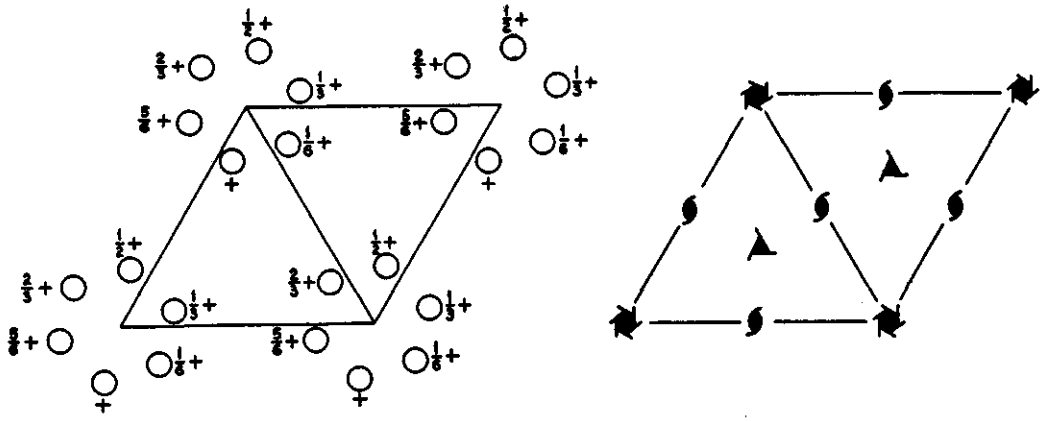




Origin on 6

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	d	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},z$; $y,y-x,z$; $x-y,x,z$.	$hkil$: No conditions
				Special:
3	c	2	$\frac{1}{2},0,z$; $0,\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},z$.	$hkil$: No conditions
2	b	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},z$.	
1	a	6	$0,0,z$.	

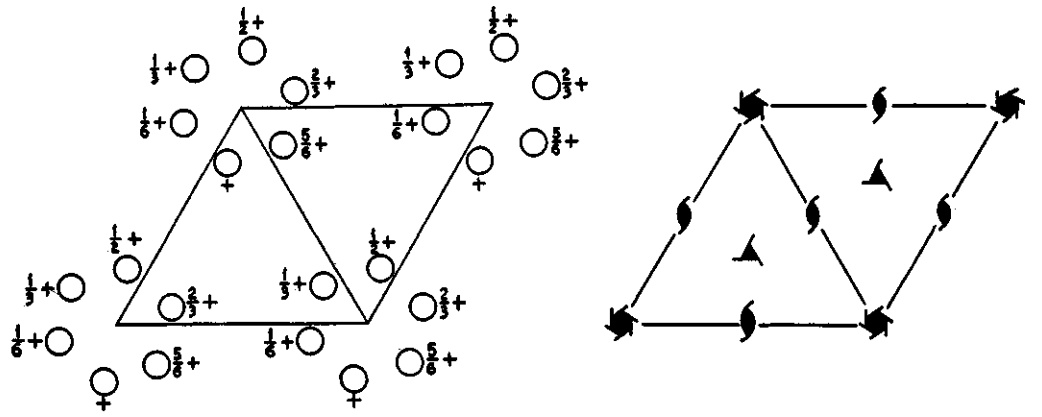
Hexagonal 6 — $P\,6_1$ — No. 169 — $P6_1$ C_6^2



Origin on 6_1

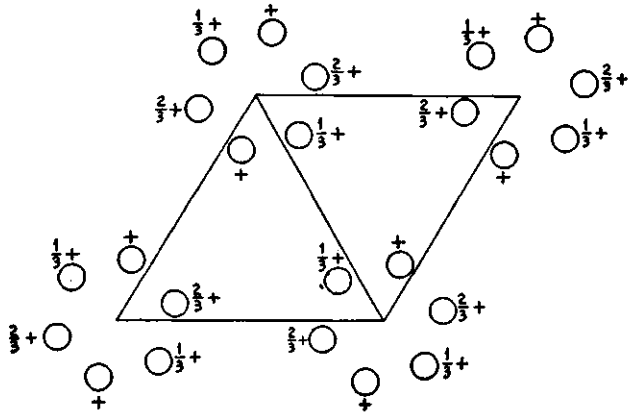
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions			Conditions limiting possible reflections
						General:
6	a	1	x,y,z;	$\bar{y},x-y,\frac{1}{3}+z$;	$y-x,\bar{x},\frac{2}{3}+z$;	$hkil$: No conditions
			$\bar{x},\bar{y},\frac{1}{2}+z$;	$y,y-x,\frac{5}{6}+z$;	$x-y,x,\frac{1}{6}+z$.	$000l$: $l=6n$

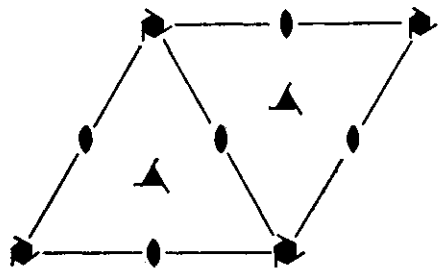
Hexagonal 6 — $P\,6_5$ — No. 170 — $P6_5$ C_6^3



Origin on 6_5

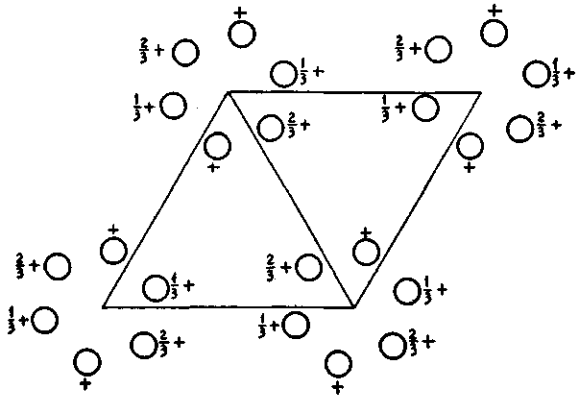
						General:
6	a	1	x,y,z;	$\bar{y},x-y,\frac{2}{3}+z$;	$y-x,\bar{x},\frac{1}{3}+z$;	$hkil$: No conditions
			$\bar{x},\bar{y},\frac{1}{2}+z$;	$y,y-x,\frac{1}{6}+z$;	$x-y,x,\frac{5}{6}+z$.	$000l$: $l=6n$

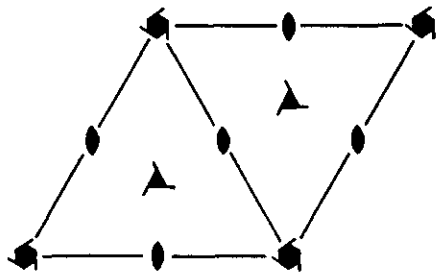




Origin on 6_2

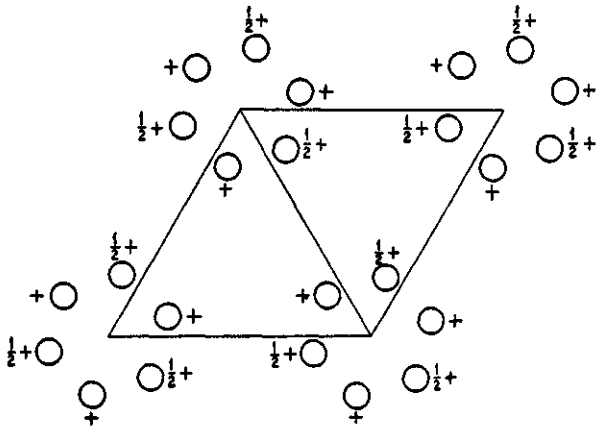
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	c	1	x,y,z; $\bar{y},x-y,\frac{2}{3}+z$; $y-x,\bar{x},\frac{1}{3}+z$; $\bar{x},\bar{y},z$; $y,y-x,\frac{2}{3}+z$; $x-y,x,\frac{1}{3}+z$.	$hkil$: No conditions $000l$: $l=3n$
				Special:
3	b	2	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},0,\frac{2}{3}+z$; $0,\frac{1}{2},\frac{1}{3}+z$.	$hkil$: If $h=2n$ and $k=2n$, then $l=3n$
3	a	2	$0,0,z$; $0,0,\frac{1}{3}+z$; $0,0,\frac{2}{3}+z$.	$hkil$: $l=3n$

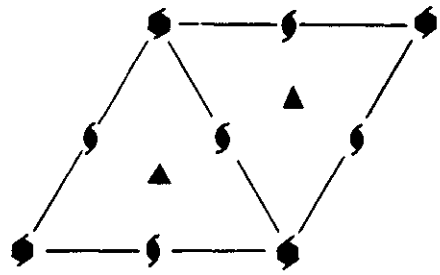




Origin on 6_4

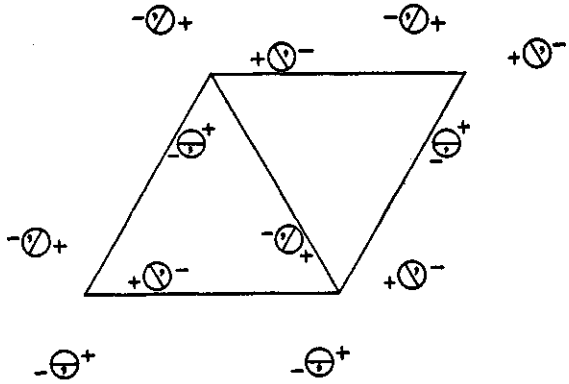
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	c	1	x,y,z; $\bar{y},x-y,\frac{1}{3}+z$; $y-x,\bar{x},\frac{2}{3}+z$; $\bar{x},\bar{y},z$; $y,y-x,\frac{1}{3}+z$; $x-y,x,\frac{2}{3}+z$.	$hkil$: No conditions $000l$: $l=3n$
				Special:
3	b	2	$\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},0,\frac{1}{3}+z$; $0,\frac{1}{2},\frac{2}{3}+z$.	$hkil$: If $h=2n$ and $k=2n$, then $l=3n$
3	a	2	$0,0,z$; $0,0,\frac{1}{3}+z$; $0,0,\frac{2}{3}+z$.	$hkil$: $l=3n$

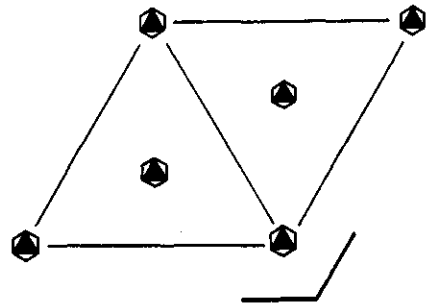




Origin on 6_3

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	c	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,y-x,\frac{1}{2}+z$; $x-y,x,\frac{1}{2}+z$.	$hkil$: No conditions $000l$: $l=2n$
				Special: as above, plus
2	b	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$.	$hkil$: If $h-k=3n$, then $l=2n$
2	a	3	$0,0,z$; $0,0,\frac{1}{2}+z$.	$hkil$: $l=2n$

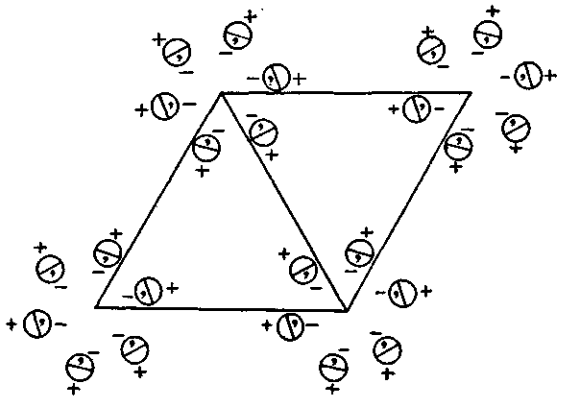


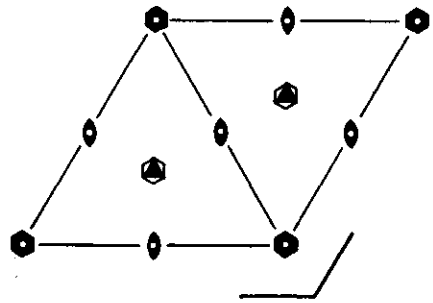


Origin at $\bar{6}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	l	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $x,y,\bar{z}$; $\bar{y},x-y,\bar{z}$; $y-x,\bar{x},\bar{z}$.	$hkil$: No conditions
				Special:
3	k	m	$x,y,\frac{1}{2}$; $\bar{y},x-y,\frac{1}{2}$; $y-x,\bar{x},\frac{1}{2}$.	$hkil$: No conditions
3	j	m	$x,y,0$; $\bar{y},x-y,0$; $y-x,\bar{x},0$.	
2	i	3	$\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$.	
2	h	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\bar{z}$.	
2	g	3	$0,0,z$; $0,0,\bar{z}$.	
1	f	$\bar{6}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$.	
1	e	$\bar{6}$	$\frac{2}{3},\frac{1}{3},0$.	
1	d	$\bar{6}$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$.	
1	c	$\bar{6}$	$\frac{1}{3},\frac{2}{3},0$.	
1	b	$\bar{6}$	$0,0,\frac{1}{2}$.	
1	a	$\bar{6}$	$0,0,0$.	

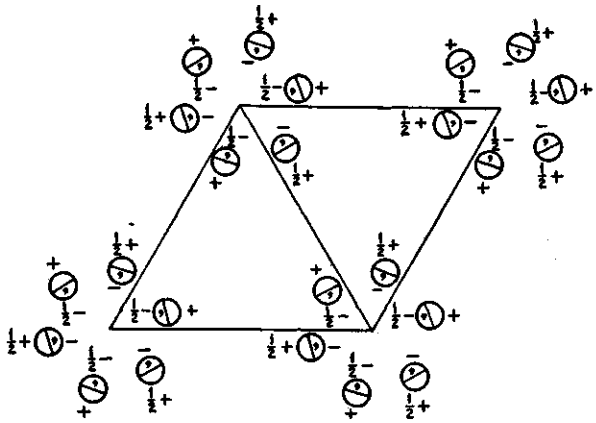
No. 175 $P\,6/m$ $6/m$ Hexagonal

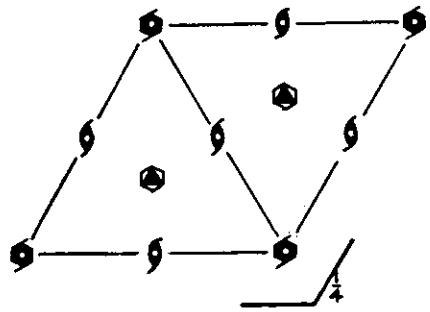




Origin at centre ($6/m$)

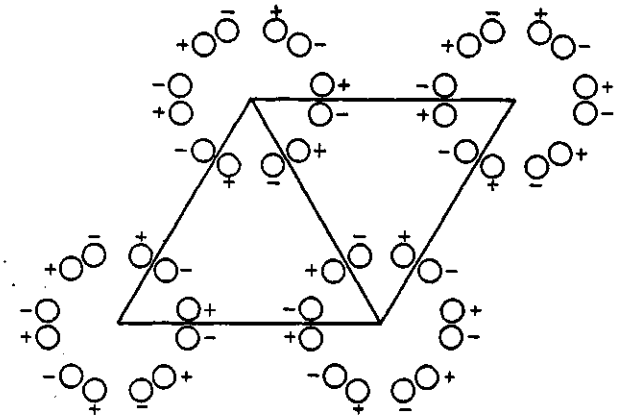
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	l	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$; $\bar{x},\bar{y},z$; $y,y-x,z$; $x-y,x,z$; $x,y,\bar{z}$; $\bar{y},x-y,\bar{z}$; $y-x,\bar{x},\bar{z}$.	*hkil*: No conditions
				Special:
6	k	m	$x,y,\frac{1}{2}$; $\bar{y},x-y,\frac{1}{2}$; $y-x,\bar{x},\frac{1}{2}$; $\bar{x},\bar{y},\frac{1}{2}$; $y,y-x,\frac{1}{2}$; $x-y,x,\frac{1}{2}$.	*hkil*: No conditions
6	j	m	$x,y,0$; $\bar{y},x-y,0$; $y-x,\bar{x},0$; $\bar{x},\bar{y},0$; $y,y-x,0$; $x-y,x,0$.	
6	i	2	$\frac{1}{2},0,z$; $0,\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	
4	h	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},z$; $\frac{1}{3},\frac{2}{3},\bar{z}$; $\frac{2}{3},\frac{1}{3},\bar{z}$.	
3	g	$2/m$	$\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
3	f	$2/m$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$.	
2	e	6	$0,0,z$; $0,0,\bar{z}$.	
2	d	$\bar{6}$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}$.	
2	c	$\bar{6}$	$\frac{1}{3},\frac{2}{3},0$; $\frac{2}{3},\frac{1}{3},0$.	
1	b	$6/m$	$0,0,\frac{1}{2}$.	
1	a	$6/m$	$0,0,0$.	

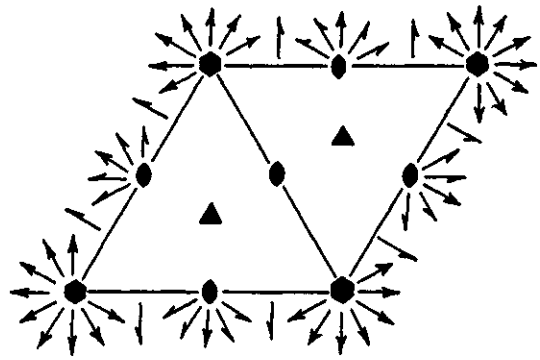




Origin at centre ($\bar{3}$)

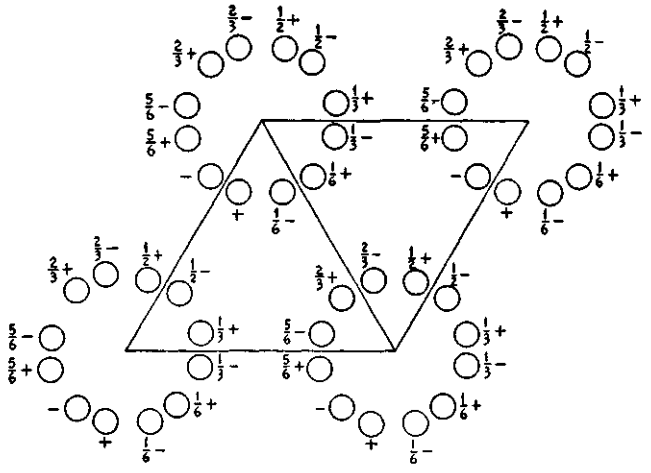
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	*i*	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,y-x,\frac{1}{2}+z$; $x-y,x,\frac{1}{2}+z$; $x,y,\frac{1}{2}-z$; $\bar{y},x-y,\frac{1}{2}-z$; $y-x,\bar{x},\frac{1}{2}-z$.	*hkil*: No conditions $000l$: $l=2n$
				Special: as above, plus
6	*h*	*m*	$x,y,\frac{1}{4}$; $\bar{y},x-y,\frac{1}{4}$; $y-x,\bar{x},\frac{1}{4}$; $\bar{x},\bar{y},\frac{3}{4}$; $y,y-x,\frac{3}{4}$; $x-y,x,\frac{3}{4}$.	no extra conditions
6	*g*	$\bar{1}$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	*hkil*: $l=2n$
4	*f*	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}-z$.	*hkil*: If $h-k=3n$, then $l=2n$
4	*e*	3	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	*hkil*: $l=2n$
2	*d*	$\bar{6}$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$; $\frac{1}{3},\frac{2}{3},\frac{3}{4}$.	*hkil*: If $h-k=3n$, then $l=2n$
2	*c*	$\bar{6}$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$; $\frac{2}{3},\frac{1}{3},\frac{3}{4}$.	
2	*b*	$\bar{3}$	$0,0,0$; $0,0,\frac{1}{2}$.	*hkil*: $l=2n$
2	*a*	$\bar{6}$	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	

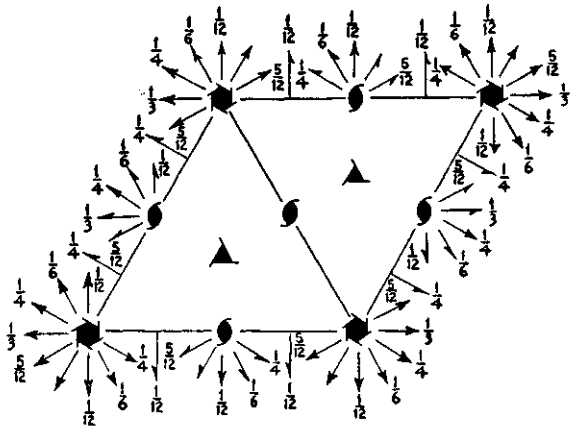




Origin at 622

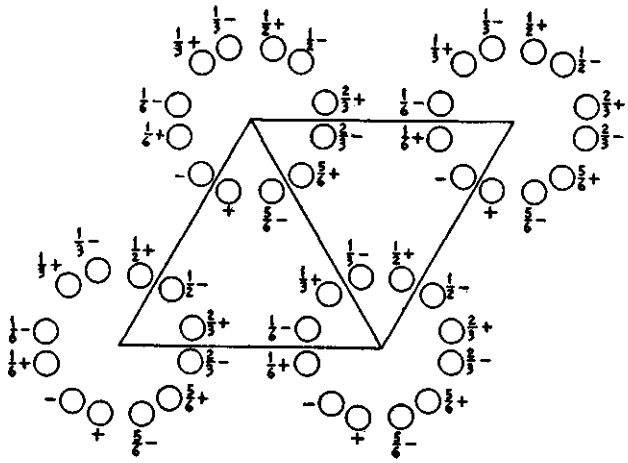
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	n	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},z$; $y,y-x,z$; $x-y,x,z$; $y,x,\bar{z}$; $\bar{x},y-x,\bar{z}$; $x-y,\bar{y},\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $x,x-y,\bar{z}$; $y-x,y,\bar{z}$.	No conditions
				Special:
6	m	2	$x,\bar{x},\frac{1}{2}$; $x,2x,\frac{1}{2}$; $2\bar{x},\bar{x},\frac{1}{2}$; $\bar{x},x,\frac{1}{2}$; $\bar{x},2\bar{x},\frac{1}{2}$; $2x,x,\frac{1}{2}$.	No conditions
6	l	2	$x,\bar{x},0$; $x,2x,0$; $2\bar{x},\bar{x},0$; $\bar{x},x,0$; $\bar{x},2\bar{x},0$; $2x,x,0$.	
6	k	2	$x,0,\frac{1}{2}$; $0,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $\bar{x},0,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$; $x,x,\frac{1}{2}$.	
6	j	2	$x,0,0$; $0,x,0$; $\bar{x},\bar{x},0$; $\bar{x},0,0$; $0,\bar{x},0$; $x,x,0$.	
6	i	2	$\frac{1}{2},0,z$; $0,\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	
4	h	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},z$; $\frac{1}{3},\frac{2}{3},\bar{z}$; $\frac{2}{3},\frac{1}{3},\bar{z}$.	
3	g	222	$\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
3	f	222	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$.	
2	e	6	$0,0,z$; $0,0,\bar{z}$.	
2	d	32	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}$.	
2	c	32	$\frac{1}{3},\frac{2}{3},0$; $\frac{2}{3},\frac{1}{3},0$.	
1	b	622	$0,0,\frac{1}{2}$.	
1	a	622	$0,0,0$.	

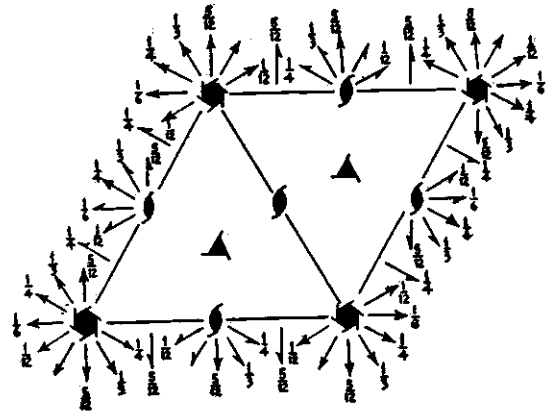




Origin at 6_121 [2-axis normal to $(\bar{2}110)$]

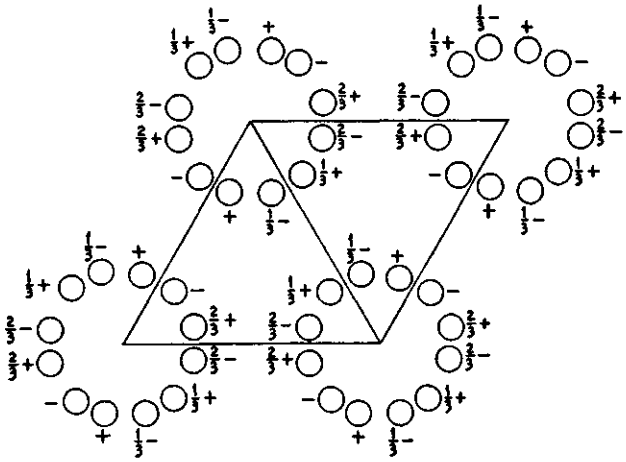
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	c	1	x,y,z; $\bar{y},x-y,\frac{1}{3}+z$; $y-x,\bar{x},\frac{2}{3}+z$; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,y-x,\frac{5}{6}+z$; $x-y,x,\frac{1}{6}+z$; $y,x,\frac{1}{3}-z$; $\bar{x},y-x,\frac{2}{3}-z$; $x-y,\bar{y},\bar{z}$; $\bar{y},\bar{x},\frac{5}{6}-z$; $x,x-y,\frac{1}{6}-z$; $y-x,y,\frac{1}{2}-z$.	$hkil$: No conditions $000l$: $l=6n$
				Special: as above, plus
6	b	2	$x,2x,\frac{1}{4}$; $2\bar{x},\bar{x},\frac{7}{12}$; $x,\bar{x},\frac{11}{12}$; $\bar{x},2\bar{x},\frac{3}{4}$; $2x,x,\frac{1}{12}$; $\bar{x},x,\frac{5}{12}$.	$hh2\bar{h}l$: $l=6n$ or $6n\pm1$ or $6n\pm2$
6	a	2	$x,0,0$; $0,x,\frac{1}{3}$; $\bar{x},\bar{x},\frac{2}{3}$; $\bar{x},0,\frac{1}{2}$; $0,\bar{x},\frac{5}{6}$; $x,x,\frac{1}{6}$.	$h\bar{h}0l$: $l=6n$ or $6n\pm1$ or $6n\pm2$

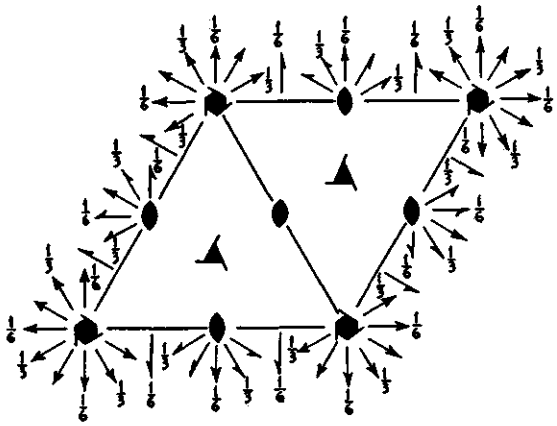




Origin at $6_5 21$ [2-axis normal to $(\bar{2}110)$]

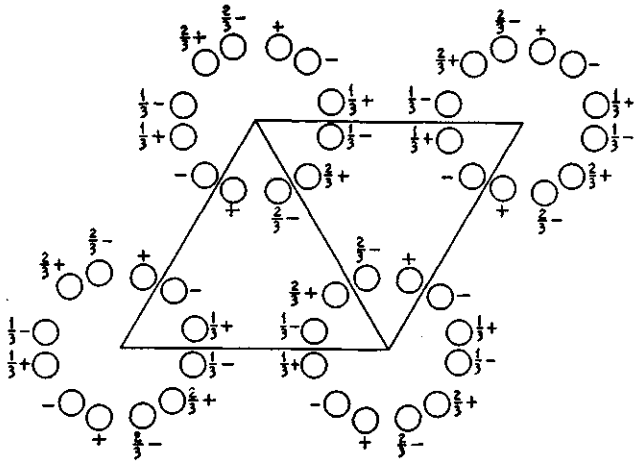
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	c	1	x,y,z; $\bar{y},x-y,\frac{2}{3}+z$; $y-x,\bar{x},\frac{1}{3}+z$; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,y-x,\frac{1}{6}+z$; $x-y,x,\frac{5}{6}+z$; $y,x,\frac{2}{3}-z$; $\bar{x},y-x,\frac{1}{3}-z$; $x-y,\bar{y},\bar{z}$; $\bar{y},\bar{x},\frac{1}{6}-z$; $x,x-y,\frac{5}{6}-z$; $y-x,y,\frac{1}{2}-z$.	$hkil$: No conditions $000l$: $l=6n$
				Special: as above, plus
6	b	2	$x,2x,\frac{3}{4}$; $2\bar{x},\bar{x},\frac{5}{12}$; $x,\bar{x},\frac{1}{12}$; $\bar{x},2\bar{x},\frac{1}{4}$; $2x,x,\frac{11}{12}$; $\bar{x},x,\frac{7}{12}$.	$hh2\bar{h}l$: $l=6n$ or $6n\pm1$ or $6n\pm2$
6	a	2	$x,0,0$; $0,x,\frac{2}{3}$; $\bar{x},\bar{x},\frac{1}{3}$; $\bar{x},0,\frac{1}{2}$; $0,\bar{x},\frac{1}{6}$; $x,x,\frac{5}{6}$.	$h\bar{h}0l$: $l=6n$ or $6n\pm1$ or $6n\pm2$

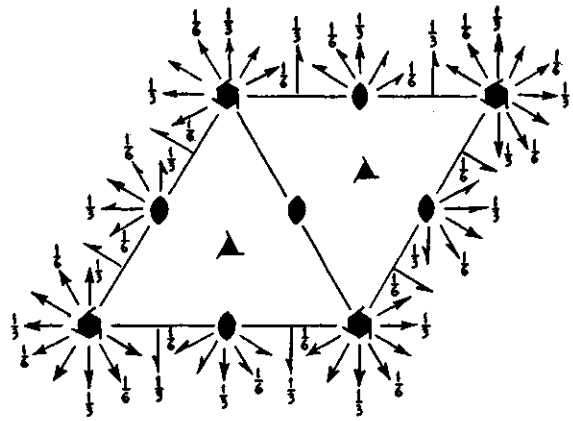




Origin at 6_222 [2-axes normal to $(\bar{2}110)$ and $(01\bar{1}0)$]

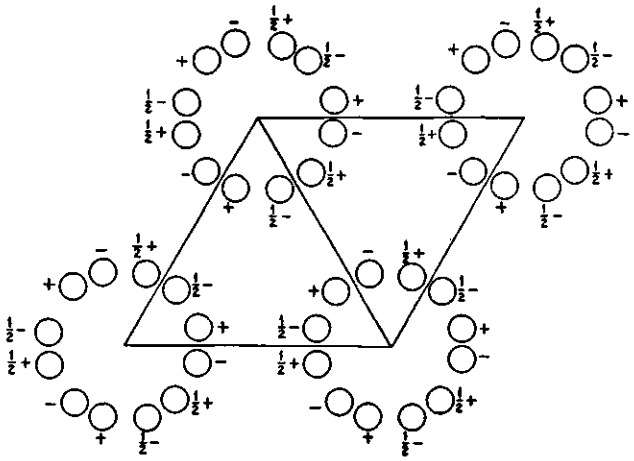
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	k	1	x,y,z; $\bar{y},x-y,\frac{2}{3}+z$; $y-x,\bar{x},\frac{1}{3}+z$; $\bar{x},\bar{y},z$; $y,y-x,\frac{2}{3}+z$; $x-y,x,\frac{1}{3}+z$; $y,x,\frac{2}{3}-z$; $\bar{x},y-x,\frac{1}{3}-z$; $x-y,\bar{y},\bar{z}$; $\bar{y},\bar{x},\frac{2}{3}-z$; $x,x-y,\frac{1}{3}-z$; $y-x,y,\bar{z}$.	$hkil$: No conditions $000l$: $l=3n$
				Special: as above, plus
6	j	2	$x,2x,\frac{1}{2}$; $2\bar{x},\bar{x},\frac{1}{6}$; $x,\bar{x},\frac{5}{6}$; $\bar{x},2\bar{x},\frac{1}{2}$; $2x,x,\frac{1}{6}$; $\bar{x},x,\frac{5}{6}$.	no extra conditions
6	i	2	$x,2x,0$; $2\bar{x},\bar{x},\frac{2}{3}$; $x,\bar{x},\frac{1}{3}$; $\bar{x},2\bar{x},0$; $2x,x,\frac{2}{3}$; $\bar{x},x,\frac{1}{3}$.	
6	h	2	$x,0,\frac{1}{2}$; $0,x,\frac{1}{6}$; $\bar{x},\bar{x},\frac{5}{6}$; $\bar{x},0,\frac{1}{2}$; $0,\bar{x},\frac{1}{6}$; $x,x,\frac{5}{6}$.	
6	g	2	$x,0,0$; $0,x,\frac{2}{3}$; $\bar{x},\bar{x},\frac{1}{3}$; $\bar{x},0,0$; $0,\bar{x},\frac{2}{3}$; $x,x,\frac{1}{3}$.	
6	f	2	$\frac{1}{2},0,z$; $0,\frac{1}{2},\frac{2}{3}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{3}+z$; $\frac{1}{2},0,\bar{z}$; $0,\frac{1}{2},\frac{2}{3}-z$; $\frac{1}{2},\frac{1}{2},\frac{1}{3}-z$.	$hkil$: If $h=2n$ and $k=2n$, then $l=3n$
6	e	2	$0,0,z$; $0,0,\frac{1}{3}+z$; $0,0,\frac{2}{3}+z$; $0,0,\bar{z}$; $0,0,\frac{1}{3}-z$; $0,0,\frac{2}{3}-z$.	$hkil$: $l=3n$
3	d	222	$\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{6}$; $\frac{1}{2},\frac{1}{2},\frac{5}{6}$.	$hkil$: If $h=2n$ and $k=2n$, then $l=3n$
3	c	222	$\frac{1}{2},0,0$; $0,\frac{1}{2},\frac{2}{3}$; $\frac{1}{2},\frac{1}{2},\frac{1}{3}$.	
3	b	222	$0,0,\frac{1}{2}$; $0,0,\frac{5}{6}$; $0,0,\frac{1}{6}$.	$hkil$: $l=3n$
3	a	222	$0,0,0$; $0,0,\frac{1}{3}$; $0,0,\frac{2}{3}$.	

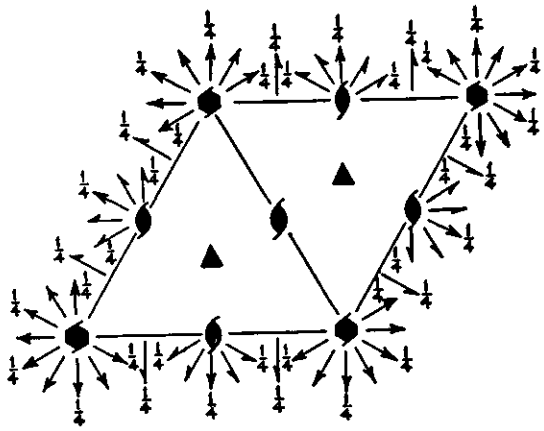




Origin at 6_422 [2-axes normal to $(\bar{2}110)$ and $(01\bar{1}0)$]

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	k	1	x,y,z; $\bar{y},x-y,\frac{1}{3}+z$; $y-x,\bar{x},\frac{2}{3}+z$; $\bar{x},\bar{y},z$; $y,y-x,\frac{1}{3}+z$; $x-y,x,\frac{2}{3}+z$; $y,x,\frac{1}{3}-z$; $\bar{x},y-x,\frac{2}{3}-z$; $x-y,\bar{y},\bar{z}$; $\bar{y},\bar{x},\frac{1}{3}-z$; $x,x-y,\frac{2}{3}-z$; $y-x,y,\bar{z}$.	$hkil$: No conditions $000l$: $l=3n$
				Special: as above, plus
6	j	2	$x,2x,\frac{1}{2}$; $2\bar{x},\bar{x},\frac{5}{6}$; $x,\bar{x},\frac{1}{6}$; $\bar{x},2\bar{x},\frac{1}{2}$; $2x,x,\frac{5}{6}$; $\bar{x},x,\frac{1}{6}$.	no extra conditions
6	i	2	$x,2x,0$; $2\bar{x},\bar{x},\frac{1}{3}$; $x,\bar{x},\frac{2}{3}$; $\bar{x},2\bar{x},0$; $2x,x,\frac{1}{3}$; $\bar{x},x,\frac{2}{3}$.	
6	h	2	$x,0,\frac{1}{2}$; $0,x,\frac{5}{6}$; $\bar{x},\bar{x},\frac{1}{6}$; $\bar{x},0,\frac{1}{2}$; $0,\bar{x},\frac{5}{6}$; $x,x,\frac{1}{6}$.	
6	g	2	$x,0,0$; $0,x,\frac{1}{3}$; $\bar{x},\bar{x},\frac{2}{3}$; $\bar{x},0,0$; $0,\bar{x},\frac{1}{3}$; $x,x,\frac{2}{3}$.	
6	f	2	$\frac{1}{2},0,z$; $0,\frac{1}{2},\frac{1}{3}+z$; $\frac{1}{2},\frac{1}{2},\frac{2}{3}+z$; $\frac{1}{2},0,\bar{z}$; $0,\frac{1}{2},\frac{1}{3}-z$; $\frac{1}{2},\frac{1}{2},\frac{2}{3}-z$.	$hkil$: If $h=2n$ and $k=2n$, then $l=3n$
6	e	2	$0,0,z$; $0,0,\frac{1}{3}+z$; $0,0,\frac{2}{3}+z$; $0,0,\bar{z}$; $0,0,\frac{1}{3}-z$; $0,0,\frac{2}{3}-z$.	$hkil$: $l=3n$
3	d	222	$\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{5}{6}$; $\frac{1}{2},\frac{1}{2},\frac{1}{6}$.	$hkil$: If $h=2n$ and $k=2n$, then $l=3n$
3	c	222	$\frac{1}{2},0,0$; $0,\frac{1}{2},\frac{1}{3}$; $\frac{1}{2},\frac{1}{2},\frac{2}{3}$.	
3	b	222	$0,0,\frac{1}{2}$; $0,0,\frac{5}{6}$; $0,0,\frac{1}{6}$.	$hkil$: $l=3n$
3	a	222	$0,0,0$; $0,0,\frac{1}{3}$; $0,0,\frac{2}{3}$.	



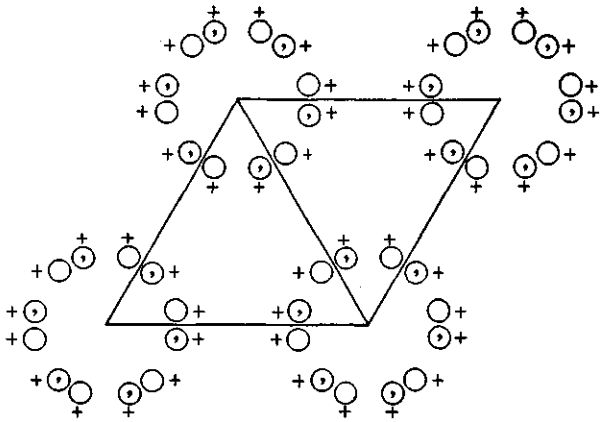


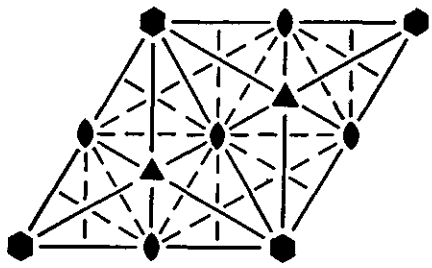
Origin at 6_321

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	i	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $y,x,\bar{z}$; $\bar{x},y-x,\bar{z}$; $x-y,\bar{y},\bar{z}$; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,y-x,\frac{1}{2}+z$; $x-y,x,\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}-z$; $x,x-y,\frac{1}{2}-z$; $y-x,y,\frac{1}{2}-z$.	$hkil$: No conditions $000l$: $l=2n$
				Special: as above, plus
6	h	2	$x,2x,\frac{1}{4}$; $2\bar{x},\bar{x},\frac{1}{4}$; $x,\bar{x},\frac{1}{4}$; $\bar{x},2\bar{x},\frac{3}{4}$; $2x,x,\frac{3}{4}$; $\bar{x},x,\frac{3}{4}$.	$hh2\bar{h}l$: $l=2n$
6	g	2	$x,0,0$; $0,x,0$; $\bar{x},\bar{x},0$; $\bar{x},0,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$; $x,x,\frac{1}{2}$.	$h\bar{h}0l$: $l=2n$
4	f	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}-z$.	$hkil$: If $h-k=3n$, then $l=2n$
4	e	3	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	$hkil$: $l=2n$
2	d	32	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$; $\frac{2}{3},\frac{1}{3},\frac{1}{4}$.	$hkil$: If $h-k=3n$, then $l=2n$
2	c	32	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$; $\frac{2}{3},\frac{1}{3},\frac{3}{4}$.	
2	b	32	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	$hkil$: $l=2n$
2	a	32	$0,0,0$; $0,0,\frac{1}{2}$.	

$P6mm$ C_{6v}^{1}

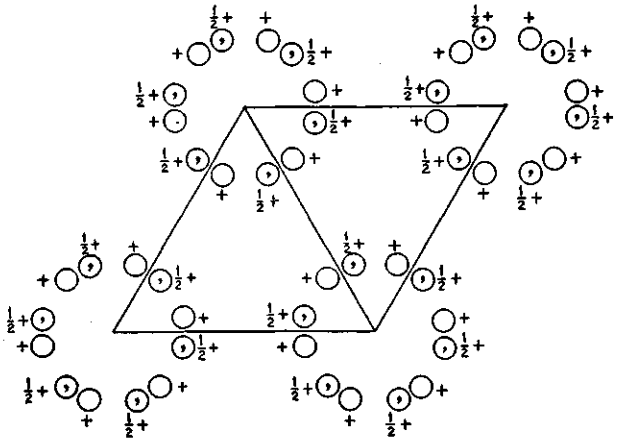
No. 183 $P\,6\,m\,m$ $6\,m\,m$ Hexagonal

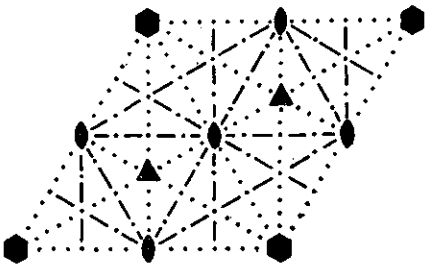




Origin on $6mm$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	f	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},z$; $y,y-x,z$; $x-y,x,z$; y,x,z; $\bar{x},y-x,z$; $x-y,\bar{y},z$; $\bar{y},\bar{x},z$; $x,x-y,z$; $y-x,y,z$.	No conditions
				Special:
6	e	m	$x,\bar{x},z$; $x,2x,z$; $2\bar{x},\bar{x},z$; $\bar{x},x,z$; $\bar{x},2\bar{x},z$; $2x,x,z$.	No conditions
6	d	m	$x,0,z$; $0,x,z$; $\bar{x},\bar{x},z$; $\bar{x},0,z$; $0,\bar{x},z$; x,x,z.	
3	c	mm	$\frac{1}{2},0,z$; $0,\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},z$.	
2	b	$3m$	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},z$.	
1	a	$6mm$	$0,0,z$.	



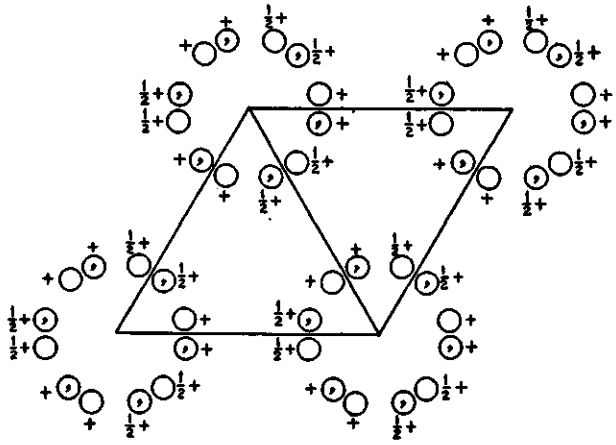


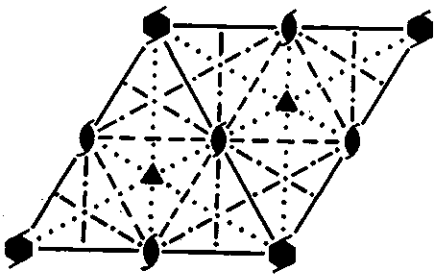
Origin on 6

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions			Conditions limiting possible reflections
						General:
12	d	1	x,y,z;	$\bar{y},x-y,z$;	$y-x,\bar{x},z$;	$hkil$: No conditions
			$\bar{x},\bar{y},z$;	$y,y-x,z$;	$x-y,x,z$;	$hh2\bar{h}l$: $l=2n$
			$y,x,\frac{1}{2}+z$;	$\bar{x},y-x,\frac{1}{2}+z$;	$x-y,\bar{y},\frac{1}{2}+z$;	$h\bar{h}0l$: $l=2n$
			$\bar{y},\bar{x},\frac{1}{2}+z$;	$x,x-y,\frac{1}{2}+z$;	$y-x,y,\frac{1}{2}+z$.	
						Special: as above, plus
6	c	2	$\frac{1}{2},0,z$;	$0,\frac{1}{2},z$;	$\frac{1}{2},\frac{1}{2},z$;	
			$\frac{1}{2},0,\frac{1}{2}+z$;	$0,\frac{1}{2},\frac{1}{2}+z$;	$\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$.	
4	b	3	$\frac{1}{3},\frac{2}{3},z$;	$\frac{2}{3},\frac{1}{3},z$;	$\frac{1}{3},\frac{2}{3},\frac{1}{2}+z$;	$\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$.	$hkil$: $l=2n$
2	a	6	$0,0,z$;	$0,0,\frac{1}{2}+z$.		

$P6_3cm$ C_{6v}^3

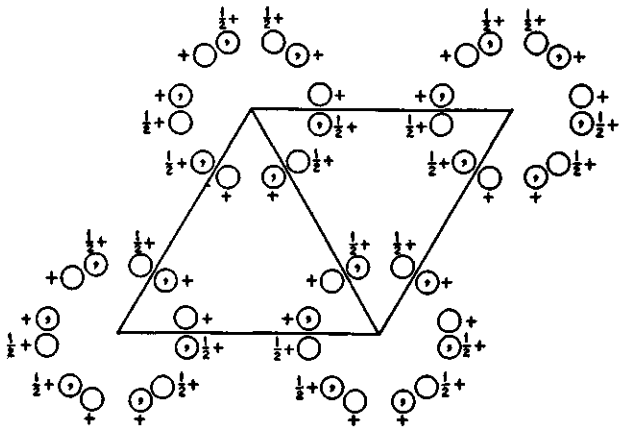
No. 185 $P\,6_3\,c\,m$ $6\,m\,m$ Hexagonal

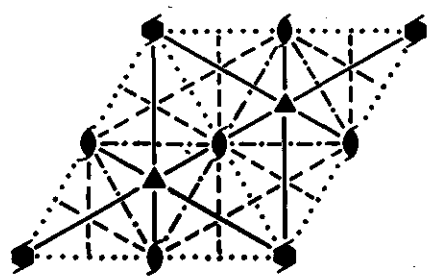




Origin on $6_3(3m)$

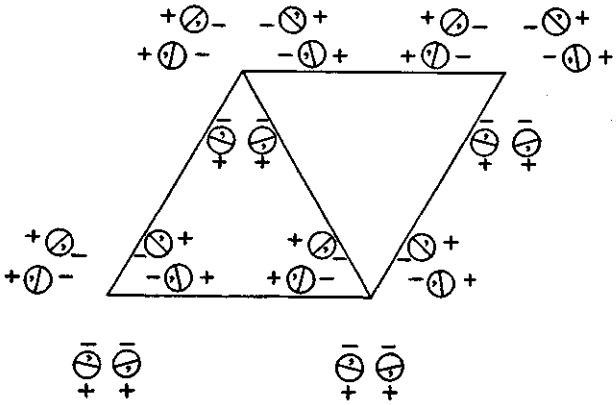
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	d	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; y,x,z; $\bar{x},y-x,z$; $x-y,\bar{y},z$; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,y-x,\frac{1}{2}+z$; $x-y,x,\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}+z$; $x,x-y,\frac{1}{2}+z$; $y-x,y,\frac{1}{2}+z$.	$hkil$: No conditions $hh2\bar{h}l$: No conditions $h\bar{h}0l$: $l=2n$
				Special: as above, plus
6	c	m	$x,0,z$; $0,x,z$; $\bar{x},\bar{x},z$; $\bar{x},0,\frac{1}{2}+z$; $0,\bar{x},\frac{1}{2}+z$; $x,x,\frac{1}{2}+z$.	no extra conditions
4	b	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},z$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}+z$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$.	$hkil$: $l=2n$
2	a	$3m$	$0,0,z$; $0,0,\frac{1}{2}+z$.	

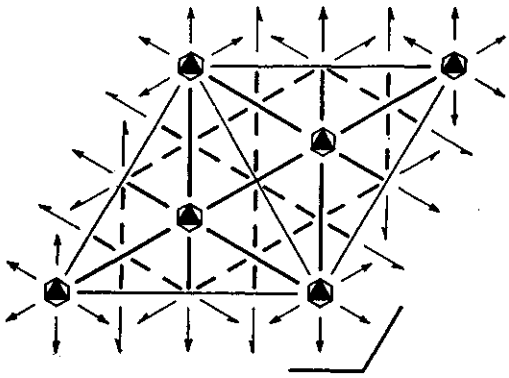




Origin on $6_3(3m)$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions			Conditions limiting possible reflections
						General:
12	*d*	1	x,y,z;	$\bar{y},x-y,z$;	$y-x,\bar{x},z$;	*hkil*: No conditions
			$\bar{y},\bar{x},z$;	$x,x-y,z$;	$y-x,y,z$;	*hh*2*h̄l*: $l=2n$
			$\bar{x},\bar{y},\frac{1}{2}+z$;	$y,y-x,\frac{1}{2}+z$;	$x-y,x,\frac{1}{2}+z$;	*hh̄*0*l*: No conditions
			$y,x,\frac{1}{2}+z$;	$\bar{x},y-x,\frac{1}{2}+z$;	$x-y,\bar{y},\frac{1}{2}+z$.	
						Special: as above, plus
6	*c*	*m*	$x,\bar{x},z$;	$x,2x,z$;	$2\bar{x},\bar{x},z$;	no extra conditions
			$\bar{x},x,\frac{1}{2}+z$;	$\bar{x},2\bar{x},\frac{1}{2}+z$;	$2x,x,\frac{1}{2}+z$.	
2	*b*	3*m*	$\frac{1}{3},\frac{2}{3},z$;	$\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$.		*hkil*: If $h-k=3n$, then $l=2n$
2	*a*	3*m*	$0,0,z$;	$0,0,\frac{1}{2}+z$.		*hkil*: $l=2n$

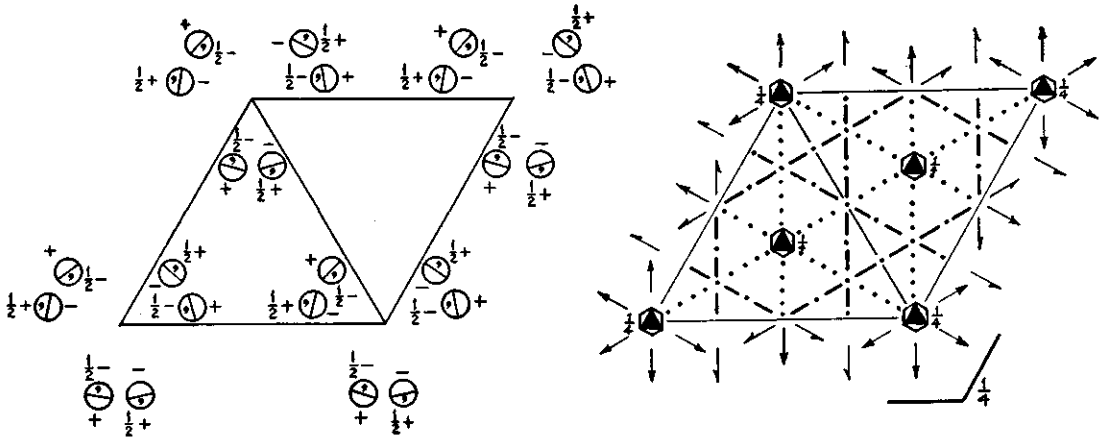




Origin at $\bar{6}m2$

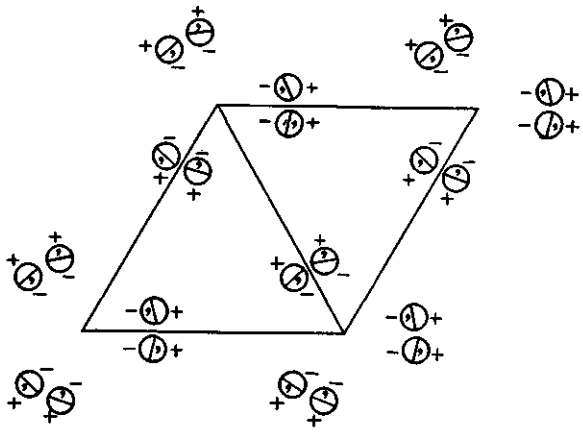
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	o	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $x,y,\bar{z}$; $\bar{y},x-y,\bar{z}$; $y-x,\bar{x},\bar{z}$; $\bar{y},\bar{x},z$; $x,x-y,z$; $y-x,y,z$; $\bar{y},\bar{x},\bar{z}$; $x,x-y,\bar{z}$; $y-x,y,\bar{z}$.	No conditions
				Special:
6	n	m	$x,\bar{x},z$; $x,2x,z$; $2\bar{x},\bar{x},z$; $x,\bar{x},\bar{z}$; $x,2x,\bar{z}$; $2\bar{x},\bar{x},\bar{z}$.	No conditions
6	m	m	$x,y,\frac{1}{2}$; $\bar{y},x-y,\frac{1}{2}$; $y-x,\bar{x},\frac{1}{2}$; $\bar{y},\bar{x},\frac{1}{2}$; $x,x-y,\frac{1}{2}$; $y-x,y,\frac{1}{2}$.	
6	l	m	$x,y,0$; $\bar{y},x-y,0$; $y-x,\bar{x},0$; $\bar{y},\bar{x},0$; $x,x-y,0$; $y-x,y,0$.	
3	k	mm	$x,\bar{x},\frac{1}{2}$; $x,2x,\frac{1}{2}$; $2\bar{x},\bar{x},\frac{1}{2}$.	
3	j	mm	$x,\bar{x},0$; $x,2x,0$; $2\bar{x},\bar{x},0$.	
2	i	$3m$	$\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$.	
2	h	$3m$	$\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\bar{z}$.	
2	g	$3m$	$0,0,z$; $0,0,\bar{z}$.	

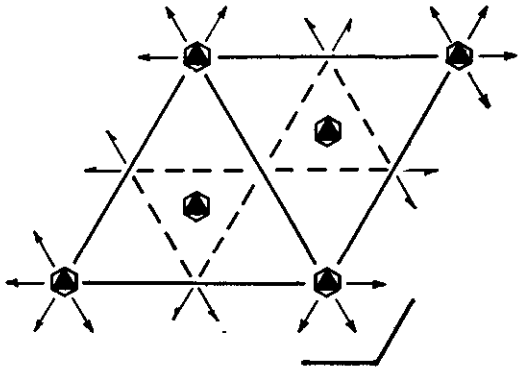
1	f	$\bar{6}m2$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$.
1	e	$\bar{6}m2$	$\frac{2}{3},\frac{1}{3},0$.
1	d	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$.
1	c	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},0$.
1	b	$\bar{6}m2$	$0,0,\frac{1}{2}$.
1	a	$\bar{6}m2$	$0,0,0$.



Origin at 312

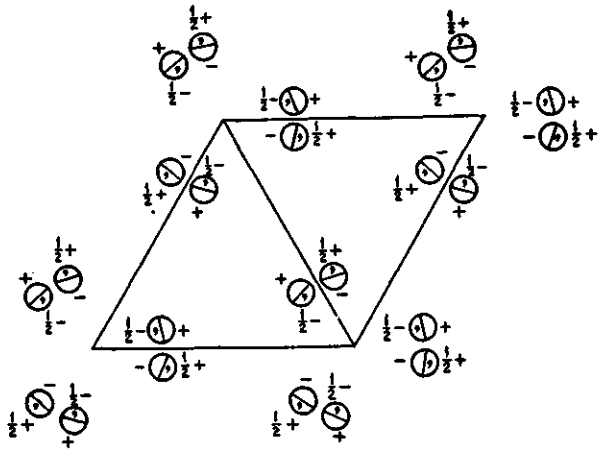
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	l	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $x,y,\frac{1}{2}-z$; $\bar{y},x-y,\frac{1}{2}-z$; $y-x,\bar{x},\frac{1}{2}-z$; $\bar{y},\bar{x},\frac{1}{2}+z$; $x,x-y,\frac{1}{2}+z$; $y-x,y,\frac{1}{2}+z$; $\bar{y},\bar{x},\bar{z}$; $x,x-y,\bar{z}$; $y-x,y,\bar{z}$.	$hkil$: No conditions $hh2\bar{h}l$: No conditions $h\bar{h}0l$: $l=2n$
				Special: as above, plus
6	k	m	$x,y,\frac{1}{4}$; $\bar{y},x-y,\frac{1}{4}$; $y-x,\bar{x},\frac{1}{4}$; $\bar{y},\bar{x},\frac{3}{4}$; $x,x-y,\frac{3}{4}$; $y-x,y,\frac{3}{4}$.	no extra conditions
6	j	2	$x,\bar{x},0$; $x,2x,0$; $2\bar{x},\bar{x},0$; $x,\bar{x},\frac{1}{2}$; $x,2x,\frac{1}{2}$; $2\bar{x},\bar{x},\frac{1}{2}$.	$hkil$: $l=2n$
4	i	3	$\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}-z$.	
4	h	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\bar{z}$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}+z$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}-z$.	
4	g	3	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	
2	f	$\bar{6}$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$; $\frac{2}{3},\frac{1}{3},\frac{3}{4}$.	
2	e	32	$\frac{2}{3},\frac{1}{3},0$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}$.	
2	d	$\bar{6}$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$; $\frac{1}{3},\frac{2}{3},\frac{3}{4}$.	
2	c	32	$\frac{1}{3},\frac{2}{3},0$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}$.	
2	b	$\bar{6}$	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	
2	a	32	$0,0,0$; $0,0,\frac{1}{2}$.	

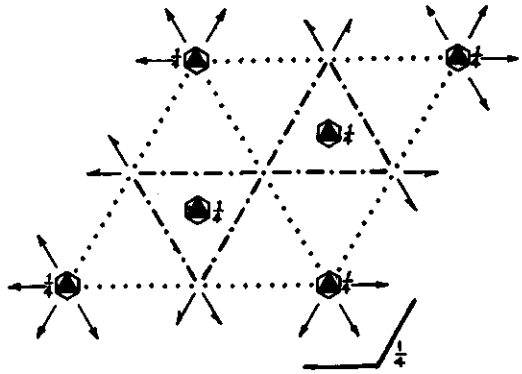




Origin at $\bar{6}2m$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	l	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $x,y,\bar{z}$; $\bar{y},x-y,\bar{z}$; $y-x,\bar{x},\bar{z}$; y,x,z; $\bar{x},y-x,z$; $x-y,\bar{y},z$; $y,x,\bar{z}$; $\bar{x},y-x,\bar{z}$; $x-y,\bar{y},\bar{z}$.	No conditions
				Special:
6	k	m	$x,y,\frac{1}{2}$; $\bar{y},x-y,\frac{1}{2}$; $y-x,\bar{x},\frac{1}{2}$; $y,x,\frac{1}{2}$; $\bar{x},y-x,\frac{1}{2}$; $x-y,\bar{y},\frac{1}{2}$.	No conditions
6	j	m	$x,y,0$; $\bar{y},x-y,0$; $y-x,\bar{x},0$; $y,x,0$; $\bar{x},y-x,0$; $x-y,\bar{y},0$.	
6	i	m	$x,0,z$; $0,x,z$; $\bar{x},\bar{x},z$; $x,0,\bar{z}$; $0,x,\bar{z}$; $\bar{x},\bar{x},\bar{z}$.	
4	h	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\bar{z}$; $\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$.	
3	g	mm	$x,0,\frac{1}{2}$; $0,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$.	
3	f	mm	$x,0,0$; $0,x,0$; $\bar{x},\bar{x},0$.	
2	e	$3m$	$0,0,z$; $0,0,\bar{z}$.	
2	d	$\bar{6}$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}$.	
2	c	$\bar{6}$	$\frac{1}{3},\frac{2}{3},0$; $\frac{2}{3},\frac{1}{3},0$.	
1	b	$\bar{6}m2$	$0,0,\frac{1}{2}$.	
1	a	$\bar{6}m2$	$0,0,0$.	



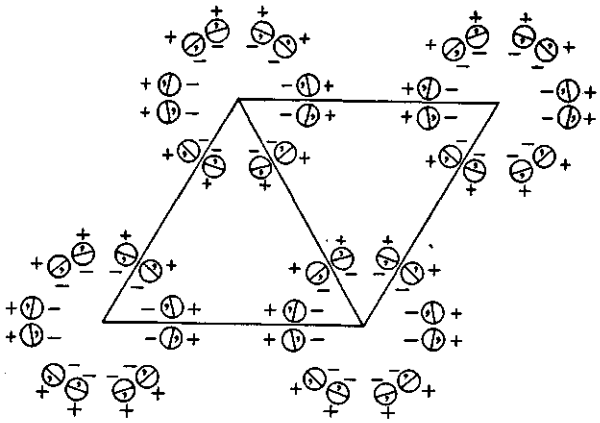


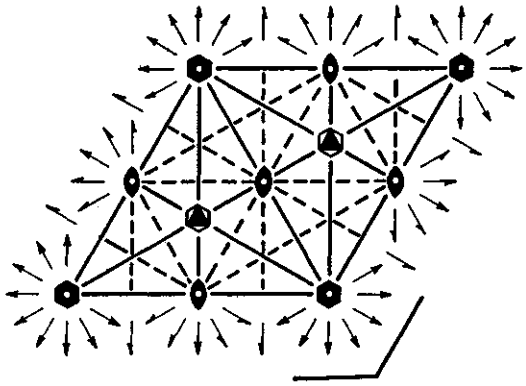
Origin at 321

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	i	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $x,y,\frac{1}{2}-z$; $\bar{y},x-y,\frac{1}{2}-z$; $y-x,\bar{x},\frac{1}{2}-z$; $y,x,\frac{1}{2}+z$; $\bar{x},y-x,\frac{1}{2}+z$; $x-y,\bar{y},\frac{1}{2}+z$; $y,x,\bar{z}$; $\bar{x},y-x,\bar{z}$; $x-y,\bar{y},\bar{z}$.	$hkil$: No conditions $hh2\bar{h}l$: $l=2n$ $h\bar{h}0l$: No conditions
				Special: as above, plus
6	h	m	$x,y,\frac{1}{4}$; $\bar{y},x-y,\frac{1}{4}$; $y-x,\bar{x},\frac{1}{4}$; $y,x,\frac{3}{4}$; $\bar{x},y-x,\frac{3}{4}$; $x-y,\bar{y},\frac{3}{4}$.	no extra conditions
6	g	2	$x,0,0$; $0,x,0$; $\bar{x},\bar{x},0$; $x,0,\frac{1}{2}$; $0,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$.	$hkil$: $l=2n$
4	f	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}-z$.	$hkil$: If $h-k=3n$, then $l=2n$
4	e	3	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	$hkil$: $l=2n$
2	d	$\bar{6}$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$; $\frac{1}{3},\frac{2}{3},\frac{3}{4}$.	$hkil$: If $h-k=3n$, then $l=2n$
2	c	$\bar{6}$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$; $\frac{2}{3},\frac{1}{3},\frac{3}{4}$.	
2	b	$\bar{6}$	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	$hkil$: $l=2n$
2	a	32	$0,0,0$; $0,0,\frac{1}{2}$.	

$P6/mmm$ D_{6h}^{1}

No. 191 $P\,6/m\,2/m\,2/m$ $6/m\,m\,m$ Hexagonal





Origin at centre ($6/mmm$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	r	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; y,x,z; $\bar{x},y-x,z$; $x-y,\bar{y},z$; $\bar{x},\bar{y},z$; $y,y-x,z$; $x-y,x,z$; $\bar{y},\bar{x},z$; $x,x-y,z$; $y-x,y,z$; $x,y,\bar{z}$; $\bar{y},x-y,\bar{z}$; $y-x,\bar{x},\bar{z}$; $y,x,\bar{z}$; $\bar{x},y-x,\bar{z}$; $x-y,\bar{y},\bar{z}$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $x,x-y,\bar{z}$; $y-x,y,\bar{z}$.	No conditions
				Special:
12	q	m	$x,y,\frac{1}{2}$; $\bar{y},x-y,\frac{1}{2}$; $y-x,\bar{x},\frac{1}{2}$; $y,x,\frac{1}{2}$; $\bar{x},y-x,\frac{1}{2}$; $x-y,\bar{y},\frac{1}{2}$; $\bar{x},\bar{y},\frac{1}{2}$; $y,y-x,\frac{1}{2}$; $x-y,x,\frac{1}{2}$; $\bar{y},\bar{x},\frac{1}{2}$; $x,x-y,\frac{1}{2}$; $y-x,y,\frac{1}{2}$.	No conditions
12	p	m	$x,y,0$; $\bar{y},x-y,0$; $y-x,\bar{x},0$; $y,x,0$; $\bar{x},y-x,0$; $x-y,\bar{y},0$; $\bar{x},\bar{y},0$; $y,y-x,0$; $x-y,x,0$; $\bar{y},\bar{x},0$; $x,x-y,0$; $y-x,y,0$.	
12	o	m	$x,2x,z$; $2\bar{x},\bar{x},z$; $x,\bar{x},z$; $\bar{x},2\bar{x},z$; $2x,x,z$; $\bar{x},x,z$; $x,2x,\bar{z}$; $2\bar{x},\bar{x},\bar{z}$; $x,\bar{x},\bar{z}$; $\bar{x},2\bar{x},\bar{z}$; $2x,x,\bar{z}$; $\bar{x},x,\bar{z}$.	
12	n	m	$x,0,z$; $0,x,z$; $\bar{x},\bar{x},z$; $\bar{x},0,z$; $0,\bar{x},z$; x,x,z; $x,0,\bar{z}$; $0,x,\bar{z}$; $\bar{x},\bar{x},\bar{z}$; $\bar{x},0,\bar{z}$; $0,\bar{x},\bar{z}$; $x,x,\bar{z}$.	
6	m	mm	$x,2x,\frac{1}{2}$; $2\bar{x},\bar{x},\frac{1}{2}$; $x,\bar{x},\frac{1}{2}$; $\bar{x},2\bar{x},\frac{1}{2}$; $2x,x,\frac{1}{2}$; $\bar{x},x,\frac{1}{2}$.	
6	l	mm	$x,2x,0$; $2\bar{x},\bar{x},0$; $x,\bar{x},0$; $\bar{x},2\bar{x},0$; $2x,x,0$; $\bar{x},x,0$.	
6	k	mm	$x,0,\frac{1}{2}$; $0,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $\bar{x},0,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$; $x,x,\frac{1}{2}$.	
6	j	mm	$x,0,0$; $0,x,0$; $\bar{x},\bar{x},0$; $\bar{x},0,0$; $0,\bar{x},0$; $x,x,0$.	
6	i	mm	$\frac{1}{2},0,z$; $0,\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},0,\bar{z}$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\bar{z}$.	

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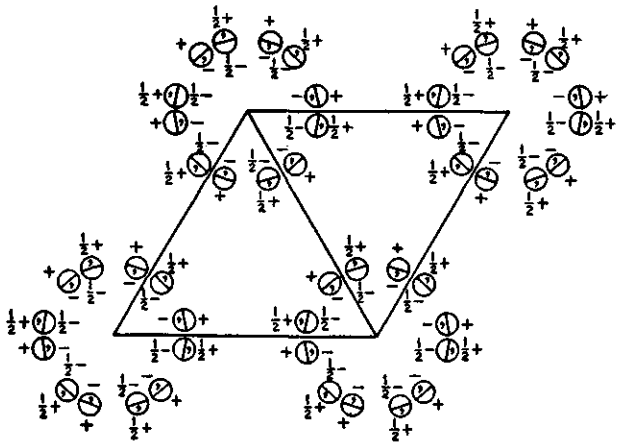
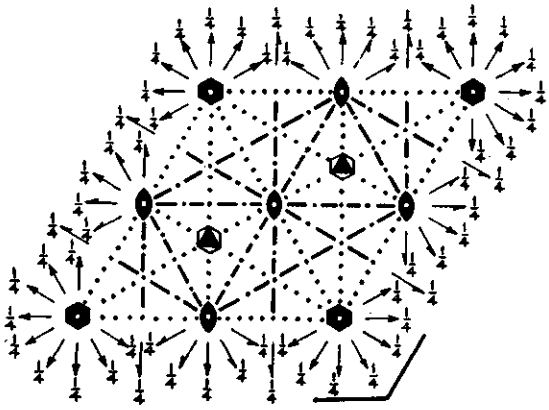
4	h	$3m$	$\frac{1}{3},\frac{2}{3},z;\ \frac{2}{3},\frac{1}{3},z;\ \frac{1}{3},\frac{2}{3},\bar{z};\ \frac{2}{3},\frac{1}{3},\bar{z}.$
3	g	mmm	$\frac{1}{2},0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$
3	f	mmm	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ \frac{1}{2},\frac{1}{2},0.$
2	e	$6mm$	$0,0,z;\ 0,0,\bar{z}.$
2	d	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{1}{2};\ \frac{2}{3},\frac{1}{3},\frac{1}{2}.$
2	c	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},0;\ \frac{2}{3},\frac{1}{3},0.$
1	b	$6/mmm$	$0,0,\frac{1}{2}.$
1	a	$6/mmm$	$0,0,0.$

$P\,6/m\,c\,c$ D_{6h}^{2}

No. 192 $P\,6/m\,2/c\,2/c$ $6/m\,m\,m$ Hexagonal





Origin at centre ($6/m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	m	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $x,y,\bar{z}$; $\bar{y},x-y,\bar{z}$; $y-x,\bar{x},\bar{z}$; $\bar{x},\bar{y},z$; $y,y-x,z$; $x-y,x,z$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$; $y,x,\frac{1}{2}+z$; $\bar{x},y-x,\frac{1}{2}+z$; $x-y,\bar{y},\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}+z$; $x,x-y,\frac{1}{2}+z$; $y-x,y,\frac{1}{2}+z$; $y,x,\frac{1}{2}-z$; $\bar{x},y-x,\frac{1}{2}-z$; $x-y,\bar{y},\frac{1}{2}-z$; $\bar{y},\bar{x},\frac{1}{2}-z$; $x,x-y,\frac{1}{2}-z$; $y-x,y,\frac{1}{2}-z$.	$hkil$: No conditions $hh2\bar{h}l$: $l=2n$ $h\bar{h}0l$: $l=2n$
				Special: as above, plus
12	l	m	$x,y,0$; $\bar{y},x-y,0$; $y-x,\bar{x},0$; $y,x,\frac{1}{2}$; $\bar{x},y-x,\frac{1}{2}$; $x-y,\bar{y},\frac{1}{2}$; $\bar{x},\bar{y},0$; $y,y-x,0$; $x-y,x,0$; $\bar{y},\bar{x},\frac{1}{2}$; $x,x-y,\frac{1}{2}$; $y-x,y,\frac{1}{2}$.	no extra conditions
12	k	2	$x,2x,\frac{1}{4}$; $2\bar{x},\bar{x},\frac{1}{4}$; $x,\bar{x},\frac{1}{4}$; $x,2x,\frac{3}{4}$; $2\bar{x},\bar{x},\frac{3}{4}$; $x,\bar{x},\frac{3}{4}$; $\bar{x},2\bar{x},\frac{3}{4}$; $2x,x,\frac{3}{4}$; $\bar{x},x,\frac{3}{4}$; $\bar{x},2\bar{x},\frac{1}{4}$; $2x,x,\frac{1}{4}$; $\bar{x},x,\frac{1}{4}$.	
12	j	2	$x,0,\frac{1}{4}$; $0,x,\frac{1}{4}$; $\bar{x},\bar{x},\frac{1}{4}$; $x,0,\frac{3}{4}$; $0,x,\frac{3}{4}$; $\bar{x},\bar{x},\frac{3}{4}$; $\bar{x},0,\frac{1}{4}$; $0,\bar{x},\frac{1}{4}$; $x,x,\frac{1}{4}$; $\bar{x},0,\frac{3}{4}$; $0,\bar{x},\frac{3}{4}$; $x,x,\frac{3}{4}$.	
12	i	2	$\frac{1}{2},0,z$; $0,\frac{1}{2},z$; $\frac{1}{2},\frac{1}{2},z$; $\frac{1}{2},0,\frac{1}{2}+z$; $0,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2},0,\bar{z}$; $0,\frac{1}{2},\bar{z}$; $\frac{1}{2},\frac{1}{2},\bar{z}$; $\frac{1}{2},0,\frac{1}{2}-z$; $0,\frac{1}{2},\frac{1}{2}-z$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-z$.	$hkil$: $l=2n$
8	h	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\bar{z}$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}+z$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}-z$; $\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}-z$.	
6	g	$2/m$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
6	f	222	$\frac{1}{2},0,\frac{1}{4}$; $0,\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},0,\frac{3}{4}$; $0,\frac{1}{2},\frac{3}{4}$; $\frac{1}{2},\frac{1}{2},\frac{3}{4}$.	

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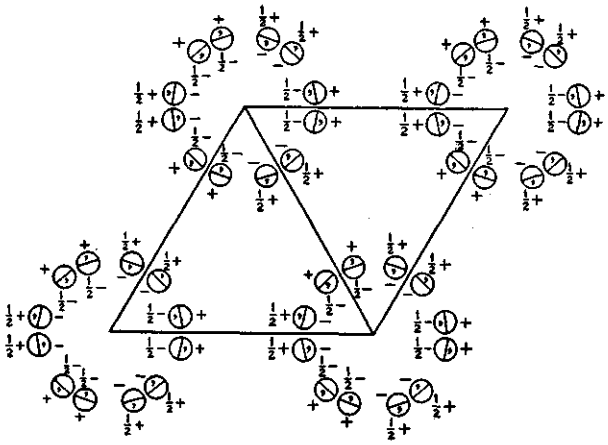
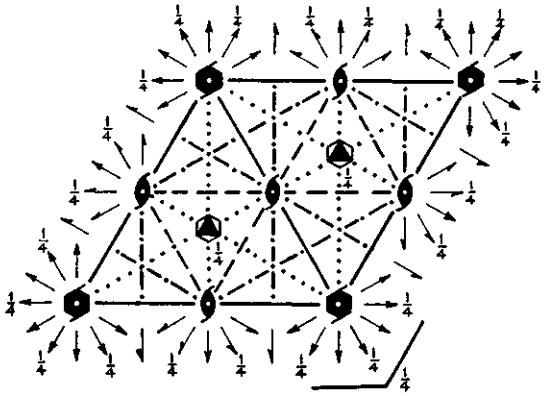
4	e	6	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	
4	d	$\bar{6}$	$\frac{1}{3},\frac{2}{3},0$; $\frac{2}{3},\frac{1}{3},0$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}$.	
4	c	32	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$; $\frac{2}{3},\frac{1}{3},\frac{1}{4}$; $\frac{1}{3},\frac{2}{3},\frac{3}{4}$; $\frac{2}{3},\frac{1}{3},\frac{3}{4}$.	$hkil$: $l=2n$
2	b	$6/m$	$0,0,0$; $0,0,\frac{1}{2}$.	
2	a	62	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	

$P\,6_3/m\,c\,m$ D_{6h}^3

No. 193 $P\,6_3/m\,2/c\,2/m$ $6/m\,m\,m$ Hexagonal





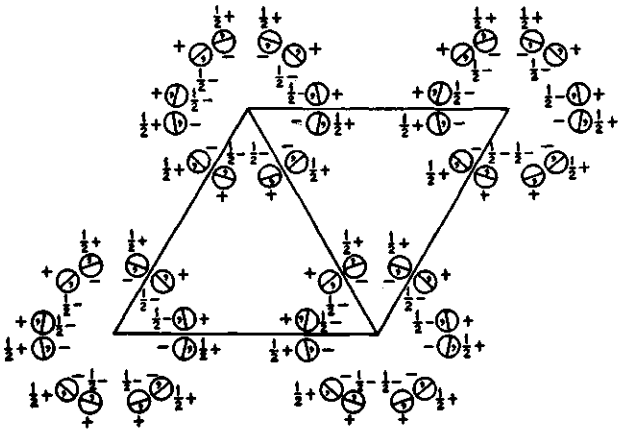
Origin at centre ($\bar{3}1m$)

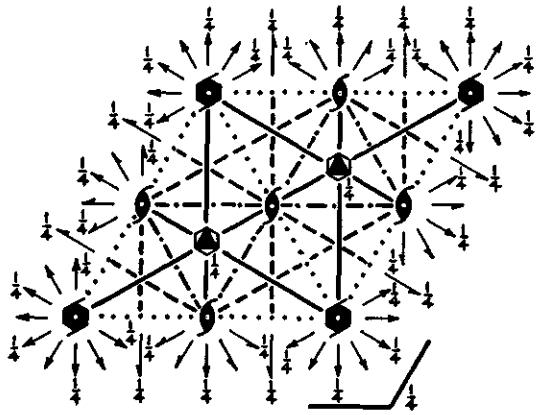
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	l	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; y,x,z; $\bar{x},y-x,z$; $x-y,\bar{y},z$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $x,x-y,\bar{z}$; $y-x,y,\bar{z}$; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,y-x,\frac{1}{2}+z$; $x-y,x,\frac{1}{2}+z$; $x,y,\frac{1}{2}-z$; $\bar{y},x-y,\frac{1}{2}-z$; $y-x,\bar{x},\frac{1}{2}-z$; $\bar{y},\bar{x},\frac{1}{2}+z$; $x,x-y,\frac{1}{2}+z$; $y-x,y,\frac{1}{2}+z$; $y,x,\frac{1}{2}-z$; $\bar{x},y-x,\frac{1}{2}-z$; $x-y,\bar{y},\frac{1}{2}-z$.	$hkil$: No conditions $hh2\bar{h}l$: No conditions $h\bar{h}0l$: $l=2n$
				Special: as above, plus
12	k	m	$x,0,z$; $0,x,z$; $\bar{x},\bar{x},z$; $\bar{x},0,\frac{1}{2}+z$; $0,\bar{x},\frac{1}{2}+z$; $x,x,\frac{1}{2}+z$; $\bar{x},0,\bar{z}$; $0,\bar{x},\bar{z}$; $x,x,\bar{z}$; $x,0,\frac{1}{2}-z$; $0,x,\frac{1}{2}-z$; $\bar{x},\bar{x},\frac{1}{2}-z$.	no extra conditions
12	j	m	$x,y,\frac{1}{4}$; $\bar{y},x-y,\frac{1}{4}$; $y-x,\bar{x},\frac{1}{4}$; $y,x,\frac{1}{4}$; $\bar{x},y-x,\frac{1}{4}$; $x-y,\bar{y},\frac{1}{4}$; $\bar{x},\bar{y},\frac{3}{4}$; $y,y-x,\frac{3}{4}$; $x-y,x,\frac{3}{4}$; $\bar{y},\bar{x},\frac{3}{4}$; $x,x-y,\frac{3}{4}$; $y-x,y,\frac{3}{4}$.	
12	i	2	$x,2x,0$; $2\bar{x},\bar{x},0$; $x,\bar{x},0$; $\bar{x},2\bar{x},0$; $2x,x,0$; $\bar{x},x,0$; $x,2x,\frac{1}{2}$; $2\bar{x},\bar{x},\frac{1}{2}$; $x,\bar{x},\frac{1}{2}$; $\bar{x},2\bar{x},\frac{1}{2}$; $2x,x,\frac{1}{2}$; $\bar{x},x,\frac{1}{2}$.	$hkil$: $l=2n$
8	h	3	$\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\bar{z}$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}+z$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}-z$; $\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}-z$.	
6	g	mm	$x,0,\frac{1}{4}$; $0,x,\frac{1}{4}$; $\bar{x},\bar{x},\frac{1}{4}$; $\bar{x},0,\frac{3}{4}$; $0,\bar{x},\frac{3}{4}$; $x,x,\frac{3}{4}$.	no extra conditions

(*continued on next page*)

6	f	$2/m$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ \frac{1}{2},\frac{1}{2},0;\ \frac{1}{2},0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	
4	e	6	$0,0,z;\ 0,0,\bar{z};\ 0,0,\frac{1}{2}+z;\ 0,0,\frac{1}{2}-z.$	
4	d	32	$\frac{1}{3},\frac{2}{3},0;\ \frac{2}{3},\frac{1}{3},0;\ \frac{1}{3},\frac{2}{3},\frac{1}{2};\ \frac{2}{3},\frac{1}{3},\frac{1}{2}.$	$hkil$: $l=2n$
4	c	$\bar{6}$	$\frac{1}{3},\frac{2}{3},\frac{1}{4};\ \frac{2}{3},\frac{1}{3},\frac{1}{4};\ \frac{1}{3},\frac{2}{3},\frac{3}{4};\ \frac{2}{3},\frac{1}{3},\frac{3}{4}.$	
2	b	$\bar{3}m$	$0,0,0;\ 0,0,\frac{1}{2}.$	
2	a	$\bar{6}m2$	$0,0,\frac{1}{4};\ 0,0,\frac{3}{4}.$	

$P6_3/mmc$ D_{6h}^4 No. 194 $P\,6_3/m\,2/m\,2/c$ $6/m\,m\,m$ Hexagonal





Origin at centre ($\bar{3}m1$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	l	1	x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{y},\bar{x},z$; $x,x-y,z$; $y-x,y,z$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$; $y,x,\bar{z}$; $\bar{x},y-x,\bar{z}$; $x-y,\bar{y},\bar{z}$; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,y-x,\frac{1}{2}+z$; $x-y,x,\frac{1}{2}+z$; $x,y,\frac{1}{2}-z$; $\bar{y},x-y,\frac{1}{2}-z$; $y-x,\bar{x},\frac{1}{2}-z$; $y,x,\frac{1}{2}+z$; $\bar{x},y-x,\frac{1}{2}+z$; $x-y,\bar{y},\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}-z$; $x,x-y,\frac{1}{2}-z$; $y-x,y,\frac{1}{2}-z$.	$hkil$: No conditions $hh2\bar{h}l$: $l=2n$ $h\bar{h}0l$: No conditions
				Special: as above, plus
12	k	m	$x,2x,z$; $2\bar{x},\bar{x},z$; $x,\bar{x},z$; $\bar{x},2\bar{x},\bar{z}$; $2x,x,\bar{z}$; $\bar{x},x,\bar{z}$; $\bar{x},2\bar{x},\frac{1}{2}+z$; $2x,x,\frac{1}{2}+z$; $\bar{x},x,\frac{1}{2}+z$; $x,2x,\frac{1}{2}-z$; $2\bar{x},\bar{x},\frac{1}{2}-z$; $x,\bar{x},\frac{1}{2}-z$.	no extra conditions
12	j	m	$x,y,\frac{1}{4}$; $\bar{y},x-y,\frac{1}{4}$; $y-x,\bar{x},\frac{1}{4}$; $\bar{y},\bar{x},\frac{1}{4}$; $x,x-y,\frac{1}{4}$; $y-x,y,\frac{1}{4}$; $\bar{x},\bar{y},\frac{3}{4}$; $y,y-x,\frac{3}{4}$; $x-y,x,\frac{3}{4}$; $y,x,\frac{3}{4}$; $\bar{x},y-x,\frac{3}{4}$; $x-y,\bar{y},\frac{3}{4}$.	
12	i	2	$x,0,0$; $0,x,0$; $\bar{x},\bar{x},0$; $x,0,\frac{1}{2}$; $0,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $\bar{x},0,0$; $0,\bar{x},0$; $x,x,0$; $\bar{x},0,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$; $x,x,\frac{1}{2}$.	$hkil$: $l=2n$
6	h	mm	$x,2x,\frac{1}{4}$; $2\bar{x},\bar{x},\frac{1}{4}$; $x,\bar{x},\frac{1}{4}$; $\bar{x},2\bar{x},\frac{3}{4}$; $2x,x,\frac{3}{4}$; $\bar{x},x,\frac{3}{4}$.	no extra conditions
6	g	$2/m$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	$hkil$: $l=2n$
4	f	$3m$	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}-z$.	$hkil$: If $h-k=3n$, then $l=2n$
4	e	$3m$	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	$hkil$: $l=2n$

(*continued on next page*)

2	d	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$;	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$.	*hkil*: If $h-k=3n$, then $l=2n$
2	c	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$;	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$.	
2	b	$\bar{6}m2$	$0,0,\frac{1}{4}$;	$0,0,\frac{3}{4}$.	*hkil*: $l=2n$
2	a	$\bar{3}m$	$0,0,0$;	$0,0,\frac{1}{2}$.	

Y

$P23$ T^1

No. 195 $P\,2\,3$ 2 3 Cubic

Origin at 23

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
12	j	1	x,y,z; z,x,y; y,z,x; $x,\bar{y},\bar{z}$; $z,\bar{x},\bar{y}$; $y,\bar{z},\bar{x}$; $\bar{x},y,\bar{z}$; $\bar{z},x,\bar{y}$; $\bar{y},z,\bar{x}$; $\bar{x},\bar{y},z$; $\bar{z},\bar{x},y$; $\bar{y},\bar{z},x$.	No conditions
				Special:
6	i	2	$x,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},x$; $\bar{x},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\bar{x},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\bar{x}$.	No conditions
6	h	2	$x,\frac{1}{2},0$; $0,x,\frac{1}{2}$; $\frac{1}{2},0,x$; $\bar{x},\frac{1}{2},0$; $0,\bar{x},\frac{1}{2}$; $\frac{1}{2},0,\bar{x}$.	
6	g	2	$x,0,\frac{1}{2}$; $\frac{1}{2},x,0$; $0,\frac{1}{2},x$; $\bar{x},0,\frac{1}{2}$; $\frac{1}{2},\bar{x},0$; $0,\frac{1}{2},\bar{x}$.	
6	f	2	$x,0,0$; $0,x,0$; $0,0,x$; $\bar{x},0,0$; $0,\bar{x},0$; $0,0,\bar{x}$.	
4	e	3	x,x,x; $x,\bar{x},\bar{x}$; $\bar{x},x,\bar{x}$; $\bar{x},\bar{x},x$.	
3	d	222	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	
3	c	222	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	
1	b	23	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
1	a	23	$0,0,0$.	

$F23$ T^2

No. 196 $F\,2\,3$ 2 3 Cubic

Origin at 23

$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0;)+$

				General:
48	h	1	x,y,z; z,x,y; y,z,x; $x,\bar{y},\bar{z}$; $z,\bar{x},\bar{y}$; $y,\bar{z},\bar{x}$; $\bar{x},y,\bar{z}$; $\bar{z},x,\bar{y}$; $\bar{y},z,\bar{x}$; $\bar{x},\bar{y},z$; $\bar{z},\bar{x},y$; $\bar{y},\bar{z},x$.	hkl: $h+k, k+l, (l+h)=2n$ $h00$: $(h=2n)$; ↻
				Special: as above only
24	g	2	$x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},x,\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},x$; $\bar{x},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\bar{x},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\bar{x}$.	
24	f	2	$x,0,0$; $0,x,0$; $0,0,x$; $\bar{x},0,0$; $0,\bar{x},0$; $0,0,\bar{x}$.	
16	e	3	x,x,x; $x,\bar{x},\bar{x}$; $\bar{x},x,\bar{x}$; $\bar{x},\bar{x},x$.	
4	d	23	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$.	
4	c	23	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$.	
4	b	23	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
4	a	23	$0,0,0$.	

Origin at 23

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+$	Conditions limiting possible reflections
				General:
24	f	1	$x,y,z;\ z,x,y;\ y,z,x;\ x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ \bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x.$	hkl: $h+k+l=2n$ $h00$: $(h=2n)$; ↻
				Special: as above only
12	e	2	$x,\tfrac{1}{2},0;\ 0,x,\tfrac{1}{2};\ \tfrac{1}{2},0,x;\ \bar{x},\tfrac{1}{2},0;\ 0,\bar{x},\tfrac{1}{2};\ \tfrac{1}{2},0,\bar{x}.$	
12	d	2	$x,0,0;\ 0,x,0;\ 0,0,x;\ \bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x}.$	
8	c	3	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x.$	
6	b	222	$0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0.$	
2	a	23	$0,0,0.$	

Origin on 3, halfway between three pairs of non-intersecting 2_1-axes

				General:
12	b	1	$x,y,z;\ z,x,y;\ y,z,x;$ $\tfrac{1}{2}+x,\tfrac{1}{2}-y,\bar{z};\ \tfrac{1}{2}+z,\tfrac{1}{2}-x,\bar{y};\ \tfrac{1}{2}+y,\tfrac{1}{2}-z,\bar{x};$ $\bar{x},\tfrac{1}{2}+y,\tfrac{1}{2}-z;\ \bar{z},\tfrac{1}{2}+x,\tfrac{1}{2}-y;\ \bar{y},\tfrac{1}{2}+z,\tfrac{1}{2}-x;$ $\tfrac{1}{2}-x,\bar{y},\tfrac{1}{2}+z;\ \tfrac{1}{2}-z,\bar{x},\tfrac{1}{2}+y;\ \tfrac{1}{2}-y,\bar{z},\tfrac{1}{2}+x.$	hkl: No conditions $h00$: $h=2n$; ↻
				Special: as above only
4	a	3	$x,x,x;\ \tfrac{1}{2}+x,\tfrac{1}{2}-x,\bar{x};\ \bar{x},\tfrac{1}{2}+x,\tfrac{1}{2}-x;\ \tfrac{1}{2}-x,\bar{x},\tfrac{1}{2}+x.$	

$I2_13$ T^5

No. 199 $I\,2_1\,3$ 2 3 Cubic

Origin on 3, halfway between 3 pairs of non-intersecting 2-axes

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Conditions limiting possible reflections
24	c	1	$x,y,z;$	$z,x,y;$	$y,z,x;$	General:
			$\frac{1}{2}+x,\frac{1}{2}-y,\bar{z};$	$\frac{1}{2}+z,\frac{1}{2}-x,\bar{y};$	$\frac{1}{2}+y,\frac{1}{2}-z,\bar{x};$	hkl: $h+k+l=2n$
			$\bar{x},\frac{1}{2}+y,\frac{1}{2}-z;$	$\bar{z},\frac{1}{2}+x,\frac{1}{2}-y;$	$\bar{y},\frac{1}{2}+z,\frac{1}{2}-x;$	$h00$: $(h=2n)$; ↻
			$\frac{1}{2}-x,\bar{y},\frac{1}{2}+z;$	$\frac{1}{2}-z,\bar{x},\frac{1}{2}+y;$	$\frac{1}{2}-y,\bar{z},\frac{1}{2}+x.$	
						Special: as above only
12	b	2	$x,0,\frac{1}{4};$ $\frac{1}{4},x,0;$ $0,\frac{1}{4},x;$ $\bar{x},\frac{1}{2},\frac{1}{4};$ $\frac{1}{4},\bar{x},\frac{1}{2};$ $\frac{1}{2},\frac{1}{4},\bar{x}.$			
8	a	3	$x,x,x;$ $\frac{1}{2}+x,\frac{1}{2}-x,\bar{x};$ $\bar{x},\frac{1}{2}+x,\frac{1}{2}-x;$ $\frac{1}{2}-x,\bar{x},\frac{1}{2}+x.$			

$Pm3$ T_h^1

No. 200 $P\,2/m\,\bar{3}$ $m\,3$ Cubic

Origin at centre (m3)

								Conditions
24	l	1	$x,y,z;$	$z,x,y;$	$y,z,x;$	$\bar{x},\bar{y},\bar{z};$	$\bar{z},\bar{x},\bar{y};$	$\bar{y},\bar{z},\bar{x};$	General:
			$x,\bar{y},\bar{z};$	$z,\bar{x},\bar{y};$	$y,\bar{z},\bar{x};$	$\bar{x},y,z;$	$\bar{z},x,y;$	$\bar{y},z,x;$	No conditions
			$\bar{x},y,\bar{z};$	$\bar{z},x,\bar{y};$	$\bar{y},z,\bar{x};$	$x,\bar{y},z;$	$z,\bar{x},y;$	$y,\bar{z},x;$	
			$\bar{x},\bar{y},z;$	$\bar{z},\bar{x},y;$	$\bar{y},\bar{z},x;$	$x,y,\bar{z};$	$z,x,\bar{y};$	$y,z,\bar{x}.$	
									Special:
12	k	m	$\frac{1}{2},y,z;$	$z,\frac{1}{2},y;$	$y,z,\frac{1}{2};$	$\frac{1}{2},\bar{y},\bar{z};$	$\bar{z},\frac{1}{2},\bar{y};$	$\bar{y},\bar{z},\frac{1}{2};$	No conditions
			$\frac{1}{2},y,\bar{z};$	$\bar{z},\frac{1}{2},y;$	$y,\bar{z},\frac{1}{2};$	$\frac{1}{2},\bar{y},z;$	$z,\frac{1}{2},\bar{y};$	$\bar{y},z,\frac{1}{2}.$	
12	j	m	$0,y,z;$	$z,0,y;$	$y,z,0;$	$0,\bar{y},\bar{z};$	$\bar{z},0,\bar{y};$	$\bar{y},\bar{z},0;$	
			$0,y,\bar{z};$	$\bar{z},0,y;$	$y,\bar{z},0;$	$0,\bar{y},z;$	$z,0,\bar{y};$	$\bar{y},z,0.$	
8	i	3	$x,x,x;$	$x,\bar{x},\bar{x};$	$\bar{x},x,\bar{x};$	$\bar{x},\bar{x},x;$			
			$\bar{x},\bar{x},\bar{x};$	$\bar{x},x,x;$	$x,\bar{x},x;$	$x,x,\bar{x}.$			
6	h	mm	$x,\frac{1}{2},\frac{1}{2};$	$\frac{1}{2},x,\frac{1}{2};$	$\frac{1}{2},\frac{1}{2},x;$	$\bar{x},\frac{1}{2},\frac{1}{2};$	$\frac{1}{2},\bar{x},\frac{1}{2};$	$\frac{1}{2},\frac{1}{2},\bar{x}.$	
6	g	mm	$x,\frac{1}{2},0;$	$0,x,\frac{1}{2};$	$\frac{1}{2},0,x;$	$\bar{x},\frac{1}{2},0;$	$0,\bar{x},\frac{1}{2};$	$\frac{1}{2},0,\bar{x}.$	
6	f	mm	$x,0,\frac{1}{2};$	$\frac{1}{2},x,0;$	$0,\frac{1}{2},x;$	$\bar{x},0,\frac{1}{2};$	$\frac{1}{2},\bar{x},0;$	$0,\frac{1}{2},\bar{x}.$	
6	e	mm	$x,0,0;$	$0,x,0;$	$0,0,x;$	$\bar{x},0,0;$	$0,\bar{x},0;$	$0,0,\bar{x}.$	
3	d	mmm	$\frac{1}{2},0,0;$	$0,\frac{1}{2},0;$	$0,0,\frac{1}{2}.$				
3	c	mmm	$0,\frac{1}{2},\frac{1}{2};$	$\frac{1}{2},0,\frac{1}{2};$	$\frac{1}{2},\frac{1}{2},0.$				
1	b	$m3$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}.$						
1	a	$m3$	$0,0,0.$						

Origin at 23, at $\bar{\frac{1}{4}},\bar{\frac{1}{4}},\bar{\frac{1}{4}}$ from centre ($\bar{3}$) (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	h	1	$x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;$ $z,x,y;\ z,\bar{x},\bar{y};\ \bar{z},x,\bar{y};\ \bar{z},\bar{x},y;$ $y,z,x;\ y,\bar{z},\bar{x};\ \bar{y},z,\bar{x};\ \bar{y},\bar{z},x;$ $\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z;\ \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z;$ $\frac{1}{2}-z,\frac{1}{2}-x,\frac{1}{2}-y;\ \frac{1}{2}-z,\frac{1}{2}+x,\frac{1}{2}+y;$ $\frac{1}{2}-y,\frac{1}{2}-z,\frac{1}{2}-x;\ \frac{1}{2}-y,\frac{1}{2}+z,\frac{1}{2}+x;$ $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z;$ $\frac{1}{2}+z,\frac{1}{2}-x,\frac{1}{2}+y;\ \frac{1}{2}+z,\frac{1}{2}+x,\frac{1}{2}-y;$ $\frac{1}{2}+y,\frac{1}{2}-z,\frac{1}{2}+x;\ \frac{1}{2}+y,\frac{1}{2}+z,\frac{1}{2}-x.$	hkl: No conditions $0kl$: $k+l=2n$; ↻
				Special: as above, plus
12	g	2	$x,\frac{1}{2},0;\ 0,x,\frac{1}{2};\ \frac{1}{2},0,x;\ \frac{1}{2}+x,0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2}+x,0;\ 0,\frac{1}{2},\frac{1}{2}+x;$ $\bar{x},\frac{1}{2},0;\ 0,\bar{x},\frac{1}{2};\ \frac{1}{2},0,\bar{x};\ \frac{1}{2}-x,0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2}-x,0;\ 0,\frac{1}{2},\frac{1}{2}-x.$	hkl: $h+k+l=2n$
12	f	2	$x,0,0;\ 0,x,0;\ 0,0,x;\ \frac{1}{2}+x,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},\frac{1}{2}+x,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}+x;$ $\bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x};\ \frac{1}{2}-x,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},\frac{1}{2}-x,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}-x.$	
8	e	3	$x,x,x;\ \frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}-x;$ $x,\bar{x},\bar{x};\ \frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}+x;$ $\bar{x},x,\bar{x};\ \frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}+x;$ $\bar{x},\bar{x},x;\ \frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}-x.$	no extra conditions
6	d	222	$0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0;\ \frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}.$	hkl: $h+k+l=2n$
4	c	$\bar{3}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{3}{4}.$	hkl: $h+k,k+l,(l+h)=2n$
4	b	$\bar{3}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\frac{3}{4},\frac{1}{4}.$	
2	a	23	$0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	hkl: $h+k+l=2n$

Origin at centre ($\bar{3}$), at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 23 (compare previous page for alternative origin)

Number of positions,	Wyckoff notation,	and point symmetry	Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	h	1	x,y,z; $x,\frac{1}{2}-y,\frac{1}{2}-z$; $\frac{1}{2}-x,y,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}-y,z$; z,x,y; $z,\frac{1}{2}-x,\frac{1}{2}-y$; $\frac{1}{2}-z,x,\frac{1}{2}-y$; $\frac{1}{2}-z,\frac{1}{2}-x,y$; y,z,x; $y,\frac{1}{2}-z,\frac{1}{2}-x$; $\frac{1}{2}-y,z,\frac{1}{2}-x$; $\frac{1}{2}-y,\frac{1}{2}-z,x$; $\bar{x},\bar{y},\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}+z$; $\frac{1}{2}+x,\bar{y},\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\bar{z},\bar{x},\bar{y}$; $\bar{z},\frac{1}{2}+x,\frac{1}{2}+y$; $\frac{1}{2}+z,\bar{x},\frac{1}{2}+y$; $\frac{1}{2}+z,\frac{1}{2}+x,\bar{y}$; $\bar{y},\bar{z},\bar{x}$; $\bar{y},\frac{1}{2}+z,\frac{1}{2}+x$; $\frac{1}{2}+y,\bar{z},\frac{1}{2}+x$; $\frac{1}{2}+y,\frac{1}{2}+z,\bar{x}$.	hkl: No conditions $0kl$: $k+l=2n$; ↻
				Special: as above, plus
12	g	2	$x,\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},x,\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},x$; $\frac{1}{2}+x,\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{2}+x,\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}+x$; $\bar{x},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\bar{x},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\bar{x}$; $\frac{1}{2}-x,\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{2}-x,\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}-x$.	hkl: $h+k+l=2n$
12	f	2	$x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},x,\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},x$; $\frac{1}{2}+x,\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{2}+x,\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}+x$; $\bar{x},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\bar{x},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\bar{x}$; $\frac{1}{2}-x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{2}-x,\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}-x$.	
8	e	3	x,x,x; $x,\frac{1}{2}-x,\frac{1}{2}-x$; $\frac{1}{2}-x,x,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}-x,x$; $\bar{x},\bar{x},\bar{x}$; $\bar{x},\frac{1}{2}+x,\frac{1}{2}+x$; $\frac{1}{2}+x,\bar{x},\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+x,\bar{x}$.	no extra conditions
6	d	222	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{3}{4}$.	hkl: $h+k+l=2n$
4	c	$\bar{3}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	hkl: $h+k,k+l,(l+h)=2n$
4	b	$\bar{3}$	$0,0,0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	
2	a	23	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$.	hkl: $h+k+l=2n$

Origin at centre ($m3$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	Conditions limiting possible reflections
				General:
96	i	1	$x,y,z;\ z,x,y;\ y,z,x;\ \bar{x},\bar{y},\bar{z};\ \bar{z},\bar{x},\bar{y};\ \bar{y},\bar{z},\bar{x};$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ \bar{x},y,z;\ \bar{z},x,y;\ \bar{y},z,x;$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ x,\bar{y},z;\ z,\bar{x},y;\ y,\bar{z},x;$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ x,y,\bar{z};\ z,x,\bar{y};\ y,z,\bar{x}.$	hkl: $h+k,k+l,(l+h)=2n$ $hk0$: $(h,\ k=2n)$; ↻
				Special: as above, plus
48	h	m	$0,y,z;\ z,0,y;\ y,z,0;\ 0,\bar{y},\bar{z};\ \bar{z},0,\bar{y};\ \bar{y},\bar{z},0;$ $0,y,\bar{z};\ \bar{z},0,y;\ y,\bar{z},0;\ 0,\bar{y},z;\ z,0,\bar{y};\ \bar{y},z,0.$	no extra conditions
48	g	2	$x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},x,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},x;\ \frac{1}{2}+x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{2}+x,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{2}+x;$ $\bar{x},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\bar{x},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\bar{x};\ \frac{1}{2}-x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{2}-x,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{2}-x.$	hkl: $h,(k,l)=2n$
32	f	3	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x;$ $\bar{x},\bar{x},\bar{x};\ \bar{x},x,x;\ x,\bar{x},x;\ x,x,\bar{x}.$	no extra conditions
24	e	mm	$x,0,0;\ 0,x,0;\ 0,0,x;\ \bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x}.$	
24	d	$2/m$	$0,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},0;\ \frac{1}{2},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{2},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{2}.$	hkl: $h,(k,l)=2n$
8	c	23	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{3}{4},\frac{3}{4},\frac{3}{4}.$	
4	b	$m3$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}.$	no extra conditions
4	a	$m3$	$0,0,0.$	

Origin at 23, at $\bar{\tfrac{1}{8}},\bar{\tfrac{1}{4}},\bar{\tfrac{1}{8}}$ from centre ($\bar{3}$) (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0)+$				Conditions limiting possible reflections
							General:
96	g	1	$x,y,z;$	$\bar{x},y,\bar{z};$	$\tfrac{1}{4}-x,\tfrac{1}{4}-y,\tfrac{1}{4}-z;$	$\tfrac{1}{4}+x,\tfrac{1}{4}-y,\tfrac{1}{4}+z;$	hkl: $h+k,k+l,(l+h)=2n$
			$z,x,y;$	$\bar{z},x,\bar{y};$	$\tfrac{1}{4}-z,\tfrac{1}{4}-x,\tfrac{1}{4}-y;$	$\tfrac{1}{4}+z,\tfrac{1}{4}-x,\tfrac{1}{4}+y;$	$0kl$: $(k,l=2n)$; $k+l=4n$
			$y,z,x;$	$\bar{y},z,\bar{x};$	$\tfrac{1}{4}-y,\tfrac{1}{4}-z,\tfrac{1}{4}-x;$	$\tfrac{1}{4}+y,\tfrac{1}{4}-z,\tfrac{1}{4}+x;$	C
			$x,\bar{y},\bar{z};$	$\bar{x},\bar{y},z;$	$\tfrac{1}{4}-x,\tfrac{1}{4}+y,\tfrac{1}{4}+z;$	$\tfrac{1}{4}+x,\tfrac{1}{4}+y,\tfrac{1}{4}-z;$	
			$z,\bar{x},\bar{y};$	$\bar{z},\bar{x},y;$	$\tfrac{1}{4}-z,\tfrac{1}{4}+x,\tfrac{1}{4}+y;$	$\tfrac{1}{4}+z,\tfrac{1}{4}+x,\tfrac{1}{4}-y;$	
			$y,\bar{z},\bar{x};$	$\bar{y},\bar{z},x;$	$\tfrac{1}{4}-y,\tfrac{1}{4}+z,\tfrac{1}{4}+x;$	$\tfrac{1}{4}+y,\tfrac{1}{4}+z,\tfrac{1}{4}-x.$	
							Special: as above, plus
48	f	2	$x,0,0;$	$\bar{x},0,0;$	$\tfrac{1}{4}-x,\tfrac{1}{4},\tfrac{1}{4};$	$\tfrac{1}{4}+x,\tfrac{1}{4},\tfrac{1}{4};$	hkl: $h+k+l=2n+1$ or $4n$
			$0,x,0;$	$0,\bar{x},0;$	$\tfrac{1}{4},\tfrac{1}{4}-x,\tfrac{1}{4};$	$\tfrac{1}{4},\tfrac{1}{4}+x,\tfrac{1}{4};$	
			$0,0,x;$	$0,0,\bar{x};$	$\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}-x;$	$\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}+x.$	
32	e	3	$x,x,x;$	$\tfrac{1}{4}-x,\tfrac{1}{4}-x,\tfrac{1}{4}-x;$			no extra conditions
			$x,\bar{x},\bar{x};$	$\tfrac{1}{4}-x,\tfrac{1}{4}+x,\tfrac{1}{4}+x;$			
			$\bar{x},x,\bar{x};$	$\tfrac{1}{4}+x,\tfrac{1}{4}-x,\tfrac{1}{4}+x;$			
			$\bar{x},\bar{x},x;$	$\tfrac{1}{4}+x,\tfrac{1}{4}+x,\tfrac{1}{4}-x.$			
16	d	$\bar{3}$	$\tfrac{5}{8},\tfrac{5}{8},\tfrac{5}{8};$	$\tfrac{5}{8},\tfrac{7}{8},\tfrac{7}{8};$	$\tfrac{7}{8},\tfrac{5}{8},\tfrac{7}{8};$	$\tfrac{7}{8},\tfrac{7}{8},\tfrac{5}{8}.$	hkl: $h=2n+1$, $(k=2n+1)$, $(l=2n+1)$; $4n+2$ or $4n+2$, $4n+2$ or $4n$, $4n$
16	c	$\bar{3}$	$\tfrac{1}{8},\tfrac{1}{8},\tfrac{1}{8};$	$\tfrac{1}{8},\tfrac{3}{8},\tfrac{3}{8};$	$\tfrac{3}{8},\tfrac{1}{8},\tfrac{3}{8};$	$\tfrac{3}{8},\tfrac{3}{8},\tfrac{1}{8}.$	
8	b	23	$\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2};$	$\tfrac{3}{4},\tfrac{3}{4},\tfrac{3}{4}.$			hkl: $h+k+l=2n+1$ or $4n$
8	a	23	$0,0,0;$	$\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}.$			

Origin at centre ($\bar{3}$), at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from 23 (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	Conditions limiting possible reflections
				General:
96	g	1	$x,y,z;\ x,\frac{1}{4}-y,\frac{1}{4}-z;\ \frac{1}{4}-x,y,\frac{1}{4}-z;\ \frac{1}{4}-x,\frac{1}{4}-y,z;$ $z,x,y;\ z,\frac{1}{4}-x,\frac{1}{4}-y;\ \frac{1}{4}-z,x,\frac{1}{4}-y;\ \frac{1}{4}-z,\frac{1}{4}-x,y;$ $y,z,x;\ y,\frac{1}{4}-z,\frac{1}{4}-x;\ \frac{1}{4}-y,z,\frac{1}{4}-x;\ \frac{1}{4}-y,\frac{1}{4}-z,x;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},\frac{3}{4}+y,\frac{3}{4}+z;\ \frac{3}{4}+x,\bar{y},\frac{3}{4}+z;\ \frac{3}{4}+x,\frac{3}{4}+y,\bar{z};$ $\bar{z},\bar{x},\bar{y};\ \bar{z},\frac{3}{4}+x,\frac{3}{4}+y;\ \frac{3}{4}+z,\bar{x},\frac{3}{4}+y;\ \frac{3}{4}+z,\frac{3}{4}+x,\bar{y};$ $\bar{y},\bar{z},\bar{x};\ \bar{y},\frac{3}{4}+z,\frac{3}{4}+x;\ \frac{3}{4}+y,\bar{z},\frac{3}{4}+x;\ \frac{3}{4}+y,\frac{3}{4}+z,\bar{x}.$	hkl: $h+k,k+l,(l+h)=2n$ $0kl$: $(k,l=2n)$; $k+l=4n$ $\circlearrowright$
				Special: as above, plus
48	f	2	$x,\frac{1}{8},\frac{1}{8};\ \bar{x},\frac{7}{8},\frac{7}{8};\ \frac{1}{4}-x,\frac{1}{8},\frac{1}{8};\ \frac{3}{4}+x,\frac{7}{8},\frac{7}{8};$ $\frac{1}{8},x,\frac{1}{8};\ \frac{7}{8},\bar{x},\frac{7}{8};\ \frac{1}{8},\frac{1}{4}-x,\frac{1}{8};\ \frac{7}{8},\frac{3}{4}+x,\frac{7}{8};$ $\frac{1}{8},\frac{1}{8},x;\ \frac{7}{8},\frac{7}{8},\bar{x};\ \frac{1}{8},\frac{1}{8},\frac{1}{4}-x;\ \frac{7}{8},\frac{7}{8},\frac{3}{4}+x.$	hkl: $h+k+l=2n+1$ or 4n
32	e	3	$x,x,x;\ \bar{x},\bar{x},\bar{x};$ $x,\frac{1}{4}-x,\frac{1}{4}-x;\ \bar{x},\frac{3}{4}+x,\frac{3}{4}+x;$ $\frac{1}{4}-x,x,\frac{1}{4}-x;\ \frac{3}{4}+x,\bar{x},\frac{3}{4}+x;$ $\frac{1}{4}-x,\frac{1}{4}-x,x;\ \frac{3}{4}+x,\frac{3}{4}+x,\bar{x}.$	no extra conditions
16	d	$\bar{3}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2};\ \frac{1}{2},\frac{3}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{2},\frac{3}{4};\ \frac{3}{4},\frac{3}{4},\frac{1}{2}.$	hkl: $h=2n+1$, $(k=2n+1)$, $(l=2n+1)$; $4n+2$ or $4n+2$, $4n+2$; $4n$ or $4n$, $4n$
16	c	$\bar{3}$	$0,0,0;\ 0,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},0.$	
8	b	23	$\frac{5}{8},\frac{5}{8},\frac{5}{8};\ \frac{3}{8},\frac{3}{8},\frac{3}{8}.$	hkl: $h+k+l=2n+1$ or $4n$
8	a	23	$\frac{1}{8},\frac{1}{8},\frac{1}{8};\ \frac{7}{8},\frac{7}{8},\frac{7}{8}.$	

$Im3$ T_h^5

No. 204 $I\,2/m\,\bar{3}$ $m\,3$ Cubic

Origin at centre ($m3$)

Number of positions, Wyckoff notation and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
48	h	1	$x,y,z;\ z,x,y;\ y,z,x;\ \bar{x},\bar{y},\bar{z};\ \bar{z},\bar{x},\bar{y};\ \bar{y},\bar{z},\bar{x};$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ \bar{x},y,z;\ \bar{z},x,y;\ \bar{y},z,x;$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ x,\bar{y},z;\ z,\bar{x},y;\ y,\bar{z},x;$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ x,y,\bar{z};\ z,x,\bar{y};\ y,z,\bar{x}.$	hkl: $h+k+l=2n$ $0kl$: $(k+l=2n)$ $\circlearrowright$
				Special: as above, plus
24	g	m	$0,y,z;\ z,0,y;\ y,z,0;\ 0,\bar{y},\bar{z};\ \bar{z},0,\bar{y};\ \bar{y},\bar{z},0;$ $0,y,\bar{z};\ \bar{z},0,y;\ y,\bar{z},0;\ 0,\bar{y},z;\ z,0,\bar{y};\ \bar{y},z,0.$	no extra conditions
16	f	3	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x;$ $\bar{x},\bar{x},\bar{x};\ \bar{x},x,x;\ x,\bar{x},x;\ x,x,\bar{x}.$	
12	e	mm	$x,0,\frac{1}{2};\ \frac{1}{2},x,0;\ 0,\frac{1}{2},x;\ \bar{x},0,\frac{1}{2};\ \frac{1}{2},\bar{x},0;\ 0,\frac{1}{2},\bar{x}.$	
12	d	mm	$x,0,0;\ 0,x,0;\ 0,0,x;\ \bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x}.$	
8	c	$\bar{3}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\frac{3}{4},\frac{1}{4}.$	hkl: $h,k,(l)=2n$
6	b	mmm	$0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0.$	no extra conditions
2	a	$m3$	$0,0,0.$	

$Pa3$ T_h^6

No. 205 $P\,2_1/a\,\bar{3}$ $m\,3$ Cubic

Origin at centre ($\bar{3}$)

				General:
24	d	1	$x,y,z;\ \frac{1}{2}+x,\frac{1}{2}-y,\bar{z};\ \bar{x},\frac{1}{2}+y,\frac{1}{2}-z;\ \frac{1}{2}-x,\bar{y},\frac{1}{2}+z;$ $z,x,y;\ \frac{1}{2}+z,\frac{1}{2}-x,\bar{y};\ \bar{z},\frac{1}{2}+x,\frac{1}{2}-y;\ \frac{1}{2}-z,\bar{x},\frac{1}{2}+y;$ $y,z,x;\ \frac{1}{2}+y,\frac{1}{2}-z,\bar{x};\ \bar{y},\frac{1}{2}+z,\frac{1}{2}-x;\ \frac{1}{2}-y,\bar{z},\frac{1}{2}+x;$ $\bar{x},\bar{y},\bar{z};\ \frac{1}{2}-x,\frac{1}{2}+y,z;\ x,\frac{1}{2}-y,\frac{1}{2}+z;\ \frac{1}{2}+x,y,\frac{1}{2}-z;$ $\bar{z},\bar{x},\bar{y};\ \frac{1}{2}-z,\frac{1}{2}+x,y;\ z,\frac{1}{2}-x,\frac{1}{2}+y;\ \frac{1}{2}+z,x,\frac{1}{2}-y;$ $\bar{y},\bar{z},\bar{x};\ \frac{1}{2}-y,\frac{1}{2}+z,x;\ y,\frac{1}{2}-z,\frac{1}{2}+x;\ \frac{1}{2}+y,z,\frac{1}{2}-x.$	hkl: No conditions $0kl$: $k=2n$ $h0l$: $(l=2n)$ $hk0$: $(h=2n)$ h, k, l not permutable
				Special: as above, plus
8	c	3	$x,x,x;\ \frac{1}{2}+x,\frac{1}{2}-x,\bar{x};\ \bar{x},\frac{1}{2}+x,\frac{1}{2}-x;\ \frac{1}{2}-x,\bar{x},\frac{1}{2}+x;$ $\bar{x},\bar{x},\bar{x};\ \frac{1}{2}-x,\frac{1}{2}+x,x;\ x,\frac{1}{2}-x,\frac{1}{2}+x;\ \frac{1}{2}+x,x,\frac{1}{2}-x.$	no extra conditions
4	b	$\bar{3}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}.$	hkl: $h+k,k+l,(l+h)=2n$
4	a	$\bar{3}$	$0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0.$	

Origin at centre ($\bar{3}$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+$	Conditions limiting possible reflections
				General:
48	e	1	$x,y,z;\ x,\bar{y},\tfrac{1}{2}-z;\ \tfrac{1}{2}-x,y,\bar{z};\ \bar{x},\tfrac{1}{2}-y,z;$ $z,x,y;\ z,\bar{x},\tfrac{1}{2}-y;\ \tfrac{1}{2}-z,x,\bar{y};\ \bar{z},\tfrac{1}{2}-x,y;$ $y,z,x;\ y,\bar{z},\tfrac{1}{2}-x;\ \tfrac{1}{2}-y,z,\bar{x};\ \bar{y},\tfrac{1}{2}-z,x;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},y,\tfrac{1}{2}+z;\ \tfrac{1}{2}+x,\bar{y},z;\ x,\tfrac{1}{2}+y,\bar{z};$ $\bar{z},\bar{x},\bar{y};\ \bar{z},x,\tfrac{1}{2}+y;\ \tfrac{1}{2}+z,\bar{x},y;\ z,\tfrac{1}{2}+x,\bar{y};$ $\bar{y},\bar{z},\bar{x};\ \bar{y},z,\tfrac{1}{2}+x;\ \tfrac{1}{2}+y,\bar{z},x;\ y,\tfrac{1}{2}+z,\bar{x}.$	hkl: $h+k+l=2n$ $0kl$: $k,(l)=2n$ $\circlearrowright$
				Special: as above, plus
24	d	2	$x,0,\tfrac{1}{4};\ \bar{x},0,\tfrac{3}{4};\ x,\tfrac{1}{2},\tfrac{3}{4};\ \bar{x},\tfrac{1}{2},\tfrac{1}{4};$ $\tfrac{1}{4},x,0;\ \tfrac{3}{4},\bar{x},0;\ \tfrac{3}{4},x,\tfrac{1}{2};\ \tfrac{1}{4},\bar{x},\tfrac{1}{2};$ $0,\tfrac{1}{4},x;\ 0,\tfrac{3}{4},\bar{x};\ \tfrac{1}{2},\tfrac{3}{4},x;\ \tfrac{1}{2},\tfrac{1}{4},\bar{x}.$	no extra conditions
16	c	3	$x,x,x;\ \tfrac{1}{2}+x,\tfrac{1}{2}-x,\bar{x};\ \bar{x},\tfrac{1}{2}+x,\tfrac{1}{2}-x;\ \tfrac{1}{2}-x,\bar{x},\tfrac{1}{2}+x;$ $\bar{x},\bar{x},\bar{x};\ \tfrac{1}{2}-x,\tfrac{1}{2}+x,x;\ x,\tfrac{1}{2}-x,\tfrac{1}{2}+x;\ \tfrac{1}{2}+x,x,\tfrac{1}{2}-x.$	
8	b	$\bar{3}$	$\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{3}{4},\tfrac{3}{4};\ \tfrac{3}{4},\tfrac{1}{4},\tfrac{3}{4};\ \tfrac{3}{4},\tfrac{3}{4},\tfrac{1}{4}.$	hkl: $h,k,(l)=2n$
8	a	$\bar{3}$	$0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0.$	

Origin at 43

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	k	1	x,y,z; z,x,y; y,z,x; $\bar{x},\bar{z},\bar{y}$; $\bar{y},\bar{x},\bar{z}$; $\bar{z},\bar{y},\bar{x}$; $x,\bar{y},\bar{z}$; $z,\bar{x},\bar{y}$; $y,\bar{z},\bar{x}$; $\bar{x},z,y$; $\bar{y},x,z$; $\bar{z},y,x$; $\bar{x},y,\bar{z}$; $\bar{z},x,\bar{y}$; $\bar{y},z,\bar{x}$; $x,\bar{z},y$; $y,\bar{x},z$; $z,\bar{y},x$; $\bar{x},\bar{y},z$; $\bar{z},\bar{x},y$; $\bar{y},\bar{z},x$; $x,z,\bar{y}$; $y,x,\bar{z}$; $z,y,\bar{x}$.	hkl: } No conditions $h00$: } $\circlearrowright$
				Special:
12	j	2	$\frac{1}{2},x,x$; $x,\frac{1}{2},x$; $x,x,\frac{1}{2}$; $\frac{1}{2},x,\bar{x}$; $\bar{x},\frac{1}{2},x$; $x,\bar{x},\frac{1}{2}$; $\frac{1}{2},\bar{x},\bar{x}$; $\bar{x},\frac{1}{2},\bar{x}$; $\bar{x},\bar{x},\frac{1}{2}$; $\frac{1}{2},\bar{x},x$; $x,\frac{1}{2},\bar{x}$; $\bar{x},x,\frac{1}{2}$.	
12	i	2	$0,x,x$; $x,0,x$; $x,x,0$; $0,x,\bar{x}$; $\bar{x},0,x$; $x,\bar{x},0$; $0,\bar{x},\bar{x}$; $\bar{x},0,\bar{x}$; $\bar{x},\bar{x},0$; $0,\bar{x},x$; $x,0,\bar{x}$; $\bar{x},x,0$.	
12	h	2	$x,\frac{1}{2},0$; $0,x,\frac{1}{2}$; $\frac{1}{2},0,x$; $x,0,\frac{1}{2}$; $\frac{1}{2},x,0$; $0,\frac{1}{2},x$; $\bar{x},\frac{1}{2},0$; $0,\bar{x},\frac{1}{2}$; $\frac{1}{2},0,\bar{x}$; $\bar{x},0,\frac{1}{2}$; $\frac{1}{2},\bar{x},0$; $0,\frac{1}{2},\bar{x}$.	
8	g	3	x,x,x; $x,\bar{x},\bar{x}$; $\bar{x},x,\bar{x}$; $\bar{x},\bar{x},x$; $\bar{x},\bar{x},\bar{x}$; $\bar{x},x,x$; $x,\bar{x},x$; $x,x,\bar{x}$.	No conditions
6	f	4	$x,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},x$; $\bar{x},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\bar{x},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\bar{x}$.	
6	e	4	$x,0,0$; $0,x,0$; $0,0,x$; $\bar{x},0,0$; $0,\bar{x},0$; $0,0,\bar{x}$.	
3	d	42	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	
3	c	42	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	
1	b	43	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
1	a	43	$0,0,0$.	

Origin at 23

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	m	1	x,y,z; $\bar{x},y,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}-z,\frac{1}{2}-y$; $\frac{1}{2}+x,\frac{1}{2}-z,\frac{1}{2}+y$; z,x,y; $\bar{z},x,\bar{y}$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$; y,z,x; $\bar{y},z,\bar{x}$; $\frac{1}{2}-z,\frac{1}{2}-y,\frac{1}{2}-x$; $\frac{1}{2}+z,\frac{1}{2}-y,\frac{1}{2}+x$; $x,\bar{y},\bar{z}$; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+z,\frac{1}{2}+y$; $\frac{1}{2}+x,\frac{1}{2}+z,\frac{1}{2}-y$; $z,\bar{x},\bar{y}$; $\bar{z},\bar{x},y$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}-z$; $y,\bar{z},\bar{x}$; $\bar{y},\bar{z},x$; $\frac{1}{2}-z,\frac{1}{2}+y,\frac{1}{2}+x$; $\frac{1}{2}+z,\frac{1}{2}+y,\frac{1}{2}-x$.	hkl: No conditions $h00$: $h=2n$ $\circlearrowleft$
				Special: as above, plus
12	l	2	$\frac{1}{4},x,\frac{1}{2}+x$; $\frac{1}{4},\bar{x},\frac{1}{2}-x$; $\frac{3}{4},x,\frac{1}{2}-x$; $\frac{3}{4},\bar{x},\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{4},x$; $\frac{1}{2}-x,\frac{1}{4},\bar{x}$; $\frac{1}{2}-x,\frac{3}{4},x$; $\frac{1}{2}+x,\frac{3}{4},\bar{x}$; $x,\frac{1}{2}+x,\frac{1}{4}$; $\bar{x},\frac{1}{2}-x,\frac{1}{4}$; $x,\frac{1}{2}-x,\frac{3}{4}$; $\bar{x},\frac{1}{2}+x,\frac{3}{4}$.	no extra conditions
12	k	2	$\frac{1}{4},x,\frac{1}{2}-x$; $\frac{1}{4},\bar{x},\frac{1}{2}+x$; $\frac{3}{4},x,\frac{1}{2}+x$; $\frac{3}{4},\bar{x},\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{4},x$; $\frac{1}{2}+x,\frac{1}{4},\bar{x}$; $\frac{1}{2}+x,\frac{3}{4},x$; $\frac{1}{2}-x,\frac{3}{4},\bar{x}$; $x,\frac{1}{2}-x,\frac{1}{4}$; $\bar{x},\frac{1}{2}+x,\frac{1}{4}$; $x,\frac{1}{2}+x,\frac{3}{4}$; $\bar{x},\frac{1}{2}-x,\frac{3}{4}$.	
12	j	2	$x,\frac{1}{2},0$; $\bar{x},\frac{1}{2},0$; $\frac{1}{2}+x,\frac{1}{2},0$; $\frac{1}{2}-x,\frac{1}{2},0$; $0,x,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$; $0,\frac{1}{2}+x,\frac{1}{2}$; $0,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2},0,x$; $\frac{1}{2},0,\bar{x}$; $\frac{1}{2},0,\frac{1}{2}+x$; $\frac{1}{2},0,\frac{1}{2}-x$.	hkl: h or k or $l=2n$
12	i	2	$x,0,\frac{1}{2}$; $\bar{x},0,\frac{1}{2}$; $\frac{1}{2}+x,0,\frac{1}{2}$; $\frac{1}{2}-x,0,\frac{1}{2}$; $\frac{1}{2},x,0$; $\frac{1}{2},\bar{x},0$; $\frac{1}{2},\frac{1}{2}+x,0$; $\frac{1}{2},\frac{1}{2}-x,0$; $0,\frac{1}{2},x$; $0,\frac{1}{2},\bar{x}$; $0,\frac{1}{2},\frac{1}{2}+x$; $0,\frac{1}{2},\frac{1}{2}-x$.	
12	h	2	$x,0,0$; $\bar{x},0,0$; $\frac{1}{2}+x,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2},\frac{1}{2}$; $0,x,0$; $0,\bar{x},0$; $\frac{1}{2},\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}-x,\frac{1}{2}$; $0,0,x$; $0,0,\bar{x}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+x$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-x$.	hkl: $h+k+l=2n$
8	g	3	x,x,x; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}-x$; $x,\bar{x},\bar{x}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}+x$; $\bar{x},x,\bar{x}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}+x$; $\bar{x},\bar{x},x$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}-x$.	no extra conditions
6	f	222	$\frac{1}{4},\frac{1}{2},0$; $0,\frac{1}{4},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{4}$; $\frac{3}{4},\frac{1}{2},0$; $0,\frac{3}{4},\frac{1}{2}$; $\frac{1}{2},0,\frac{3}{4}$.	hkl: $h=2n+1$, $k=2n+1$, $l=2n$ or $2n+1$, $4n+2$, $4n$; $2n$, $2n$, $2n$ or $2n$, $2n$, $2n$; h,k,l permutable
6	e	222	$\frac{1}{4},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{4},0$; $0,\frac{1}{2},\frac{1}{4}$; $\frac{3}{4},0,\frac{1}{2}$; $\frac{1}{2},\frac{3}{4},0$; $0,\frac{1}{2},\frac{3}{4}$.	
6	d	222	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	hkl: $h+k+l=2n$
4	c	32	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{3}{4}$.	hkl: $h+k,k+l,(l+h)=2n$
4	b	32	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$.	
2	a	23	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	hkl: $h+k+l=2n$

Origin at 43

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	Conditions limiting possible reflections
				General:
96	j	1	$x,y,z;\ z,x,y;\ y,z,x;\ \bar{x},\bar{z},\bar{y};\ \bar{y},\bar{x},\bar{z};\ \bar{z},\bar{y},\bar{x};$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ \bar{x},z,y;\ \bar{y},x,z;\ \bar{z},y,x;$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ x,\bar{z},y;\ y,\bar{x},z;\ z,\bar{y},x;$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ x,z,\bar{y};\ y,x,\bar{z};\ z,y,\bar{x}.$	hkl: $h+k,k+l,(l+h)=2n$ $h00$: $(h=2n)$ $\mathcal{C}$
				Special: as above, plus
48	i	2	$x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},x,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},x;\ \bar{x},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\bar{x},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\bar{x};$ $x,\frac{1}{4},\frac{3}{4};\ \frac{3}{4},x,\frac{1}{4};\ \frac{1}{4},\frac{3}{4},x;\ \bar{x},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\bar{x},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\bar{x}.$	hkl: $h,(k,l)=2n$
48	h	2	$\frac{1}{2},x,x;\ x,\frac{1}{2},x;\ x,x,\frac{1}{2};\ \frac{1}{2},x,\bar{x};\ \bar{x},\frac{1}{2},x;\ x,\bar{x},\frac{1}{2};$ $\frac{1}{2},\bar{x},\bar{x};\ \bar{x},\frac{1}{2},\bar{x};\ \bar{x},\bar{x},\frac{1}{2};\ \frac{1}{2},\bar{x},x;\ x,\frac{1}{2},\bar{x};\ \bar{x},x,\frac{1}{2}.$	no extra conditions
48	g	2	$0,x,x;\ x,0,x;\ x,x,0;\ 0,x,\bar{x};\ \bar{x},0,x;\ x,\bar{x},0;$ $0,\bar{x},\bar{x};\ \bar{x},0,\bar{x};\ \bar{x},\bar{x},0;\ 0,\bar{x},x;\ x,0,\bar{x};\ \bar{x},x,0.$	
32	f	3	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x;$ $\bar{x},\bar{x},\bar{x};\ \bar{x},x,x;\ x,\bar{x},x;\ x,x,\bar{x}.$	
24	e	4	$x,0,0;\ 0,x,0;\ 0,0,x;\ \bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x}.$	
24	d	222	$0,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},0;\ \frac{1}{2},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{2},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{2}.$	hkl: $h,(k,l)=2n$
8	c	23	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{3}{4},\frac{3}{4},\frac{3}{4}.$	
4	b	43	$\frac{1}{2},\frac{1}{2},\frac{1}{2}.$	no extra conditions
4	a	43	$0,0,0.$	

Origin at 23

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	Conditions limiting possible reflections
				General:
96	h	1	$x,y,z;\ \bar{x},y,\bar{z};\ \frac{1}{4}-x,\frac{1}{4}-z,\frac{1}{4}-y;\ \frac{1}{4}+x,\frac{1}{4}-z,\frac{1}{4}+y;$ $z,x,y;\ \bar{z},x,\bar{y};\ \frac{1}{4}-y,\frac{1}{4}-x,\frac{1}{4}-z;\ \frac{1}{4}+y,\frac{1}{4}-x,\frac{1}{4}+z;$ $y,z,x;\ \bar{y},z,\bar{x};\ \frac{1}{4}-z,\frac{1}{4}-y,\frac{1}{4}-x;\ \frac{1}{4}+z,\frac{1}{4}-y,\frac{1}{4}+x;$ $x,\bar{y},\bar{z};\ \bar{x},\bar{y},z;\ \frac{1}{4}-x,\frac{1}{4}+z,\frac{1}{4}+y;\ \frac{1}{4}+x,\frac{1}{4}+z,\frac{1}{4}-y;$ $z,\bar{x},\bar{y};\ \bar{z},\bar{x},y;\ \frac{1}{4}-y,\frac{1}{4}+x,\frac{1}{4}+z;\ \frac{1}{4}+y,\frac{1}{4}+x,\frac{1}{4}-z;$ $y,\bar{z},\bar{x};\ \bar{y},\bar{z},x;\ \frac{1}{4}-z,\frac{1}{4}+y,\frac{1}{4}+x;\ \frac{1}{4}+z,\frac{1}{4}+y,\frac{1}{4}-x.$	hkl: $h+k, k+l, (l+h)=2n$ $h00$: $h=4n$ $\circlearrowleft$
				Special: as above, plus
48	g	2	$\frac{1}{8},x,\frac{1}{4}-x;\ \frac{1}{8},\bar{x},\frac{3}{4}+x;\ \frac{7}{8},x,\frac{3}{4}+x;\ \frac{7}{8},\bar{x},\frac{1}{4}-x;$ $\frac{1}{4}-x,\frac{1}{8},x;\ \frac{3}{4}+x,\frac{1}{8},\bar{x};\ \frac{3}{4}+x,\frac{7}{8},x;\ \frac{1}{4}-x,\frac{7}{8},\bar{x};$ $x,\frac{1}{4}-x,\frac{1}{8};\ \bar{x},\frac{3}{4}+x,\frac{1}{8};\ x,\frac{3}{4}+x,\frac{7}{8};\ \bar{x},\frac{1}{4}-x,\frac{7}{8}.$	no extra conditions
48	f	2	$x,0,0;\ \bar{x},0,0;\ \frac{1}{4}+x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4}-x,\frac{1}{4},\frac{1}{4};$ $0,x,0;\ 0,\bar{x},0;\ \frac{1}{4},\frac{1}{4}+x,\frac{1}{4};\ \frac{1}{4},\frac{1}{4}-x,\frac{1}{4};$ $0,0,x;\ 0,0,\bar{x};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}+x;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}-x.$	hkl: $h+k+l=2n+1$ or $4n$
32	e	3	$x,x,x;\ \frac{1}{4}-x,\frac{1}{4}-x,\frac{1}{4}-x;$ $x,\bar{x},\bar{x};\ \frac{1}{4}-x,\frac{1}{4}+x,\frac{1}{4}+x;$ $\bar{x},x,\bar{x};\ \frac{1}{4}+x,\frac{1}{4}-x,\frac{1}{4}+x;$ $\bar{x},\bar{x},x;\ \frac{1}{4}+x,\frac{1}{4}+x,\frac{1}{4}-x.$	$hk0$: $h+k=4n$
16	d	32	$\frac{5}{8},\frac{5}{8},\frac{5}{8};\ \frac{5}{8},\frac{3}{8},\frac{3}{8};\ \frac{3}{8},\frac{5}{8},\frac{3}{8};\ \frac{3}{8},\frac{3}{8},\frac{5}{8}.$	hkl: $h=2n+1$, $(k=2n+1)$, $(l=2n+1)$; $4n+2$ or $4n+2$ or $4n+2$; $4n$ or $4n$ or $4n$
16	c	32	$\frac{1}{8},\frac{1}{8},\frac{1}{8};\ \frac{1}{8},\frac{7}{8},\frac{7}{8};\ \frac{7}{8},\frac{1}{8},\frac{7}{8};\ \frac{7}{8},\frac{7}{8},\frac{1}{8}.$	
8	b	23	$\frac{1}{2},\frac{1}{2},\frac{1}{2};\ \frac{3}{4},\frac{3}{4},\frac{3}{4}.$	hkl: $h+k+l=2n+1$ or $4n$
8	a	23	$0,0,0;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}.$	

Origin at 43

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
48	j	1	$x,y,z;\ z,x,y;\ y,z,x;\ \bar{x},\bar{z},\bar{y};\ \bar{y},\bar{x},\bar{z};\ \bar{z},\bar{y},\bar{x};$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ \bar{x},z,y;\ \bar{y},x,z;\ \bar{z},y,x;$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ x,\bar{z},y;\ y,\bar{x},z;\ z,\bar{y},x;$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ x,z,\bar{y};\ y,x,\bar{z};\ z,y,\bar{x}.$	hkl: $h+k+l=2n$ $h00$: $(h=2n)$ $\circlearrowright$
				Special: as above, plus
24	i	2	$\frac{1}{4},x,\frac{1}{2}-x;\ \frac{1}{4},\bar{x},\frac{1}{2}+x;\ \frac{1}{4},\frac{1}{2}+x,x;\ \frac{1}{4},\frac{1}{2}-x,\bar{x};$ $\frac{1}{2}-x,\frac{1}{4},x;\ \frac{1}{2}+x,\frac{1}{4},\bar{x};\ x,\frac{1}{4},\frac{1}{2}+x;\ \bar{x},\frac{1}{4},\frac{1}{2}-x;$ $x,\frac{1}{2}-x,\frac{1}{4};\ \bar{x},\frac{1}{2}+x,\frac{1}{4};\ \frac{1}{2}+x,x,\frac{1}{4};\ \frac{1}{2}-x,\bar{x},\frac{1}{4}.$	no extra conditions
24	h	2	$0,x,x;\ x,0,x;\ x,x,0;\ 0,x,\bar{x};\ \bar{x},0,x;\ x,\bar{x},0;$ $0,\bar{x},\bar{x};\ \bar{x},0,\bar{x};\ \bar{x},\bar{x},0;\ 0,\bar{x},x;\ x,0,\bar{x};\ \bar{x},x,0.$	
24	g	2	$x,\frac{1}{2},0;\ 0,x,\frac{1}{2};\ \frac{1}{2},0,x;\ x,0,\frac{1}{2};\ \frac{1}{2},x,0;\ 0,\frac{1}{2},x;$ $\bar{x},\frac{1}{2},0;\ 0,\bar{x},\frac{1}{2};\ \frac{1}{2},0,\bar{x};\ \bar{x},0,\frac{1}{2};\ \frac{1}{2},\bar{x},0;\ 0,\frac{1}{2},\bar{x}.$	
16	f	3	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x;$ $\bar{x},\bar{x},\bar{x};\ \bar{x},x,x;\ x,\bar{x},x;\ x,x,\bar{x}.$	
12	e	4	$x,0,0;\ 0,x,0;\ 0,0,x;\ \bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x}.$	
12	d	222	$\frac{1}{4},\frac{1}{2},0;\ 0,\frac{1}{4},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{4};\ \frac{1}{4},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{4},0;\ 0,\frac{1}{2},\frac{1}{4}.$	
8	c	32	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\frac{3}{4},\frac{1}{4}.$	hkl: $h,k,(l)=2n$
6	b	42	$0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0.$	no extra conditions
2	a	43	$0,0,0.$	

Origin on 3, at $\frac{1}{4}$ translation from each of three non-intersecting 4_3-axes and three non-intersecting 2_1-axes

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	e	1	x,y,z; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}-x,\bar{y},\frac{1}{2}+z$; z,x,y; $\frac{1}{2}+z,\frac{1}{2}-x,\bar{y}$; $\bar{z},\frac{1}{2}+x,\frac{1}{2}-y$; $\frac{1}{2}-z,\bar{x},\frac{1}{2}+y$; y,z,x; $\frac{1}{2}+y,\frac{1}{2}-z,\bar{x}$; $\bar{y},\frac{1}{2}+z,\frac{1}{2}-x$; $\frac{1}{2}-y,\bar{z},\frac{1}{2}+x$; $\frac{1}{4}-x,\frac{1}{4}-z,\frac{1}{4}-y$; $\frac{3}{4}+x,\frac{3}{4}-z,\frac{1}{4}+y$; $\frac{1}{4}-y,\frac{1}{4}-x,\frac{1}{4}-z$; $\frac{3}{4}+y,\frac{3}{4}-x,\frac{1}{4}+z$; $\frac{1}{4}-z,\frac{1}{4}-y,\frac{1}{4}-x$; $\frac{3}{4}+z,\frac{3}{4}-y,\frac{1}{4}+x$; $\frac{3}{4}-x,\frac{1}{4}+z,\frac{3}{4}+y$; $\frac{1}{4}+x,\frac{3}{4}+z,\frac{3}{4}-y$; $\frac{3}{4}-y,\frac{1}{4}+x,\frac{3}{4}+z$; $\frac{1}{4}+y,\frac{3}{4}+x,\frac{3}{4}-z$; $\frac{3}{4}-z,\frac{1}{4}+y,\frac{3}{4}+x$; $\frac{1}{4}+z,\frac{3}{4}+y,\frac{3}{4}-x$.	hkl: No conditions $h00$: $h=4n$ $\circlearrowright$
				Special: as above, plus
12	d	2	$\frac{1}{8},x,\frac{1}{4}-x$; $\frac{3}{8},\bar{x},\frac{3}{4}-x$; $\frac{5}{8},\frac{1}{2}-x,\frac{3}{4}+x$; $\frac{7}{8},\frac{1}{2}+x,\frac{1}{4}+x$; $\frac{1}{4}-x,\frac{1}{8},x$; $\frac{3}{4}-x,\frac{3}{8},\bar{x}$; $\frac{3}{4}+x,\frac{5}{8},\frac{1}{2}-x$; $\frac{1}{4}+x,\frac{7}{8},\frac{1}{2}+x$; $x,\frac{1}{4}-x,\frac{1}{8}$; $\bar{x},\frac{3}{4}-x,\frac{3}{8}$; $\frac{1}{2}-x,\frac{3}{4}+x,\frac{5}{8}$; $\frac{1}{2}+x,\frac{1}{4}+x,\frac{7}{8}$.	no extra conditions
8	c	3	x,x,x; $\frac{1}{4}-x,\frac{1}{4}-x,\frac{1}{4}-x$; $\frac{1}{2}+x,\frac{1}{2}-x,\bar{x}$; $\frac{3}{4}-x,\frac{1}{4}+x,\frac{3}{4}+x$; $\bar{x},\frac{1}{2}+x,\frac{1}{2}-x$; $\frac{3}{4}+x,\frac{3}{4}-x,\frac{1}{4}+x$; $\frac{1}{2}-x,\bar{x},\frac{1}{2}+x$; $\frac{1}{4}+x,\frac{3}{4}+x,\frac{3}{4}-x$.	
4	b	32	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$; $\frac{1}{8},\frac{7}{8},\frac{3}{8}$; $\frac{3}{8},\frac{1}{8},\frac{7}{8}$; $\frac{7}{8},\frac{3}{8},\frac{1}{8}$.	hkl: $h=2n+1$, $k=2n+1$, $l=2n+1$ or $2n+1$, $2n+1$, $2n$ $2n+1$, $4n+2$, $4n$ or $4n+2$, $4n+2$, $4n$ h,k,l permutable
4	a	32	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$; $\frac{5}{8},\frac{3}{8},\frac{7}{8}$; $\frac{7}{8},\frac{5}{8},\frac{3}{8}$; $\frac{3}{8},\frac{7}{8},\frac{5}{8}$.	

z

Origin on 3, at $\frac{1}{4}$ translation from each of three non-intersecting 4_1-axes and three non-intersecting 2_1-axes

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	e	1	x,y,z; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}-x,\bar{y},\frac{1}{2}+z$; z,x,y; $\frac{1}{2}+z,\frac{1}{2}-x,\bar{y}$; $\bar{z},\frac{1}{2}+x,\frac{1}{2}-y$; $\frac{1}{2}-z,\bar{x},\frac{1}{2}+y$; y,z,x; $\frac{1}{2}+y,\frac{1}{2}-z,\bar{x}$; $\bar{y},\frac{1}{2}+z,\frac{1}{2}-x$; $\frac{1}{2}-y,\bar{z},\frac{1}{2}+x$; $\frac{3}{4}-x,\frac{3}{4}-z,\frac{3}{4}-y$; $\frac{1}{4}+x,\frac{1}{4}-z,\frac{3}{4}+y$; $\frac{3}{4}-y,\frac{3}{4}-x,\frac{3}{4}-z$; $\frac{1}{4}+y,\frac{1}{4}-x,\frac{3}{4}+z$; $\frac{3}{4}-z,\frac{3}{4}-y,\frac{3}{4}-x$; $\frac{1}{4}+z,\frac{1}{4}-y,\frac{3}{4}+x$; $\frac{1}{4}-x,\frac{3}{4}+z,\frac{1}{4}+y$; $\frac{3}{4}+x,\frac{1}{4}+z,\frac{1}{4}-y$; $\frac{1}{4}-y,\frac{3}{4}+x,\frac{1}{4}+z$; $\frac{3}{4}+y,\frac{1}{4}+x,\frac{1}{4}-z$; $\frac{1}{4}-z,\frac{3}{4}+y,\frac{1}{4}+x$; $\frac{3}{4}+z,\frac{1}{4}+y,\frac{1}{4}-x$.	hkl: No conditions $h00$: $h=4n$ $\circlearrowright$
				Special: as above, plus
12	d	2	$\frac{1}{8},x,\frac{1}{4}+x$; $\frac{3}{8},\bar{x},\frac{3}{4}+x$; $\frac{7}{8},\frac{1}{2}+x,\frac{1}{4}-x$; $\frac{5}{8},\frac{1}{2}-x,\frac{3}{4}-x$; $\frac{1}{4}+x,\frac{1}{8},x$; $\frac{3}{4}+x,\frac{3}{8},\bar{x}$; $\frac{1}{4}-x,\frac{7}{8},\frac{1}{2}+x$; $\frac{3}{4}-x,\frac{5}{8},\frac{1}{2}-x$; $x,\frac{1}{4}+x,\frac{1}{8}$; $\bar{x},\frac{3}{4}+x,\frac{3}{8}$; $\frac{1}{2}+x,\frac{1}{4}-x,\frac{7}{8}$; $\frac{1}{2}-x,\frac{3}{4}-x,\frac{5}{8}$.	no extra conditions
8	c	3	x,x,x; $\frac{3}{4}-x,\frac{3}{4}-x,\frac{3}{4}-x$; $\frac{1}{2}+x,\frac{1}{2}-x,\bar{x}$; $\frac{1}{4}-x,\frac{3}{4}+x,\frac{1}{4}+x$; $\bar{x},\frac{1}{2}+x,\frac{1}{2}-x$; $\frac{1}{4}+x,\frac{1}{4}-x,\frac{3}{4}+x$; $\frac{1}{2}-x,\bar{x},\frac{1}{2}+x$; $\frac{3}{4}+x,\frac{1}{4}+x,\frac{1}{4}-x$.	
4	b	32	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$; $\frac{1}{8},\frac{3}{8},\frac{5}{8}$; $\frac{5}{8},\frac{1}{8},\frac{3}{8}$; $\frac{3}{8},\frac{5}{8},\frac{1}{8}$.	hkl: $h=2n+1$, $k=2n+1$, $l=2n+1$ } $\begin{matrix}2n+1\\ \text{or } 2n+1\\ 2n\end{matrix}$ } $\begin{matrix}2n+1\\ \text{or } 4n+2\\ 4n\end{matrix}$ } $\begin{matrix}4n+2\\ \text{or } 4n+2\\ 4n+2\end{matrix}$ } $\begin{matrix}4n\\ \text{or } 4n\\ 4n\end{matrix}$ }
4	a	32	$\frac{3}{8},\frac{3}{8},\frac{3}{8}$; $\frac{7}{8},\frac{1}{8},\frac{5}{8}$; $\frac{5}{8},\frac{7}{8},\frac{1}{8}$; $\frac{1}{8},\frac{5}{8},\frac{7}{8}$.	h,k,l permutable

Origin on 3, at $\frac{1}{4}$ translation from each of three non-intersecting 4_1-axes and three non-intersecting 2-axes

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
48	i	1	$x,y,z;\ \frac{1}{2}+x,\frac{1}{2}-y,\bar{z};\ \bar{x},\frac{1}{2}+y,\frac{1}{2}-z;\ \frac{1}{2}-x,\bar{y},\frac{1}{2}+z;$ $z,x,y;\ \frac{1}{2}+z,\frac{1}{2}-x,\bar{y};\ \bar{z},\frac{1}{2}+x,\frac{1}{2}-y;\ \frac{1}{2}-z,\bar{x},\frac{1}{2}+y;$ $y,z,x;\ \frac{1}{2}+y,\frac{1}{2}-z,\bar{x};\ \bar{y},\frac{1}{2}+z,\frac{1}{2}-x;\ \frac{1}{2}-y,\bar{z},\frac{1}{2}+x;$ $\frac{1}{4}-x,\frac{1}{4}-z,\frac{1}{4}-y;\ \frac{3}{4}+x,\frac{3}{4}-z,\frac{1}{4}+y;$ $\frac{1}{4}-y,\frac{1}{4}-x,\frac{1}{4}-z;\ \frac{3}{4}+y,\frac{3}{4}-x,\frac{1}{4}+z;$ $\frac{1}{4}-z,\frac{1}{4}-y,\frac{1}{4}-x;\ \frac{3}{4}+z,\frac{3}{4}-y,\frac{1}{4}+x;$ $\frac{3}{4}-x,\frac{1}{4}+z,\frac{3}{4}+y;\ \frac{1}{4}+x,\frac{3}{4}+z,\frac{3}{4}-y;$ $\frac{3}{4}-y,\frac{1}{4}+x,\frac{3}{4}+z;\ \frac{1}{4}+y,\frac{3}{4}+x,\frac{3}{4}-z;$ $\frac{3}{4}-z,\frac{1}{4}+y,\frac{3}{4}+x;\ \frac{1}{4}+z,\frac{3}{4}+y,\frac{3}{4}-x.$	hkl: $h+k+l=2n$ $h00$: $h=4n$ $\circlearrowright$
				Special: as above, plus
24	h	2	$\frac{1}{8},x,\frac{1}{4}-x;\ \frac{5}{8},\frac{1}{2}-x,\frac{3}{4}+x;\ \frac{7}{8},\frac{1}{2}+x,\frac{1}{4}+x;\ \frac{3}{8},\bar{x},\frac{3}{4}-x;$ $\frac{1}{4}-x,\frac{1}{8},x;\ \frac{3}{4}+x,\frac{5}{8},\frac{1}{2}-x;\ \frac{1}{4}+x,\frac{7}{8},\frac{1}{2}+x;\ \frac{3}{4}-x,\frac{3}{8},\bar{x};$ $x,\frac{1}{4}-x,\frac{1}{8};\ \frac{1}{2}-x,\frac{3}{4}+x,\frac{5}{8};\ \frac{1}{2}+x,\frac{1}{4}+x,\frac{7}{8};\ \bar{x},\frac{3}{4}-x,\frac{3}{8}.$	no extra conditions
24	g	2	$\frac{1}{8},x,\frac{1}{4}+x;\ \frac{5}{8},\frac{1}{2}-x,\frac{3}{4}-x;\ \frac{7}{8},\frac{1}{2}+x,\frac{1}{4}-x;\ \frac{3}{8},\bar{x},\frac{3}{4}+x;$ $\frac{1}{4}+x,\frac{1}{8},x;\ \frac{3}{4}-x,\frac{5}{8},\frac{1}{2}-x;\ \frac{1}{4}-x,\frac{7}{8},\frac{1}{2}+x;\ \frac{3}{4}+x,\frac{3}{8},\bar{x};$ $x,\frac{1}{4}+x,\frac{1}{8};\ \frac{1}{2}-x,\frac{3}{4}-x,\frac{5}{8};\ \frac{1}{2}+x,\frac{1}{4}-x,\frac{7}{8};\ \bar{x},\frac{3}{4}+x,\frac{3}{8}.$	
24	f	2	$x,0,\frac{1}{4};\ \frac{1}{2}-x,0,\frac{3}{4};\ \frac{1}{4}-x,0,\frac{1}{4};\ \frac{1}{4}+x,0,\frac{3}{4};$ $\frac{1}{4},x,0;\ \frac{3}{4},\frac{1}{2}-x,0;\ \frac{1}{4},\frac{1}{4}-x,0;\ \frac{3}{4},\frac{1}{4}+x,0;$ $0,\frac{1}{4},x;\ 0,\frac{3}{4},\frac{1}{2}-x;\ 0,\frac{1}{4},\frac{1}{4}-x;\ 0,\frac{3}{4},\frac{1}{4}+x.$	hkl: h or k or $l=2n+1$ or $4n$
16	e	3	$x,x,x;\ \frac{1}{4}-x,\frac{1}{4}-x,\frac{1}{4}-x;$ $\frac{1}{2}+x,\frac{1}{2}-x,\bar{x};\ \frac{3}{4}-x,\frac{1}{4}+x,\frac{3}{4}+x;$ $\bar{x},\frac{1}{2}+x,\frac{1}{2}-x;\ \frac{3}{4}+x,\frac{3}{4}-x,\frac{1}{4}+x;$ $\frac{1}{2}-x,\bar{x},\frac{1}{2}+x;\ \frac{1}{4}+x,\frac{3}{4}+x,\frac{3}{4}-x.$	no extra conditions
12	d	222	$\frac{5}{8},0,\frac{1}{4};\ \frac{1}{4},\frac{5}{8},0;\ 0,\frac{1}{4},\frac{5}{8};$ $\frac{3}{8},\frac{1}{2},\frac{1}{4};\ \frac{1}{4},\frac{3}{8},\frac{1}{2};\ \frac{1}{2},\frac{1}{4},\frac{3}{8}.$	hkl: $\left.\begin{matrix}h=2n+1\\k=2n+1\\l=4n+2\end{matrix}\right\}$ or $\left.\begin{matrix}8n\pm1\\8n\pm1\\4n\end{matrix}\right\}$ or $\left.\begin{matrix}8n\pm3\\8n\pm3\\4n\end{matrix}\right\}$ or $\left.\begin{matrix}4n+2\\4n+2\\4n\end{matrix}\right\}$ or $\left.\begin{matrix}8n\\8n+4\\4n+2\end{matrix}\right\}$ or $\left.\begin{matrix}4n\\4n\\4n\end{matrix}\right\}$ h,k,l permutable
12	c	222	$\frac{1}{8},0,\frac{1}{4};\ \frac{1}{4},\frac{1}{8},0;\ 0,\frac{1}{4},\frac{1}{8};$ $\frac{7}{8},\frac{1}{2},\frac{1}{4};\ \frac{1}{4},\frac{7}{8},\frac{1}{2};\ \frac{1}{2},\frac{1}{4},\frac{7}{8}.$	
8	b	32	$\frac{7}{8},\frac{7}{8},\frac{7}{8};\ \frac{3}{8},\frac{5}{8},\frac{1}{8};\ \frac{1}{8},\frac{3}{8},\frac{5}{8};\ \frac{5}{8},\frac{1}{8},\frac{3}{8}.$	hkl: $\left.\begin{matrix}h=2n+1\\k=2n+1\\l=2n\end{matrix}\right\}$ or $\left.\begin{matrix}4n+2\\4n+2\\4n+2\end{matrix}\right\}$ or $\left.\begin{matrix}4n\\4n\\4n\end{matrix}\right\}$ h,k,l permutable
8	a	32	$\frac{1}{8},\frac{1}{8},\frac{1}{8};\ \frac{5}{8},\frac{3}{8},\frac{7}{8};\ \frac{7}{8},\frac{5}{8},\frac{3}{8};\ \frac{3}{8},\frac{7}{8},\frac{5}{8}.$	

Origin at $\bar{4}3m$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	j	1	x,y,z; z,x,y; y,z,x; x,z,y; y,x,z; z,y,x; $x,\bar{y},\bar{z}$; $z,\bar{x},\bar{y}$; $y,\bar{z},\bar{x}$; $x,\bar{z},\bar{y}$; $y,\bar{x},\bar{z}$; $z,\bar{y},\bar{x}$; $\bar{x},y,\bar{z}$; $\bar{z},x,\bar{y}$; $\bar{y},z,\bar{x}$; $\bar{x},z,\bar{y}$; $\bar{y},x,\bar{z}$; $\bar{z},y,\bar{x}$; $\bar{x},\bar{y},z$; $\bar{z},\bar{x},y$; $\bar{y},\bar{z},x$; $\bar{x},\bar{z},y$; $\bar{y},\bar{x},z$; $\bar{z},\bar{y},x$.	hkl: hhl: No conditions
				Special:
12	i	m	x,x,z; z,x,x; x,z,x; $\bar{x},x,\bar{z}$; $\bar{z},x,\bar{x}$; $\bar{x},z,\bar{x}$; $x,\bar{x},\bar{z}$; $z,\bar{x},\bar{x}$; $x,\bar{z},\bar{x}$; $\bar{x},\bar{x},z$; $\bar{z},\bar{x},x$; $\bar{x},\bar{z},x$.	No conditions
12	h	2	$x,\frac{1}{2},0$; $0,x,\frac{1}{2}$; $\frac{1}{2},0,x$; $\bar{x},\frac{1}{2},0$; $0,\bar{x},\frac{1}{2}$; $\frac{1}{2},0,\bar{x}$; $x,0,\frac{1}{2}$; $\frac{1}{2},x,0$; $0,\frac{1}{2},x$; $\bar{x},0,\frac{1}{2}$; $\frac{1}{2},\bar{x},0$; $0,\frac{1}{2},\bar{x}$.	
6	g	mm	$x,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},x$; $\bar{x},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\bar{x},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\bar{x}$.	
6	f	mm	$x,0,0$; $0,x,0$; $0,0,x$; $\bar{x},0,0$; $0,\bar{x},0$; $0,0,\bar{x}$.	
4	e	$3m$	x,x,x; $x,\bar{x},\bar{x}$; $\bar{x},x,\bar{x}$; $\bar{x},\bar{x},x$.	
3	d	$\bar{4}2m$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	
3	c	$\bar{4}2m$	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	
1	b	$\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
1	a	$\bar{4}3m$	$0,0,0$.	

Origin at $\bar{4}3m$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	Conditions limiting possible reflections
				General:
96	i	1	$x,y,z;\ z,x,y;\ y,z,x;\ x,z,y;\ y,x,z;\ z,y,x;$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ x,\bar{z},\bar{y};\ y,\bar{x},\bar{z};\ z,\bar{y},\bar{x};$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ \bar{x},z,\bar{y};\ \bar{y},x,\bar{z};\ \bar{z},y,\bar{x};$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ \bar{x},\bar{z},y;\ \bar{y},\bar{x},z;\ \bar{z},\bar{y},x.$	hkl: $h+k, k+l, (l+h)=2n$ hhl: $(h+l=2n)$ $\circlearrowright$
				Special: as above only
48	h	m	$x,x,z;\ z,x,x;\ x,z,x;\ \bar{x},x,\bar{z};\ \bar{z},x,\bar{x};\ \bar{x},z,\bar{x};$ $x,\bar{x},\bar{z};\ z,\bar{x},\bar{x};\ x,\bar{z},\bar{x};\ \bar{x},\bar{x},z;\ \bar{z},\bar{x},x;\ \bar{x},\bar{z},x.$	
24	g	mm	$x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},x,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},x;\ \bar{x},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\bar{x},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\bar{x}.$	
24	f	mm	$x,0,0;\ 0,x,0;\ 0,0,x;\ \bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x}.$	
16	e	$3m$	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x.$	
4	d	$\bar{4}3m$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}.$	
4	c	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}.$	
4	b	$\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}.$	
4	a	$\bar{4}3m$	$0,0,0.$	

Origin at $\bar{4}3m$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
48	h	1	$x,y,z;\ z,x,y;\ y,z,x;\ x,z,y;\ y,x,z;\ z,y,x;$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ x,\bar{z},\bar{y};\ y,\bar{x},\bar{z};\ z,\bar{y},\bar{x};$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ \bar{x},z,\bar{y};\ \bar{y},x,\bar{z};\ \bar{z},y,\bar{x};$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ \bar{x},\bar{z},y;\ \bar{y},\bar{x},z;\ \bar{z},\bar{y},x.$	hkl: $h+k+l=2n$ hhl: $(l=2n)$ $\circlearrowright$
				Special: as above only
24	g	m	$x,x,z;\ z,x,x;\ x,z,x;\ \bar{x},x,\bar{z};\ \bar{z},x,\bar{x};\ \bar{x},z,\bar{x};$ $x,\bar{x},\bar{z};\ z,\bar{x},\bar{x};\ x,\bar{z},\bar{x};\ \bar{x},\bar{x},z;\ \bar{z},\bar{x},x;\ \bar{x},\bar{z},x.$	
24	f	2	$x,\frac{1}{2},0;\ 0,x,\frac{1}{2};\ \frac{1}{2},0,x;\ \bar{x},\frac{1}{2},0;\ 0,\bar{x},\frac{1}{2};\ \frac{1}{2},0,\bar{x};$ $x,0,\frac{1}{2};\ \frac{1}{2},x,0;\ 0,\frac{1}{2},x;\ \bar{x},0,\frac{1}{2};\ \frac{1}{2},\bar{x},0;\ 0,\frac{1}{2},\bar{x}.$	
12	e	mm	$x,0,0;\ 0,x,0;\ 0,0,x;\ \bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x}.$	
12	d	$\bar{4}$	$\frac{1}{4},\frac{1}{2},0;\ 0,\frac{1}{4},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{4};\ \frac{1}{4},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{4},0;\ 0,\frac{1}{2},\frac{1}{4}.$	
8	c	$3m$	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x.$	
6	b	$\bar{4}2m$	$0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0.$	
2	a	$\bar{4}3m$	$0,0,0.$	

Origin at 23

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	i	1	x,y,z; z,x,y; y,z,x; $\bar{x},y,\bar{z}$; $\bar{z},x,\bar{y}$; $\bar{y},z,\bar{x}$; $x,\bar{y},\bar{z}$; $z,\bar{x},\bar{y}$; $y,\bar{z},\bar{x}$; $\bar{x},\bar{y},z$; $\bar{z},\bar{x},y$; $\bar{y},\bar{z},x$; $\frac{1}{2}+x,\frac{1}{2}+z,\frac{1}{2}+y$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+z,\frac{1}{2}+y,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}-z,\frac{1}{2}-y$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}+z,\frac{1}{2}-y,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}+z,\frac{1}{2}-y$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}-z$; $\frac{1}{2}-z,\frac{1}{2}+y,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}-z,\frac{1}{2}+y$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}-z,\frac{1}{2}-y,\frac{1}{2}+x$.	*hkl*: No conditions *hhl*: $l=2n$ $\mathcal{C}$
				Special: as above, plus
12	h	2	$x,0,\frac{1}{2}$; $\bar{x},0,\frac{1}{2}$; $\frac{1}{2}+x,0,\frac{1}{2}$; $\frac{1}{2}-x,0,\frac{1}{2}$; $\frac{1}{2},x,0$; $\frac{1}{2},\bar{x},0$; $\frac{1}{2},\frac{1}{2}+x,0$; $\frac{1}{2},\frac{1}{2}-x,0$; $0,\frac{1}{2},x$; $0,\frac{1}{2},\bar{x}$; $0,\frac{1}{2},\frac{1}{2}+x$; $0,\frac{1}{2},\frac{1}{2}-x$.	*hkl*: h or k or $l=2n$
12	g	2	$x,\frac{1}{2},0$; $\bar{x},\frac{1}{2},0$; $\frac{1}{2}+x,\frac{1}{2},0$; $\frac{1}{2}-x,\frac{1}{2},0$; $0,x,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$; $0,\frac{1}{2}+x,\frac{1}{2}$; $0,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2},0,x$; $\frac{1}{2},0,\bar{x}$; $\frac{1}{2},0,\frac{1}{2}+x$; $\frac{1}{2},0,\frac{1}{2}-x$.	
12	f	2	$x,0,0$; $\bar{x},0,0$; $\frac{1}{2}+x,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2},\frac{1}{2}$; $0,x,0$; $0,\bar{x},0$; $\frac{1}{2},\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}-x,\frac{1}{2}$; $0,0,x$; $0,0,\bar{x}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+x$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-x$.	*hkl*: $h+k+l=2n$
8	e	3	x,x,x; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}+x$; $x,\bar{x},\bar{x}$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}-x$; $\bar{x},x,\bar{x}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}-x$; $\bar{x},\bar{x},x$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}+x$.	
6	d	$\bar{4}$	$\frac{1}{4},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{4},0$; $0,\frac{1}{2},\frac{1}{4}$; $\frac{3}{4},0,\frac{1}{2}$; $\frac{1}{2},\frac{3}{4},0$; $0,\frac{1}{2},\frac{3}{4}$.	*hkl*: $\left.\begin{matrix} h=2n+1 \\ k=2n+1 \\ l=2n \end{matrix}\right\}$ or $\left.\begin{matrix} 2n+1 \\ 4n+2 \\ 4n \end{matrix}\right\}$ $\left.\begin{matrix} 2n \\ 2n \\ 2n \end{matrix}\right\}$
6	c	$\bar{4}$	$\frac{1}{4},\frac{1}{2},0$; $0,\frac{1}{4},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{4}$; $\frac{3}{4},\frac{1}{2},0$; $0,\frac{3}{4},\frac{1}{2}$; $\frac{1}{2},0,\frac{3}{4}$.	h,k,l permutable
6	b	222	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	*hkl*: $h+k+l=2n$
2	a	23	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	

Origin at 23

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	Conditions limiting possible reflections
				General:
96	h	1	$x,y,z;\ z,x,y;\ y,z,x;\ \bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ \bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;$ $x,z,\frac{1}{2}+y;\ y,x,\frac{1}{2}+z;\ z,y,\frac{1}{2}+x;$ $x,\bar{z},\frac{1}{2}-y;\ y,\bar{x},\frac{1}{2}-z;\ z,\bar{y},\frac{1}{2}-x;$ $\bar{x},z,\frac{1}{2}-y;\ \bar{y},x,\frac{1}{2}-z;\ \bar{z},y,\frac{1}{2}-x;$ $\bar{x},\bar{z},\frac{1}{2}+y;\ \bar{y},\bar{x},\frac{1}{2}+z;\ \bar{z},\bar{y},\frac{1}{2}+x.$	hkl: $h+k,k+l,(l+h)=2n$ hhl: $l,(h)=2n$ $\circlearrowright$
				Special: as above, plus
48	g	2	$x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},x,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},x;\ \bar{x},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\bar{x},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\bar{x};$ $\bar{x},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\bar{x},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\bar{x};\ x,\frac{1}{4},\frac{3}{4};\ \frac{3}{4},x,\frac{1}{4};\ \frac{1}{4},\frac{3}{4},x.$	
48	f	2	$x,0,0;\ 0,x,0;\ 0,0,x;\ x,0,\frac{1}{2};\ \frac{1}{2},x,0;\ 0,\frac{1}{2},x;$ $\bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x};\ \bar{x},0,\frac{1}{2};\ \frac{1}{2},\bar{x},0;\ 0,\frac{1}{2},\bar{x}.$	
32	e	3	$x,x,x;\ x,x,\frac{1}{2}+x;$ $x,\bar{x},\bar{x};\ x,\bar{x},\frac{1}{2}-x;$ $\bar{x},x,\bar{x};\ \bar{x},x,\frac{1}{2}-x;$ $\bar{x},\bar{x},x;\ \bar{x},\bar{x},\frac{1}{2}+x.$	hkl: $h,(k,l)=2n$
24	d	$\bar{4}$	$\frac{1}{4},0,0;\ 0,\frac{1}{4},0;\ 0,0,\frac{1}{4};\ \frac{3}{4},0,0;\ 0,\frac{3}{4},0;\ 0,0,\frac{3}{4}.$	
24	c	$\bar{4}$	$0,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},0;\ 0,\frac{1}{4},\frac{3}{4};\ \frac{3}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{3}{4},0.$	
8	b	23	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{3}{4},\frac{3}{4},\frac{3}{4}.$	
8	a	23	$0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	

Origin on 3, halfway between three pairs of non-intersecting 2-axes

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
48	e	1	x,y,z; z,x,y; y,z,x; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\frac{1}{2}+z,\frac{1}{2}-x,\bar{y}$; $\frac{1}{2}+y,\frac{1}{2}-z,\bar{x}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$; $\bar{z},\frac{1}{2}+x,\frac{1}{2}-y$; $\bar{y},\frac{1}{2}+z,\frac{1}{2}-x$; $\frac{1}{2}-x,\bar{y},\frac{1}{2}+z$; $\frac{1}{2}-z,\bar{x},\frac{1}{2}+y$; $\frac{1}{2}-y,\bar{z},\frac{1}{2}+x$; $\frac{1}{4}+x,\frac{1}{4}+z,\frac{1}{4}+y$; $\frac{1}{4}+y,\frac{1}{4}+x,\frac{1}{4}+z$; $\frac{1}{4}+z,\frac{1}{4}+y,\frac{1}{4}+x$; $\frac{3}{4}+x,\frac{1}{4}-z,\frac{3}{4}-y$; $\frac{3}{4}+y,\frac{1}{4}-x,\frac{3}{4}-z$; $\frac{3}{4}+z,\frac{1}{4}-y,\frac{3}{4}-x$; $\frac{3}{4}-x,\frac{3}{4}+z,\frac{1}{4}-y$; $\frac{3}{4}-y,\frac{3}{4}+x,\frac{1}{4}-z$; $\frac{3}{4}-z,\frac{3}{4}+y,\frac{1}{4}-x$; $\frac{1}{4}-x,\frac{3}{4}-z,\frac{3}{4}+y$; $\frac{1}{4}-y,\frac{3}{4}-x,\frac{3}{4}+z$; $\frac{1}{4}-z,\frac{3}{4}-y,\frac{3}{4}+x$.	hkl: $h+k+l=2n$ hhl: $(l=2n), 2h+l=4n$ $\circlearrowright$
				Special: as above, plus
24	d	2	$x,0,\frac{1}{4}$; $\bar{x},\frac{1}{2},\frac{1}{4}$; $\frac{1}{4}+x,\frac{1}{2},\frac{1}{4}$; $\frac{3}{4}-x,0,\frac{1}{4}$; $\frac{1}{4},x,0$; $\frac{1}{4},\bar{x},\frac{1}{2}$; $\frac{1}{4},\frac{1}{4}+x,\frac{1}{2}$; $\frac{1}{4},\frac{3}{4}-x,0$; $0,\frac{1}{4},x$; $\frac{1}{2},\frac{1}{4},\bar{x}$; $\frac{1}{2},\frac{1}{4},\frac{1}{4}+x$; $0,\frac{1}{4},\frac{3}{4}-x$.	hkl: h or k or $l=2n+1$ or $4n$
16	c	3	x,x,x; $\frac{1}{4}+x,\frac{1}{4}+x,\frac{1}{4}+x$; $\frac{1}{2}+x,\frac{1}{2}-x,\bar{x}$; $\frac{3}{4}+x,\frac{1}{4}-x,\frac{3}{4}-x$; $\bar{x},\frac{1}{2}+x,\frac{1}{2}-x$; $\frac{3}{4}-x,\frac{3}{4}+x,\frac{1}{4}-x$; $\frac{1}{2}-x,\bar{x},\frac{1}{2}+x$; $\frac{1}{4}-x,\frac{3}{4}-x,\frac{3}{4}+x$.	hkl: If h and k (and l) $=2n$, then $h+k+l=4n$
12	b	$\bar{4}$	$\frac{7}{8},0,\frac{1}{4}$; $\frac{1}{4},\frac{7}{8},0$; $0,\frac{1}{4},\frac{7}{8}$; $\frac{5}{8},0,\frac{3}{4}$; $\frac{3}{4},\frac{5}{8},0$; $0,\frac{3}{4},\frac{5}{8}$.	hkl: $\left.\begin{matrix} h=2n+1 \\ k=2n+1 \\ l=4n+2 \end{matrix}\right\}$ or $\left.\begin{matrix} 8n+1 \\ 8n\pm3 \\ 4n \end{matrix}\right\}$ $\left.\begin{matrix} 8n\pm3 \\ \text{or } 8n-1 \\ 4n \end{matrix}\right\}$ or $\left.\begin{matrix} 4n+2 \\ 4n+2 \\ 4n \end{matrix}\right\}$ $\left.\begin{matrix} 4n+2 \\ \text{or } 8n+4 \\ 8n \end{matrix}\right\}$ or $\left.\begin{matrix} 4n \\ 4n \\ 4n \end{matrix}\right\}$ h,k,l permutable
12	a	$\bar{4}$	$\frac{3}{8},0,\frac{1}{4}$; $\frac{1}{4},\frac{3}{8},0$; $0,\frac{1}{4},\frac{3}{8}$; $\frac{1}{8},0,\frac{3}{4}$; $\frac{3}{4},\frac{1}{8},0$; $0,\frac{3}{4},\frac{1}{8}$.	

$Pm3m$ O_h^1

No. 221 $P\,4/m\,\bar{3}\,2/m$ $m\,3\,m$ Cubic

Origin at centre ($m3m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
48	n	1	x,y,z; z,x,y; y,z,x; x,z,y; y,x,z; z,y,x; $x,\bar{y},\bar{z}$; $z,\bar{x},\bar{y}$; $y,\bar{z},\bar{x}$; $x,\bar{z},\bar{y}$; $y,\bar{x},\bar{z}$; $z,\bar{y},\bar{x}$; $\bar{x},y,\bar{z}$; $\bar{z},x,\bar{y}$; $\bar{y},z,\bar{x}$; $\bar{x},z,\bar{y}$; $\bar{y},x,\bar{z}$; $\bar{z},y,\bar{x}$; $\bar{x},\bar{y},z$; $\bar{z},\bar{x},y$; $\bar{y},\bar{z},x$; $\bar{x},\bar{z},y$; $\bar{y},\bar{x},z$; $\bar{z},\bar{y},x$; $\bar{x},\bar{y},\bar{z}$; $\bar{z},\bar{x},\bar{y}$; $\bar{y},\bar{z},\bar{x}$; $\bar{x},\bar{z},\bar{y}$; $\bar{y},\bar{x},\bar{z}$; $\bar{z},\bar{y},\bar{x}$; $\bar{x},y,z$; $\bar{z},x,y$; $\bar{y},z,x$; $\bar{x},z,y$; $\bar{y},x,z$; $\bar{z},y,x$; $x,\bar{y},z$; $z,\bar{x},y$; $y,\bar{z},x$; $x,\bar{z},y$; $y,\bar{x},z$; $z,\bar{y},x$; $x,y,\bar{z}$; $z,x,\bar{y}$; $y,z,\bar{x}$; $x,z,\bar{y}$; $y,x,\bar{z}$; $z,y,\bar{x}$.	hkl: hhl: $0kl$: } No conditions
				Special:
24	m	m	x,x,z; z,x,x; x,z,x; $\bar{x},\bar{x},\bar{z}$; $\bar{z},\bar{x},\bar{x}$; $\bar{x},\bar{z},\bar{x}$; $x,\bar{x},\bar{z}$; $z,\bar{x},\bar{x}$; $x,\bar{z},\bar{x}$; $\bar{x},x,z$; $\bar{z},x,x$; $\bar{x},z,x$; $\bar{x},x,\bar{z}$; $\bar{z},x,\bar{x}$; $\bar{x},z,\bar{x}$; $x,\bar{x},z$; $z,\bar{x},x$; $x,\bar{z},x$; $\bar{x},\bar{x},z$; $\bar{z},\bar{x},x$; $\bar{x},\bar{z},x$; $x,x,\bar{z}$; $z,x,\bar{x}$; $x,z,\bar{x}$.	No conditions
24	l	m	$\frac{1}{2},y,z$; $z,\frac{1}{2},y$; $y,z,\frac{1}{2}$; $\frac{1}{2},z,y$; $y,\frac{1}{2},z$; $z,y,\frac{1}{2}$; $\frac{1}{2},\bar{y},\bar{z}$; $\bar{z},\frac{1}{2},\bar{y}$; $\bar{y},\bar{z},\frac{1}{2}$; $\frac{1}{2},\bar{z},\bar{y}$; $\bar{y},\frac{1}{2},\bar{z}$; $\bar{z},\bar{y},\frac{1}{2}$; $\frac{1}{2},y,\bar{z}$; $\bar{z},\frac{1}{2},y$; $y,\bar{z},\frac{1}{2}$; $\frac{1}{2},\bar{z},y$; $y,\frac{1}{2},\bar{z}$; $\bar{z},y,\frac{1}{2}$; $\frac{1}{2},\bar{y},z$; $z,\frac{1}{2},\bar{y}$; $\bar{y},z,\frac{1}{2}$; $\frac{1}{2},z,\bar{y}$; $\bar{y},\frac{1}{2},z$; $z,\bar{y},\frac{1}{2}$.	
24	k	m	$0,y,z$; $z,0,y$; $y,z,0$; $0,z,y$; $y,0,z$; $z,y,0$; $0,\bar{y},\bar{z}$; $\bar{z},0,\bar{y}$; $\bar{y},\bar{z},0$; $0,\bar{z},\bar{y}$; $\bar{y},0,\bar{z}$; $\bar{z},\bar{y},0$; $0,y,\bar{z}$; $\bar{z},0,y$; $y,\bar{z},0$; $0,\bar{z},y$; $y,0,\bar{z}$; $\bar{z},y,0$; $0,\bar{y},z$; $z,0,\bar{y}$; $\bar{y},z,0$; $0,z,\bar{y}$; $\bar{y},0,z$; $z,\bar{y},0$.	
12	j	mm	$\frac{1}{2},x,x$; $x,\frac{1}{2},x$; $x,x,\frac{1}{2}$; $\frac{1}{2},x,\bar{x}$; $\bar{x},\frac{1}{2},x$; $x,\bar{x},\frac{1}{2}$; $\frac{1}{2},\bar{x},\bar{x}$; $\bar{x},\frac{1}{2},\bar{x}$; $\bar{x},\bar{x},\frac{1}{2}$; $\frac{1}{2},\bar{x},x$; $x,\frac{1}{2},\bar{x}$; $\bar{x},x,\frac{1}{2}$.	
12	i	mm	$0,x,x$; $x,0,x$; $x,x,0$; $0,x,\bar{x}$; $\bar{x},0,x$; $x,\bar{x},0$; $0,\bar{x},\bar{x}$; $\bar{x},0,\bar{x}$; $\bar{x},\bar{x},0$; $0,\bar{x},x$; $x,0,\bar{x}$; $\bar{x},x,0$.	
12	h	mm	$x,\frac{1}{2},0$; $0,x,\frac{1}{2}$; $\frac{1}{2},0,x$; $x,0,\frac{1}{2}$; $\frac{1}{2},x,0$; $0,\frac{1}{2},x$; $\bar{x},\frac{1}{2},0$; $0,\bar{x},\frac{1}{2}$; $\frac{1}{2},0,\bar{x}$; $\bar{x},0,\frac{1}{2}$; $\frac{1}{2},\bar{x},0$; $0,\frac{1}{2},\bar{x}$.	
8	g	$3m$	x,x,x; $x,\bar{x},\bar{x}$; $\bar{x},x,\bar{x}$; $\bar{x},\bar{x},x$; $\bar{x},\bar{x},\bar{x}$; $\bar{x},x,x$; $x,\bar{x},x$; $x,x,\bar{x}$.	
6	f	$4mm$	$x,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},x$; $\bar{x},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\bar{x},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\bar{x}$.	
6	e	$4mm$	$x,0,0$; $0,x,0$; $0,0,x$; $\bar{x},0,0$; $0,\bar{x},0$; $0,0,\bar{x}$.	
3	d	$4/mmm$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	
3	c	$4/mmm$	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	
1	b	$m3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
1	a	$m3m$	$0,0,0$.	

Origin at 43, at $\bar{\frac{1}{4}},\bar{\frac{1}{4}},\bar{\frac{1}{4}}$ from centre ($\bar{3}$) (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
48	i	1	x,y,z; z,x,y; y,z,x; $\bar{x},\bar{z},\bar{y}$; $\bar{y},\bar{x},\bar{z}$; $\bar{z},\bar{y},\bar{x}$; $x,\bar{y},\bar{z}$; $z,\bar{x},\bar{y}$; $y,\bar{z},\bar{x}$; $\bar{x},z,y$; $\bar{y},x,z$; $\bar{z},y,x$; $\bar{x},y,\bar{z}$; $\bar{z},x,\bar{y}$; $\bar{y},z,\bar{x}$; $x,\bar{z},y$; $y,\bar{x},z$; $z,\bar{y},x$; $\bar{x},\bar{y},z$; $\bar{z},\bar{x},y$; $\bar{y},\bar{z},x$; $x,z,\bar{y}$; $y,x,\bar{z}$; $z,y,\bar{x}$; $\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z$; $\frac{1}{2}-z,\frac{1}{2}-x,\frac{1}{2}-y$; $\frac{1}{2}-y,\frac{1}{2}-z,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $\frac{1}{2}-z,\frac{1}{2}+x,\frac{1}{2}+y$; $\frac{1}{2}-y,\frac{1}{2}+z,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$; $\frac{1}{2}+z,\frac{1}{2}-x,\frac{1}{2}+y$; $\frac{1}{2}+y,\frac{1}{2}-z,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}+z,\frac{1}{2}+x,\frac{1}{2}-y$; $\frac{1}{2}+y,\frac{1}{2}+z,\frac{1}{2}-x$; $\frac{1}{2}+x,\frac{1}{2}+z,\frac{1}{2}+y$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+z,\frac{1}{2}+y,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}-z,\frac{1}{2}-y$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}+z,\frac{1}{2}-y,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}+z,\frac{1}{2}-y$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}-z$; $\frac{1}{2}-z,\frac{1}{2}+y,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}-z,\frac{1}{2}+y$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}-z,\frac{1}{2}-y,\frac{1}{2}+x$.	hkl: No conditions hhl: $l=2n$; ↻ $0kl$: $k+l=2n$; ↻
				Special: as above, plus
24	h	2	$0,x,x$; $x,0,x$; $x,x,0$; $0,x,\bar{x}$; $\bar{x},0,x$; $x,\bar{x},0$; $0,\bar{x},\bar{x}$; $\bar{x},0,\bar{x}$; $\bar{x},\bar{x},0$; $0,\bar{x},x$; $x,0,\bar{x}$; $\bar{x},x,0$; $\frac{1}{2},\frac{1}{2}+x,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2},\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}-x,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2},\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}+x,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2},\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}-x,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2},\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}$.	
24	g	2	$x,0,\frac{1}{2}$; $\frac{1}{2},x,0$; $0,\frac{1}{2},x$; $x,\frac{1}{2},0$; $0,x,\frac{1}{2}$; $\frac{1}{2},0,x$; $\bar{x},0,\frac{1}{2}$; $\frac{1}{2},\bar{x},0$; $0,\frac{1}{2},\bar{x}$; $\bar{x},\frac{1}{2},0$; $0,\bar{x},\frac{1}{2}$; $\frac{1}{2},0,\bar{x}$; $\frac{1}{2}+x,\frac{1}{2},0$; $0,\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}+x$; $\frac{1}{2}-x,\frac{1}{2},0$; $0,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}-x$; $\frac{1}{2}+x,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}+x,0$; $0,\frac{1}{2},\frac{1}{2}+x$; $\frac{1}{2}-x,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}-x,0$; $0,\frac{1}{2},\frac{1}{2}-x$.	hkl: $h+k+l=2n$
16	f	3	x,x,x; $\bar{x},\bar{x},\bar{x}$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}+x$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}-x$; $x,\bar{x},\bar{x}$; $\bar{x},x,x$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}+x$; $\bar{x},x,\bar{x}$; $x,\bar{x},x$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}-x$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}+x$; $\bar{x},\bar{x},x$; $x,x,\bar{x}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}-x$.	
12	e	4	$x,0,0$; $\bar{x},0,0$; $\frac{1}{2}+x,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2},\frac{1}{2}$; $0,x,0$; $0,\bar{x},0$; $\frac{1}{2},\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}-x,\frac{1}{2}$; $0,0,x$; $0,0,\bar{x}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+x$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-x$.	
12	d	$\bar{4}$	$\frac{1}{4},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{4},0$; $0,\frac{1}{2},\frac{1}{4}$; $\frac{1}{4},\frac{1}{2},0$; $0,\frac{1}{4},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{4}$; $\frac{3}{4},0,\frac{1}{2}$; $\frac{1}{2},\frac{3}{4},0$; $0,\frac{1}{2},\frac{3}{4}$; $\frac{3}{4},\frac{1}{2},0$; $0,\frac{3}{4},\frac{1}{2}$; $\frac{1}{2},0,\frac{3}{4}$.	
8	c	$\bar{3}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{3}{4}$.	hkl: $h,\ k,\ l=2n$
6	b	42	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	hkl: $h+k+l=2n$
2	a	43	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	

Origin at centre ($\bar{3}$), at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 43 (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
48	i	1	x,y,z; $x,\frac{1}{2}-y,\frac{1}{2}-z$; $\frac{1}{2}-x,y,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}-y,z$; z,x,y; $z,\frac{1}{2}-x,\frac{1}{2}-y$; $\frac{1}{2}-z,x,\frac{1}{2}-y$; $\frac{1}{2}-z,\frac{1}{2}-x,y$; y,z,x; $y,\frac{1}{2}-z,\frac{1}{2}-x$; $\frac{1}{2}-y,z,\frac{1}{2}-x$; $\frac{1}{2}-y,\frac{1}{2}-z,x$; $\bar{x},\bar{y},\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}+z$; $\frac{1}{2}+x,\bar{y},\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$; $\bar{z},\bar{x},\bar{y}$; $\bar{z},\frac{1}{2}+x,\frac{1}{2}+y$; $\frac{1}{2}+z,\bar{x},\frac{1}{2}+y$; $\frac{1}{2}+z,\frac{1}{2}+x,\bar{y}$; $\bar{y},\bar{z},\bar{x}$; $\bar{y},\frac{1}{2}+z,\frac{1}{2}+x$; $\frac{1}{2}+y,\bar{z},\frac{1}{2}+x$; $\frac{1}{2}+y,\frac{1}{2}+z,\bar{x}$; $\frac{1}{2}+x,\frac{1}{2}+z,\frac{1}{2}+y$; $\frac{1}{2}+x,\bar{z},\bar{y}$; $\bar{x},\frac{1}{2}+z,\bar{y}$; $\bar{x},\bar{z},\frac{1}{2}+y$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+y,\bar{x},\bar{z}$; $\bar{y},\frac{1}{2}+x,\bar{z}$; $\bar{y},\bar{x},\frac{1}{2}+z$; $\frac{1}{2}+z,\frac{1}{2}+y,\frac{1}{2}+x$; $\frac{1}{2}+z,\bar{y},\bar{x}$; $\bar{z},\frac{1}{2}+y,\bar{x}$; $\bar{z},\bar{y},\frac{1}{2}+x$; $\frac{1}{2}-x,\frac{1}{2}-z,\frac{1}{2}-y$; $\frac{1}{2}-x,z,y$; $x,\frac{1}{2}-z,y$; $x,z,\frac{1}{2}-y$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}-y,x,z$; $y,\frac{1}{2}-x,z$; $y,x,\frac{1}{2}-z$; $\frac{1}{2}-z,\frac{1}{2}-y,\frac{1}{2}-x$; $\frac{1}{2}-z,y,x$; $z,\frac{1}{2}-y,x$; $z,y,\frac{1}{2}-x$.	hkl: No conditions hhl: $l=2n$; ↻ $0kl$: $k+l=2n$; ↻
				Special: as above, plus
24	h	2	$\frac{1}{4},x,x$; $\frac{1}{4},\frac{1}{2}-x,\frac{1}{2}-x$; $\frac{1}{4},x,\frac{1}{2}-x$; $\frac{1}{4},\frac{1}{2}-x,x$; $x,\frac{1}{4},x$; $\frac{1}{2}-x,\frac{1}{4},\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{4},x$; $x,\frac{1}{4},\frac{1}{2}-x$; $x,x,\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{4}$; $x,\frac{1}{2}-x,\frac{1}{4}$; $\frac{1}{2}-x,x,\frac{1}{4}$; $\frac{3}{4},\bar{x},\bar{x}$; $\frac{3}{4},\frac{1}{2}+x,\frac{1}{2}+x$; $\frac{3}{4},\bar{x},\frac{1}{2}+x$; $\frac{3}{4},\frac{1}{2}+x,\bar{x}$; $\bar{x},\frac{3}{4},\bar{x}$; $\frac{1}{2}+x,\frac{3}{4},\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{3}{4},\bar{x}$; $\bar{x},\frac{3}{4},\frac{1}{2}+x$; $\bar{x},\bar{x},\frac{3}{4}$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{3}{4}$; $\bar{x},\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{2}+x,\bar{x},\frac{3}{4}$.	
24	g	2	$x,\frac{3}{4},\frac{1}{4}$; $\frac{1}{2}-x,\frac{3}{4},\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{4},\frac{3}{4}$; $x,\frac{1}{4},\frac{3}{4}$; $\frac{1}{4},x,\frac{3}{4}$; $\frac{1}{4},\frac{1}{2}-x,\frac{3}{4}$; $\frac{3}{4},\frac{1}{2}-x,\frac{1}{4}$; $\frac{3}{4},x,\frac{1}{4}$; $\frac{3}{4},\frac{1}{4},x$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}-x$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}-x$; $\frac{1}{4},\frac{3}{4},x$; $\bar{x},\frac{1}{4},\frac{3}{4}$; $\frac{1}{2}+x,\frac{1}{4},\frac{3}{4}$; $\frac{1}{2}+x,\frac{3}{4},\frac{1}{4}$; $\bar{x},\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\bar{x},\frac{1}{4}$; $\frac{3}{4},\frac{1}{2}+x,\frac{1}{4}$; $\frac{1}{4},\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{4},\bar{x},\frac{3}{4}$; $\frac{1}{4},\frac{3}{4},\bar{x}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}+x$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}+x$; $\frac{3}{4},\frac{1}{4},\bar{x}$.	hkl: $h+k+l=2n$
16	f	3	x,x,x; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}+x$; $\bar{x},\bar{x},\bar{x}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}-x$; $x,\frac{1}{2}-x,\frac{1}{2}-x$; $\frac{1}{2}+x,\bar{x},\bar{x}$; $\bar{x},\frac{1}{2}+x,\frac{1}{2}+x$; $\frac{1}{2}-x,x,x$; $\frac{1}{2}-x,x,\frac{1}{2}-x$; $\bar{x},\frac{1}{2}+x,\bar{x}$; $\frac{1}{2}+x,\bar{x},\frac{1}{2}+x$; $x,\frac{1}{2}-x,x$; $\frac{1}{2}-x,\frac{1}{2}-x,x$; $\bar{x},\bar{x},\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+x,\bar{x}$; $x,x,\frac{1}{2}-x$.	
12	e	4	$x,\frac{1}{4},\frac{1}{4}$; $\bar{x},\frac{3}{4},\frac{3}{4}$; $\frac{1}{2}+x,\frac{3}{4},\frac{3}{4}$; $\frac{1}{2}-x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},x,\frac{1}{4}$; $\frac{3}{4},\bar{x},\frac{3}{4}$; $\frac{3}{4},\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{4},\frac{1}{2}-x,\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},x$; $\frac{3}{4},\frac{3}{4},\bar{x}$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}+x$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}-x$.	
12	d	$\bar{4}$	$0,\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},0,\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},0$; $\frac{1}{2},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{2},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}$; $0,\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},0,\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},0$; $\frac{1}{2},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{2},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}$.	
8	c	$\bar{3}$	$0,0,0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	hkl: $h,k,l=2n$
6	b	42	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{3}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$.	hkl: $h+k+l=2n$
2	a	43	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$.	

Origin at centre ($m3$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
48	l	1	x,y,z; z,x,y; y,z,x; $\bar{x},\bar{y},\bar{z}$; $\bar{z},\bar{x},\bar{y}$; $\bar{y},\bar{z},\bar{x}$; $x,\bar{y},\bar{z}$; $z,\bar{x},\bar{y}$; $y,\bar{z},\bar{x}$; $\bar{x},y,z$; $\bar{z},x,y$; $\bar{y},z,x$; $\bar{x},y,\bar{z}$; $\bar{z},x,\bar{y}$; $\bar{y},z,\bar{x}$; $x,\bar{y},z$; $z,\bar{x},y$; $y,\bar{z},x$; $\bar{x},\bar{y},z$; $\bar{z},\bar{x},y$; $\bar{y},\bar{z},x$; $x,y,\bar{z}$; $z,x,\bar{y}$; $y,z,\bar{x}$; $\frac{1}{2}+x,\frac{1}{2}+z,\frac{1}{2}+y$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+z,\frac{1}{2}+y,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}-z,\frac{1}{2}-y$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}+z,\frac{1}{2}-y,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}+z,\frac{1}{2}-y$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}-z$; $\frac{1}{2}-z,\frac{1}{2}+y,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}-z,\frac{1}{2}+y$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}-z,\frac{1}{2}-y,\frac{1}{2}+x$; $\frac{1}{2}-x,\frac{1}{2}-z,\frac{1}{2}-y$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}-z,\frac{1}{2}-y,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}+z,\frac{1}{2}+y$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}-z,\frac{1}{2}+y,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}-z,\frac{1}{2}+y$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}+z,\frac{1}{2}-y,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+z,\frac{1}{2}-y$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}-z$; $\frac{1}{2}+z,\frac{1}{2}+y,\frac{1}{2}-x$.	hkl: No conditions hhl: $l=2n$; ↻ $0kl$: No conditions
				Special: as above, plus
24	k	m	$0,y,z$; $z,0,y$; $y,z,0$; $0,y,\bar{z}$; $\bar{z},0,y$; $y,\bar{z},0$; $0,\bar{y},\bar{z}$; $\bar{z},0,\bar{y}$; $\bar{y},\bar{z},0$; $0,\bar{y},z$; $z,0,\bar{y}$; $\bar{y},z,0$; $\frac{1}{2},\frac{1}{2}+z,\frac{1}{2}+y$; $\frac{1}{2}+y,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2}+z,\frac{1}{2}+y,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}-z,\frac{1}{2}-y$; $\frac{1}{2}-y,\frac{1}{2},\frac{1}{2}-z$; $\frac{1}{2}-z,\frac{1}{2}-y,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}-z,\frac{1}{2}+y$; $\frac{1}{2}+y,\frac{1}{2},\frac{1}{2}-z$; $\frac{1}{2}-z,\frac{1}{2}+y,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}+z,\frac{1}{2}-y$; $\frac{1}{2}-y,\frac{1}{2},\frac{1}{2}+z$; $\frac{1}{2}+z,\frac{1}{2}-y,\frac{1}{2}$.	no extra conditions
24	j	2	$\frac{1}{4},x,\frac{1}{2}+x$; $\frac{1}{4},x,\frac{1}{2}-x$; $\frac{3}{4},x,\frac{1}{2}+x$; $\frac{3}{4},x,\frac{1}{2}-x$; $\frac{1}{2}+x,\frac{1}{4},x$; $\frac{1}{2}-x,\frac{1}{4},x$; $\frac{1}{2}+x,\frac{3}{4},x$; $\frac{1}{2}-x,\frac{3}{4},x$; $x,\frac{1}{2}+x,\frac{1}{4}$; $x,\frac{1}{2}-x,\frac{1}{4}$; $x,\frac{1}{2}+x,\frac{3}{4}$; $x,\frac{1}{2}-x,\frac{3}{4}$; $\frac{1}{4},\bar{x},\frac{1}{2}-x$; $\frac{1}{4},\bar{x},\frac{1}{2}+x$; $\frac{3}{4},\bar{x},\frac{1}{2}-x$; $\frac{3}{4},\bar{x},\frac{1}{2}+x$; $\frac{1}{2}-x,\frac{1}{4},\bar{x}$; $\frac{1}{2}+x,\frac{1}{4},\bar{x}$; $\frac{1}{2}-x,\frac{3}{4},\bar{x}$; $\frac{1}{2}+x,\frac{3}{4},\bar{x}$; $\bar{x},\frac{1}{2}-x,\frac{1}{4}$; $\bar{x},\frac{1}{2}+x,\frac{1}{4}$; $\bar{x},\frac{1}{2}-x,\frac{3}{4}$; $\bar{x},\frac{1}{2}+x,\frac{3}{4}$.	hkl: h or k or $l=2n$
16	i	3	x,x,x; $\bar{x},\bar{x},\bar{x}$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}+x$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}-x$; $x,\bar{x},\bar{x}$; $\bar{x},x,x$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}+x$; $\bar{x},x,\bar{x}$; $x,\bar{x},x$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}-x$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}+x$; $\bar{x},\bar{x},x$; $x,x,\bar{x}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}-x$.	hkl: $h+k+l=2n$
12	h	mm	$x,\frac{1}{2},0$; $\bar{x},\frac{1}{2},0$; $\frac{1}{2}+x,\frac{1}{2},0$; $\frac{1}{2}-x,\frac{1}{2},0$; $0,x,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$; $0,\frac{1}{2}+x,\frac{1}{2}$; $0,\frac{1}{2}-x,\frac{1}{2}$; $\frac{1}{2},0,x$; $\frac{1}{2},0,\bar{x}$; $\frac{1}{2},0,\frac{1}{2}+x$; $\frac{1}{2},0,\frac{1}{2}-x$.	hkl: h or k or $l=2n$
12	g	mm	$x,0,\frac{1}{2}$; $\bar{x},0,\frac{1}{2}$; $\frac{1}{2}+x,0,\frac{1}{2}$; $\frac{1}{2}-x,0,\frac{1}{2}$; $\frac{1}{2},x,0$; $\frac{1}{2},\bar{x},0$; $\frac{1}{2},\frac{1}{2}+x,0$; $\frac{1}{2},\frac{1}{2}-x,0$; $0,\frac{1}{2},x$; $0,\frac{1}{2},\bar{x}$; $0,\frac{1}{2},\frac{1}{2}+x$; $0,\frac{1}{2},\frac{1}{2}-x$.	
12	f	mm	$x,0,0$; $\bar{x},0,0$; $\frac{1}{2}+x,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2},\frac{1}{2}$; $0,x,0$; $0,\bar{x},0$; $\frac{1}{2},\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}-x,\frac{1}{2}$; $0,0,x$; $0,0,\bar{x}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+x$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-x$.	hkl: $h+k+l=2n$

(*continued on next page*)

(*continued*)

8	e	32	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{3}{4}$.	hkl: $h,k,l=2n$
6	d	$\bar{4}2m$	$\frac{1}{4},\frac{1}{2},0$; $0,\frac{1}{4},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{4}$; $\frac{3}{4},\frac{1}{2},0$; $0,\frac{3}{4},\frac{1}{2}$; $\frac{1}{2},0,\frac{3}{4}$.	hkl: $h=2n+1$, $k=2n+1$, $l=2n$ or $2n+1$, $4n+2$, $4n$
6	c	$\bar{4}2m$	$\frac{1}{4},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{4},0$; $0,\frac{1}{2},\frac{1}{4}$; $\frac{3}{4},0,\frac{1}{2}$; $\frac{1}{2},\frac{3}{4},0$; $0,\frac{1}{2},\frac{3}{4}$.	$2n$, or $2n$, $2n$; h,k,l permutable
6	b	mmm	$0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	hkl: $h+k+l=2n$
2	a	$m3$	$0,0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	

Origin at $\bar{4}3m$, at $\bar{\frac{1}{4}},\bar{\frac{1}{4}},\bar{\frac{1}{4}}$ from centre ($\bar{3}m$) (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
48	l	1	x,y,z; z,x,y; y,z,x; x,z,y; y,x,z; z,y,x; $x,\bar{y},\bar{z}$; $z,\bar{x},\bar{y}$; $y,\bar{z},\bar{x}$; $x,\bar{z},\bar{y}$; $y,\bar{x},\bar{z}$; $z,\bar{y},\bar{x}$; $\bar{x},y,\bar{z}$; $\bar{z},x,\bar{y}$; $\bar{y},z,\bar{x}$; $\bar{x},z,\bar{y}$; $\bar{y},x.\bar{z}$; $\bar{z},y,\bar{x}$; $\bar{x},\bar{y},z$; $\bar{z},\bar{x},y$; $\bar{y},\bar{z},x$; $\bar{x},\bar{z},y$; $\bar{y},\bar{x},z$; $\bar{z},\bar{y},x$; $\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z$; $\frac{1}{2}-z,\frac{1}{2}-x,\frac{1}{2}-y$; $\frac{1}{2}-y,\frac{1}{2}-z,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $\frac{1}{2}-z,\frac{1}{2}+x,\frac{1}{2}+y$; $\frac{1}{2}-y,\frac{1}{2}+z,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$; $\frac{1}{2}+z,\frac{1}{2}-x,\frac{1}{2}+y$; $\frac{1}{2}+y,\frac{1}{2}-z,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}+z,\frac{1}{2}+x,\frac{1}{2}-y$; $\frac{1}{2}+y,\frac{1}{2}+z,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}-z,\frac{1}{2}-y$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}-z,\frac{1}{2}-y,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}+z,\frac{1}{2}+y$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}-z,\frac{1}{2}+y,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}-z,\frac{1}{2}+y$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}+z,\frac{1}{2}-y,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+z,\frac{1}{2}-y$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}-z$; $\frac{1}{2}+z,\frac{1}{2}+y,\frac{1}{2}-x$.	*hkl*: No conditions *hhl*: No conditions $0kl$: $k+l=2n$ $\circlearrowright$
				Special: as above, plus
24	k	m	x,x,z; $x,\bar{x},\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}+z$; z,x,x; $\bar{z},x,\bar{x}$; $\frac{1}{2}-z,\frac{1}{2}-x,\frac{1}{2}-x$; $\frac{1}{2}+z,\frac{1}{2}-x,\frac{1}{2}+x$; x,z,x; $\bar{x},\bar{z},x$; $\frac{1}{2}-x,\frac{1}{2}-z,\frac{1}{2}-x$; $\frac{1}{2}+x,\frac{1}{2}-z,\frac{1}{2}+x$; $\bar{x},\bar{x},z$; $\bar{x},x,\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}-z$; $z,\bar{x},\bar{x}$; $\bar{z},\bar{x},x$; $\frac{1}{2}-z,\frac{1}{2}+x,\frac{1}{2}+x$; $\frac{1}{2}+z,\frac{1}{2}+x,\frac{1}{2}-x$; $\bar{x},z,\bar{x}$; $x,\bar{z},\bar{x}$; $\frac{1}{2}-x,\frac{1}{2}+z,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+z,\frac{1}{2}-x$.	
24	j	2	$\frac{1}{4},x,\frac{1}{2}+x$; $\frac{1}{4},\bar{x},\frac{1}{2}-x$; $\frac{3}{4},x,\frac{1}{2}-x$; $\frac{3}{4},\bar{x},\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{4},x$; $\frac{1}{2}-x,\frac{1}{4},\bar{x}$; $\frac{1}{2}-x,\frac{3}{4},x$; $\frac{1}{2}+x,\frac{3}{4},\bar{x}$; $x,\frac{1}{2}+x,\frac{1}{4}$; $\bar{x},\frac{1}{2}-x,\frac{1}{4}$; $x,\frac{1}{2}-x,\frac{3}{4}$; $\bar{x},\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{4},\frac{1}{2}+x,x$; $\frac{1}{4},\frac{1}{2}-x,\bar{x}$; $\frac{3}{4},\frac{1}{2}-x,x$; $\frac{3}{4},\frac{1}{2}+x,\bar{x}$; $x,\frac{1}{4},\frac{1}{2}+x$; $\bar{x},\frac{1}{4},\frac{1}{2}-x$; $x,\frac{3}{4},\frac{1}{2}-x$; $\bar{x},\frac{3}{4},\frac{1}{2}+x$; $\frac{1}{2}+x,x,\frac{1}{4}$; $\frac{1}{2}-x,\bar{x},\frac{1}{4}$; $\frac{1}{2}-x,x,\frac{3}{4}$; $\frac{1}{2}+x,\bar{x},\frac{3}{4}$.	no extra conditions
24	i	2	$\frac{1}{4},x,\frac{1}{2}-x$; $\frac{1}{4},\bar{x},\frac{1}{2}+x$; $\frac{3}{4},x,\frac{1}{2}+x$; $\frac{3}{4},\bar{x},\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{4},x$; $\frac{1}{2}+x,\frac{1}{4},\bar{x}$; $\frac{1}{2}+x,\frac{3}{4},x$; $\frac{1}{2}-x,\frac{3}{4},\bar{x}$; $x,\frac{1}{2}-x,\frac{1}{4}$; $\bar{x},\frac{1}{2}+x,\frac{1}{4}$; $x,\frac{1}{2}+x,\frac{3}{4}$; $\bar{x},\frac{1}{2}-x,\frac{3}{4}$; $\frac{1}{4},\frac{1}{2}-x,x$; $\frac{1}{4},\frac{1}{2}+x,\bar{x}$; $\frac{3}{4},\frac{1}{2}+x,x$; $\frac{3}{4},\frac{1}{2}-x,\bar{x}$; $x,\frac{1}{4},\frac{1}{2}-x$; $\bar{x},\frac{1}{4},\frac{1}{2}+x$; $x,\frac{3}{4},\frac{1}{2}+x$; $\bar{x},\frac{3}{4},\frac{1}{2}-x$; $\frac{1}{2}-x,x,\frac{1}{4}$; $\frac{1}{2}+x,\bar{x},\frac{1}{4}$; $\frac{1}{2}+x,x,\frac{3}{4}$; $\frac{1}{2}-x,\bar{x},\frac{3}{4}$.	
24	h	2	$x,0,\frac{1}{2}$; $x,\frac{1}{2},0$; $\frac{1}{2}+x,0,\frac{1}{2}$; $\frac{1}{2}+x,\frac{1}{2},0$; $\frac{1}{2},x,0$; $0,x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}+x,0$; $0,\frac{1}{2}+x,\frac{1}{2}$; $0,\frac{1}{2},x$; $\frac{1}{2},0,x$; $0,\frac{1}{2},\frac{1}{2}+x$; $\frac{1}{2},0,\frac{1}{2}+x$; $\bar{x},0,\frac{1}{2}$; $\bar{x},\frac{1}{2},0$; $\frac{1}{2}-x,0,\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2},0$; $\frac{1}{2},\bar{x},0$; $0,\bar{x},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}-x,0$; $0,\frac{1}{2}-x,\frac{1}{2}$; $0,\frac{1}{2},\bar{x}$; $\frac{1}{2},0,\bar{x}$; $0,\frac{1}{2},\frac{1}{2}-x$; $\frac{1}{2},0,\frac{1}{2}-x$.	
12	g	mm	$x,0,0$; $\bar{x},0,0$; $\frac{1}{2}+x,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2}-x,\frac{1}{2},\frac{1}{2}$; $0,x,0$; $0,\bar{x},0$; $\frac{1}{2},\frac{1}{2}+x,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}-x,\frac{1}{2}$; $0,0,x$; $0,0,\bar{x}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}+x$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}-x$.	*hkl*: $h+k+l=2n$
12	f	222	$\frac{1}{4},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{4},0$; $0,\frac{1}{2},\frac{1}{4}$; $\frac{1}{4},\frac{1}{2},0$; $0,\frac{1}{4},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{4}$; $\frac{3}{4},0,\frac{1}{2}$; $\frac{1}{2},\frac{3}{4},0$; $0,\frac{1}{2},\frac{3}{4}$; $\frac{3}{4},\frac{1}{2},0$; $0,\frac{3}{4},\frac{1}{2}$; $\frac{1}{2},0,\frac{3}{4}$.	

(*continued on next page*)

8	e	$3m$	$x,x,x;\ \bar{x},x,\bar{x};\ \frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}-x;\ \frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}+x;$ $x,\bar{x},\bar{x};\ \bar{x},\bar{x},x;\ \frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}+x;\ \frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}-x.$	no extra conditions
6	d	$\bar{4}2m$	$0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0;\ \frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}.$	hkl: $h+k+l=2n$
4	c	$\bar{3}m$	$\frac{3}{4},\frac{3}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{3}{4}.$	hkl: $h+k,k+l,(l+h)=2n$
4	b	$\bar{3}m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\frac{3}{4};\ \frac{3}{4},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\frac{3}{4},\frac{1}{4}.$	
2	a	$\bar{4}3m$	$0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	hkl: $h+k+l=2n$

Origin at centre ($\bar{3}m$), at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{4}3m$ (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
48	l	1	$x,y,z;\ x,\frac{1}{2}-y,\frac{1}{2}-z;\ \frac{1}{2}-x,y,\frac{1}{2}-z;\ \frac{1}{2}-x,\frac{1}{2}-y,z;$ $z,x,y;\ z,\frac{1}{2}-x,\frac{1}{2}-y;\ \frac{1}{2}-z,x,\frac{1}{2}-y;\ \frac{1}{2}-z,\frac{1}{2}-x,y;$ $y,z,x;\ y,\frac{1}{2}-z,\frac{1}{2}-x;\ \frac{1}{2}-y,z,\frac{1}{2}-x;\ \frac{1}{2}-y,\frac{1}{2}-z,x;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},\frac{1}{2}+y,\frac{1}{2}+z;\ \frac{1}{2}+x,\bar{y},\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}+y,\bar{z};$ $\bar{z},\bar{x},\bar{y};\ \bar{z},\frac{1}{2}+x,\frac{1}{2}+y;\ \frac{1}{2}+z,\bar{x},\frac{1}{2}+y;\ \frac{1}{2}+z,\frac{1}{2}+x,\bar{y};$ $\bar{y},\bar{z},\bar{x};\ \bar{y},\frac{1}{2}+z,\frac{1}{2}+x;\ \frac{1}{2}+y,\bar{z},\frac{1}{2}+x;\ \frac{1}{2}+y,\frac{1}{2}+z,\bar{x};$ $x,z,y;\ x,\frac{1}{2}-z,\frac{1}{2}-y;\ \frac{1}{2}-x,z,\frac{1}{2}-y;\ \frac{1}{2}-x,\frac{1}{2}-z,y;$ $y,x,z;\ y,\frac{1}{2}-x,\frac{1}{2}-z;\ \frac{1}{2}-y,x,\frac{1}{2}-z;\ \frac{1}{2}-y,\frac{1}{2}-x,z;$ $z,y,x;\ z,\frac{1}{2}-y,\frac{1}{2}-x;\ \frac{1}{2}-z,y,\frac{1}{2}-x;\ \frac{1}{2}-z,\frac{1}{2}-y,x;$ $\bar{x},\bar{z},\bar{y};\ \bar{x},\frac{1}{2}+z,\frac{1}{2}+y;\ \frac{1}{2}+x,\bar{z},\frac{1}{2}+y;\ \frac{1}{2}+x,\frac{1}{2}+z,\bar{y};$ $\bar{y},\bar{x},\bar{z};\ \bar{y},\frac{1}{2}+x,\frac{1}{2}+z;\ \frac{1}{2}+y,\bar{x},\frac{1}{2}+z;\ \frac{1}{2}+y,\frac{1}{2}+x,\bar{z};$ $\bar{z},\bar{y},\bar{x};\ \bar{z},\frac{1}{2}+y,\frac{1}{2}+x;\ \frac{1}{2}+z,\bar{y},\frac{1}{2}+x;\ \frac{1}{2}+z,\frac{1}{2}+y,\bar{x}.$	hkl: No conditions hhl: No conditions $0kl$: $k+l=2n$ $\circlearrowright$
				Special: as above, plus
24	k	m	$x,x,z;\ x,\frac{1}{2}-x,\frac{1}{2}-z;\ \frac{1}{2}-x,x,\frac{1}{2}-z;\ \frac{1}{2}-x,\frac{1}{2}-x,z;$ $z,x,x;\ z,\frac{1}{2}-x,\frac{1}{2}-x;\ \frac{1}{2}-z,x,\frac{1}{2}-x;\ \frac{1}{2}-z,\frac{1}{2}-x,x;$ $x,z,x;\ x,\frac{1}{2}-z,\frac{1}{2}-x;\ \frac{1}{2}-x,z,\frac{1}{2}-x;\ \frac{1}{2}-x,\frac{1}{2}-z,x;$ $\bar{x},\bar{x},\bar{z};\ \bar{x},\frac{1}{2}+x,\frac{1}{2}+z;\ \frac{1}{2}+x,\bar{x},\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}+x,\bar{z};$ $\bar{z},\bar{x},\bar{x};\ \bar{z},\frac{1}{2}+x,\frac{1}{2}+x;\ \frac{1}{2}+z,\bar{x},\frac{1}{2}+x;\ \frac{1}{2}+z,\frac{1}{2}+x,\bar{x};$ $\bar{x},\bar{z},\bar{x};\ \bar{x},\frac{1}{2}+z,\frac{1}{2}+x;\ \frac{1}{2}+x,\bar{z},\frac{1}{2}+x;\ \frac{1}{2}+x,\frac{1}{2}+z,\bar{x}.$	
24	j	2	$\frac{1}{2},\frac{1}{4}+x,\frac{3}{4}+x;\ \frac{1}{2},\frac{1}{4}-x,\frac{3}{4}-x;\ 0,\frac{1}{4}+x,\frac{3}{4}-x;\ 0,\frac{1}{4}-x,\frac{3}{4}+x;$ $\frac{3}{4}+x,\frac{1}{2},\frac{1}{4}+x;\ \frac{3}{4}-x,\frac{1}{2},\frac{1}{4}-x;\ \frac{3}{4}-x,0,\frac{1}{4}+x;\ \frac{3}{4}+x,0,\frac{1}{4}-x;$ $\frac{1}{4}+x,\frac{3}{4}+x,\frac{1}{2};\ \frac{1}{4}-x,\frac{3}{4}-x,\frac{1}{2};\ \frac{1}{4}+x,\frac{3}{4}-x,0;\ \frac{1}{4}-x,\frac{3}{4}+x,0;$ $\frac{1}{2},\frac{3}{4}-x,\frac{1}{4}-x;\ \frac{1}{2},\frac{3}{4}+x,\frac{1}{4}+x;\ 0,\frac{3}{4}-x,\frac{1}{4}+x;\ 0,\frac{3}{4}+x,\frac{1}{4}-x;$ $\frac{1}{4}-x,\frac{1}{2},\frac{3}{4}-x;\ \frac{1}{4}+x,\frac{1}{2},\frac{3}{4}+x;\ \frac{1}{4}+x,0,\frac{3}{4}-x;\ \frac{1}{4}-x,0,\frac{3}{4}+x;$ $\frac{3}{4}-x,\frac{1}{4}-x,\frac{1}{2};\ \frac{3}{4}+x,\frac{1}{4}+x,\frac{1}{2};\ \frac{3}{4}-x,\frac{1}{4}+x,0;\ \frac{3}{4}+x,\frac{1}{4}-x,0.$	no extra conditions
24	i	2	$\frac{1}{2},\frac{1}{4}+x,\frac{3}{4}-x;\ \frac{1}{2},\frac{1}{4}-x,\frac{3}{4}+x;\ 0,\frac{1}{4}+x,\frac{3}{4}+x;\ 0,\frac{1}{4}-x,\frac{3}{4}-x;$ $\frac{3}{4}-x,\frac{1}{2},\frac{1}{4}+x;\ \frac{3}{4}+x,\frac{1}{2},\frac{1}{4}-x;\ \frac{3}{4}+x,0,\frac{1}{4}+x;\ \frac{3}{4}-x,0,\frac{1}{4}-x;$ $\frac{1}{4}+x,\frac{3}{4}-x,\frac{1}{2};\ \frac{1}{4}-x,\frac{3}{4}+x,\frac{1}{2};\ \frac{1}{4}+x,\frac{3}{4}+x,0;\ \frac{1}{4}-x,\frac{3}{4}-x,0;$ $\frac{1}{2},\frac{3}{4}-x,\frac{1}{4}+x;\ \frac{1}{2},\frac{3}{4}+x,\frac{1}{4}-x;\ 0,\frac{3}{4}-x,\frac{1}{4}-x;\ 0,\frac{3}{4}+x,\frac{1}{4}+x;$ $\frac{1}{4}+x,\frac{1}{2},\frac{3}{4}-x;\ \frac{1}{4}-x,\frac{1}{2},\frac{3}{4}+x;\ \frac{1}{4}-x,0,\frac{3}{4}-x;\ \frac{1}{4}+x,0,\frac{3}{4}+x;$ $\frac{3}{4}-x,\frac{1}{4}+x,\frac{1}{2};\ \frac{3}{4}+x,\frac{1}{4}-x,\frac{1}{2};\ \frac{3}{4}-x,\frac{1}{4}-x,0;\ \frac{3}{4}+x,\frac{1}{4}+x,0.$	

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24	h	2	$x,\frac{1}{4},\frac{3}{4}$; $\bar{x},\frac{1}{4},\frac{3}{4}$; $\bar{x},\frac{3}{4},\frac{1}{4}$; $x,\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},x,\frac{1}{4}$; $\frac{3}{4},\bar{x},\frac{1}{4}$; $\frac{1}{4},\bar{x},\frac{3}{4}$; $\frac{1}{4},x,\frac{3}{4}$; $\frac{1}{4},\frac{3}{4},x$; $\frac{1}{4},\frac{3}{4},\bar{x}$; $\frac{3}{4},\frac{1}{4},\bar{x}$; $\frac{3}{4},\frac{1}{4},x$; $\frac{1}{2}+x,\frac{3}{4},\frac{1}{4}$; $\frac{1}{2}-x,\frac{3}{4},\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{4},\frac{3}{4}$; $\frac{1}{2}+x,\frac{1}{4},\frac{3}{4}$; $\frac{1}{4},\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{4},\frac{1}{2}-x,\frac{3}{4}$; $\frac{3}{4},\frac{1}{2}-x,\frac{1}{4}$; $\frac{3}{4},\frac{1}{2}+x,\frac{1}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}+x$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}-x$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}-x$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}+x$.	hkl: $h+k+l=2n$
12	g	mm	$x,\frac{1}{4},\frac{1}{4}$; $\bar{x},\frac{3}{4},\frac{3}{4}$; $\frac{1}{2}-x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{2}+x,\frac{3}{4},\frac{3}{4}$; $\frac{1}{4},x,\frac{1}{4}$; $\frac{3}{4},\bar{x},\frac{3}{4}$; $\frac{1}{4},\frac{1}{2}-x,\frac{1}{4}$; $\frac{3}{4},\frac{1}{2}+x,\frac{3}{4}$; $\frac{1}{4},\frac{1}{4},x$; $\frac{3}{4},\frac{3}{4},\bar{x}$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}-x$; $\frac{3}{4},\frac{3}{4},\frac{1}{2}+x$.	
12	f	222	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{2},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{2}$; $0,\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},0,\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},0$; $\frac{1}{2},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{2},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{2}$; $0,\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},0,\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},0$.	
8	e	$3m$	x,x,x; $x,\frac{1}{2}-x,\frac{1}{2}-x$; $\frac{1}{2}-x,x,\frac{1}{2}-x$; $\frac{1}{2}-x,\frac{1}{2}-x,x$; $\bar{x},\bar{x},\bar{x}$; $\bar{x},\frac{1}{2}+x,\frac{1}{2}+x$; $\frac{1}{2}+x,\bar{x},\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+x,\bar{x}$.	no extra conditions
6	d	$\bar{4}2m$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$; $\frac{3}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{3}{4}$.	hkl: $h+k+l=2n$
4	c	$\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	hkl: $h+k,k+l,(l+h)=2n$
4	b	$\bar{3}m$	$0,0,0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	
2	a	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$.	hkl: $h+k+l=2n$

$Fm3m$ O_h^5

No. 225 $F\,4/m\,\bar{3}\,2/m$ $m\,3\,m$ Cubic

Origin at centre ($m3m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	Conditions limiting possible reflections
				General:
192	l	1	$x,y,z;\ z,x,y;\ y,z,x;\ x,z,y;\ y,x,z;\ z,y,x;$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ x,\bar{z},\bar{y};\ y,\bar{x},\bar{z};\ z,\bar{y},\bar{x};$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ \bar{x},z,\bar{y};\ \bar{y},x,\bar{z};\ \bar{z},y,\bar{x};$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ \bar{x},\bar{z},y;\ \bar{y},\bar{x},z;\ \bar{z},\bar{y},x;$ $\bar{x},\bar{y},\bar{z};\ \bar{z},\bar{x},\bar{y};\ \bar{y},\bar{z},\bar{x};\ \bar{x},\bar{z},\bar{y};\ \bar{y},\bar{x},\bar{z};\ \bar{z},\bar{y},\bar{x};$ $\bar{x},y,z;\ \bar{z},x,y;\ \bar{y},z,x;\ \bar{x},z,y;\ \bar{y},x,z;\ \bar{z},y,x;$ $x,\bar{y},z;\ z,\bar{x},y;\ y,\bar{z},x;\ x,\bar{z},y;\ y,\bar{x},z;\ z,\bar{y},x;$ $x,y,\bar{z};\ z,x,\bar{y};\ y,z,\bar{x};\ x,z,\bar{y};\ y,x,\bar{z};\ z,y,\bar{x}.$	hkl: $h+k,k+l,(l+h)=2n$ hhl: $(l+h=2n)$; ↻ $0kl$: $(k,l=2n)$; ↻
				Special: as above, plus
96	k	m	$x,x,z;\ z,x,x;\ x,z,x;\ \bar{x},\bar{x},\bar{z};\ \bar{z},\bar{x},\bar{x};\ \bar{x},\bar{z},\bar{x};$ $x,\bar{x},\bar{z};\ z,\bar{x},\bar{x};\ x,\bar{z},\bar{x};\ \bar{x},x,z;\ \bar{z},x,x;\ \bar{x},z,x;$ $\bar{x},x,\bar{z};\ \bar{z},x,\bar{x};\ \bar{x},z,\bar{x};\ x,\bar{x},z;\ z,\bar{x},x;\ x,\bar{z},x;$ $\bar{x},\bar{x},z;\ \bar{z},\bar{x},x;\ \bar{x},\bar{z},x;\ x,x,\bar{z};\ z,x,\bar{x};\ x,z,\bar{x}.$	no extra conditions
96	j	m	$0,y,z;\ z,0,y;\ y,z,0;\ 0,z,y;\ y,0,z;\ z,y,0;$ $0,\bar{y},\bar{z};\ \bar{z},0,\bar{y};\ \bar{y},\bar{z},0;\ 0,\bar{z},\bar{y};\ \bar{y},0,\bar{z};\ \bar{z},\bar{y},0;$ $0,y,\bar{z};\ \bar{z},0,y;\ y,\bar{z},0;\ 0,\bar{z},y;\ y,0,\bar{z};\ \bar{z},y,0;$ $0,\bar{y},z;\ z,0,\bar{y};\ \bar{y},z,0;\ 0,z,\bar{y};\ \bar{y},0,z;\ z,\bar{y},0.$	
48	i	mm	$\frac{1}{2},x,x;\ x,\frac{1}{2},x;\ x,x,\frac{1}{2};\ \frac{1}{2},x,\bar{x};\ \bar{x},\frac{1}{2},x;\ x,\bar{x},\frac{1}{2};$ $\frac{1}{2},\bar{x},\bar{x};\ \bar{x},\frac{1}{2},\bar{x};\ \bar{x},\bar{x},\frac{1}{2};\ \frac{1}{2},\bar{x},x;\ x,\frac{1}{2},\bar{x};\ \bar{x},x,\frac{1}{2}.$	
48	h	mm	$0,x,x;\ x,0,x;\ x,x,0;\ 0,x,\bar{x};\ \bar{x},0,x;\ x,\bar{x},0;$ $0,\bar{x},\bar{x};\ \bar{x},0,\bar{x};\ \bar{x},\bar{x},0;\ 0,\bar{x},x;\ x,0,\bar{x};\ \bar{x},x,0.$	
48	g	mm	$x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},x,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},x;\ x,\frac{1}{4},\frac{3}{4};\ \frac{3}{4},x,\frac{1}{4};\ \frac{1}{4},\frac{3}{4},x;$ $\bar{x},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\bar{x},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\bar{x};\ \bar{x},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\bar{x},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\bar{x}.$	hkl: $h,(k,l)=2n$
32	f	$3m$	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x;$ $\bar{x},\bar{x},\bar{x};\ \bar{x},x,x;\ x,\bar{x},x;\ x,x,\bar{x}.$	no extra conditions
24	e	$4mm$	$x,0,0;\ 0,x,0;\ 0,0,x;\ \bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x}.$	
24	d	mmm	$0,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},0;\ 0,\frac{1}{4},\frac{3}{4};\ \frac{3}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{3}{4},0.$	hkl: $h,(k,l)=2n$
8	c	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{3}{4},\frac{3}{4},\frac{3}{4}.$	
4	b	$m3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}.$	no extra conditions
4	a	$m3m$	$0,0,0.$	

Origin at centre ($m3$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	Conditions limiting possible reflections
				General:
192	j	1	$x,y,z;\ z,x,y;\ y,z,x;\ \bar{x},\bar{y},\bar{z};\ \bar{z},\bar{x},\bar{y};\ \bar{y},\bar{z},\bar{x};$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ \bar{x},y,z;\ \bar{z},x,y;\ \bar{y},z,x;$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ x,\bar{y},z;\ z,\bar{x},y;\ y,\bar{z},x;$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ x,y,\bar{z};\ z,x,\bar{y};\ y,z,\bar{x};$ $x,z,\frac{1}{2}+y;\ y,x,\frac{1}{2}+z;\ z,y,\frac{1}{2}+x;$ $x,\bar{z},\frac{1}{2}-y;\ y,\bar{x},\frac{1}{2}-z;\ z,\bar{y},\frac{1}{2}-x;$ $\bar{x},z,\frac{1}{2}-y;\ \bar{y},x,\frac{1}{2}-z;\ \bar{z},y,\frac{1}{2}-x;$ $\bar{x},\bar{z},\frac{1}{2}+y;\ \bar{y},\bar{x},\frac{1}{2}+z;\ \bar{z},\bar{y},\frac{1}{2}+x;$ $\bar{x},\bar{z},\frac{1}{2}-y;\ \bar{y},\bar{x},\frac{1}{2}-z;\ \bar{z},\bar{y},\frac{1}{2}-x;$ $\bar{x},z,\frac{1}{2}+y;\ \bar{y},x,\frac{1}{2}+z;\ \bar{z},y,\frac{1}{2}+x;$ $x,\bar{z},\frac{1}{2}+y;\ y,\bar{x},\frac{1}{2}+z;\ z,\bar{y},\frac{1}{2}+x;$ $x,z,\frac{1}{2}-y;\ y,x,\frac{1}{2}-z;\ z,y,\frac{1}{2}-x.$	hkl: $h+k,k+l,(l+h)=2n$ hhl: $l,(h)=2n$; C $0kl$: $(k,l=2n)$; C
				Special: as above, plus
96	i	m	$0,y,z;\ z,0,y;\ y,z,0;\ \frac{1}{2},z,y;\ y,\frac{1}{2},z;\ z,y,\frac{1}{2};$ $0,\bar{y},\bar{z};\ \bar{z},0,\bar{y};\ \bar{y},\bar{z},0;\ \frac{1}{2},\bar{z},\bar{y};\ \bar{y},\frac{1}{2},\bar{z};\ \bar{z},\bar{y},\frac{1}{2};$ $0,y,\bar{z};\ \bar{z},0,y;\ y,\bar{z},0;\ \frac{1}{2},\bar{z},y;\ y,\frac{1}{2},\bar{z};\ \bar{z},y,\frac{1}{2};$ $0,\bar{y},z;\ z,0,\bar{y};\ \bar{y},z,0;\ \frac{1}{2},z,\bar{y};\ \bar{y},\frac{1}{2},z;\ z,\bar{y},\frac{1}{2}.$	no extra conditions
96	h	2	$\frac{1}{4},x,x;\ x,\frac{1}{4},x;\ x,x,\frac{1}{4};\ \frac{3}{4},x,x;\ x,\frac{3}{4},x;\ x,x,\frac{3}{4};$ $\frac{1}{4},\bar{x},\bar{x};\ \bar{x},\frac{1}{4},\bar{x};\ \bar{x},\bar{x},\frac{1}{4};\ \frac{3}{4},\bar{x},\bar{x};\ \bar{x},\frac{3}{4},\bar{x};\ \bar{x},\bar{x},\frac{3}{4};$ $\frac{1}{4},x,\bar{x};\ \bar{x},\frac{1}{4},x;\ x,\bar{x},\frac{1}{4};\ \frac{3}{4},x,\bar{x};\ \bar{x},\frac{3}{4},x;\ x,\bar{x},\frac{3}{4};$ $\frac{1}{4},\bar{x},x;\ x,\frac{1}{4},\bar{x};\ \bar{x},x,\frac{1}{4};\ \frac{3}{4},\bar{x},x;\ x,\frac{3}{4},\bar{x};\ \bar{x},x,\frac{3}{4}.$	
64	g	3	$x,x,x;\ \bar{x},\bar{x},\bar{x};\ x,x,\frac{1}{2}+x;\ \bar{x},\bar{x},\frac{1}{2}-x;$ $x,\bar{x},\bar{x};\ \bar{x},x,x;\ x,\bar{x},\frac{1}{2}-x;\ \bar{x},x,\frac{1}{2}+x;$ $\bar{x},x,\bar{x};\ x,\bar{x},x;\ \bar{x},x,\frac{1}{2}-x;\ x,\bar{x},\frac{1}{2}+x;$ $\bar{x},\bar{x},x;\ x,x,\bar{x};\ \bar{x},\bar{x},\frac{1}{2}+x;\ x,x,\frac{1}{2}-x.$	
48	f	4	$x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},x,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},x;\ x,\frac{1}{4},\frac{3}{4};\ \frac{3}{4},x,\frac{1}{4};\ \frac{1}{4},\frac{3}{4},x;$ $\bar{x},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\bar{x},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\bar{x};\ \bar{x},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\bar{x},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\bar{x}.$	hkl: $h,(k,l)=2n$
48	e	mm	$x,0,0;\ 0,x,0;\ 0,0,x;\ x,0,\frac{1}{2};\ \frac{1}{2},x,0;\ 0,\frac{1}{2},x;$ $\bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x};\ \bar{x},0,\frac{1}{2};\ \frac{1}{2},\bar{x},0;\ 0,\frac{1}{2},\bar{x}.$	
24	d	$4/m$	$0,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},0;\ \frac{1}{2},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{2},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{2}.$	
24	c	$\bar{4}2m$	$\frac{1}{4},0,0;\ 0,\frac{1}{4},0;\ 0,0,\frac{1}{4};\ \frac{3}{4},0,0;\ 0,\frac{3}{4},0;\ 0,0,\frac{3}{4}.$	
8	b	$m3$	$0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	
8	a	43	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{3}{4},\frac{3}{4},\frac{3}{4}.$	

$Fd3m$ O_h^7

No. 227 $F\,4_1/d\,\bar{3}\,2/m$ $m\,3\,m$ Cubic

Origin at $\bar{4}3m$, at $\bar{\frac{1}{8}},\bar{\frac{1}{8}},\bar{\frac{1}{8}}$ from centre ($\bar{3}m$) (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
192	i	1	$x,y,z;\ z,x,y;\ y,z,x;\ x,z,y;\ y,x,z;\ z,y,x;$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ x,\bar{z},\bar{y};\ y,\bar{x},\bar{z};\ z,\bar{y},\bar{x};$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ \bar{x},z,\bar{y};\ \bar{y},x,\bar{z};\ \bar{z},y,\bar{x};$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ \bar{x},\bar{z},y;\ \bar{y},\bar{x},z;\ \bar{z},\bar{y},x;$ $\frac{1}{4}-x,\frac{1}{4}-y,\frac{1}{4}-z;\ \frac{1}{4}-z,\frac{1}{4}-x,\frac{1}{4}-y;\ \frac{1}{4}-y,\frac{1}{4}-z,\frac{1}{4}-x;$ $\frac{1}{4}-x,\frac{1}{4}+y,\frac{1}{4}+z;\ \frac{1}{4}-z,\frac{1}{4}+x,\frac{1}{4}+y;\ \frac{1}{4}-y,\frac{1}{4}+z,\frac{1}{4}+x;$ $\frac{1}{4}+x,\frac{1}{4}-y,\frac{1}{4}+z;\ \frac{1}{4}+z,\frac{1}{4}-x,\frac{1}{4}+y;\ \frac{1}{4}+y,\frac{1}{4}-z,\frac{1}{4}+x;$ $\frac{1}{4}+x,\frac{1}{4}+y,\frac{1}{4}-z;\ \frac{1}{4}+z,\frac{1}{4}+x,\frac{1}{4}-y;\ \frac{1}{4}+y,\frac{1}{4}+z,\frac{1}{4}-x;$ $\frac{1}{4}-x,\frac{1}{4}-z,\frac{1}{4}-y;\ \frac{1}{4}-y,\frac{1}{4}-x,\frac{1}{4}-z;\ \frac{1}{4}-z,\frac{1}{4}-y,\frac{1}{4}-x;$ $\frac{1}{4}-x,\frac{1}{4}+z,\frac{1}{4}+y;\ \frac{1}{4}-y,\frac{1}{4}+x,\frac{1}{4}+z;\ \frac{1}{4}-z,\frac{1}{4}+y,\frac{1}{4}+x;$ $\frac{1}{4}+x,\frac{1}{4}-z,\frac{1}{4}+y;\ \frac{1}{4}+y,\frac{1}{4}-x,\frac{1}{4}+z;\ \frac{1}{4}+z,\frac{1}{4}-y,\frac{1}{4}+x;$ $\frac{1}{4}+x,\frac{1}{4}+z,\frac{1}{4}-y;\ \frac{1}{4}+y,\frac{1}{4}+x,\frac{1}{4}-z;\ \frac{1}{4}+z,\frac{1}{4}+y,\frac{1}{4}-x.$	hkl: $h+k,k+l,(l+h)=2n$ hhl: $(l+h=2n)$; ↻ $0kl$: $(k,l=2n)$; $k+l=4n$ ↻
				Special: as above, plus
96	h	2	$\frac{1}{8},x,\frac{1}{4}-x;\ \frac{1}{8},\frac{1}{4}-x,x;\ \frac{3}{8},x,\frac{1}{4}+x;\ \frac{3}{8},\frac{1}{4}+x,x;$ $\frac{1}{4}-x,\frac{1}{8},x;\ x,\frac{1}{8},\frac{1}{4}-x;\ \frac{1}{4}+x,\frac{3}{8},x;\ x,\frac{3}{8},\frac{1}{4}+x;$ $x,\frac{1}{4}-x,\frac{1}{8};\ \frac{1}{4}-x,x,\frac{1}{8};\ x,\frac{1}{4}+x,\frac{3}{8};\ \frac{1}{4}+x,x,\frac{3}{8};$ $\frac{1}{8},\bar{x},\frac{3}{4}+x;\ \frac{1}{8},\frac{3}{4}+x,\bar{x};\ \frac{3}{8},\bar{x},\frac{3}{4}-x;\ \frac{3}{8},\frac{3}{4}-x,\bar{x};$ $\frac{3}{4}+x,\frac{1}{8},\bar{x};\ \bar{x},\frac{1}{8},\frac{3}{4}+x;\ \frac{3}{4}-x,\frac{3}{8},\bar{x};\ \bar{x},\frac{3}{8},\frac{3}{4}-x;$ $\bar{x},\frac{3}{4}+x,\frac{1}{8};\ \frac{3}{4}+x,\bar{x},\frac{1}{8};\ \bar{x},\frac{3}{4}-x,\frac{3}{8};\ \frac{3}{4}-x,\bar{x},\frac{3}{8}.$	no extra conditions
96	g	m	$x,x,z;\ z,x,x;\ x,z,x;\ \bar{x},x,\bar{z};\ \bar{z},x,\bar{x};\ \bar{x},z,\bar{x};$ $x,\bar{x},\bar{z};\ z,\bar{x},\bar{x};\ x,\bar{z},\bar{x};\ \bar{x},\bar{x},z;\ \bar{z},\bar{x},x;\ \bar{x},\bar{z},x;$ $\frac{1}{4}-x,\frac{1}{4}-x,\frac{1}{4}-z;\ \frac{1}{4}-z,\frac{1}{4}-x,\frac{1}{4}-x;\ \frac{1}{4}-x,\frac{1}{4}-z,\frac{1}{4}-x;$ $\frac{1}{4}-x,\frac{1}{4}+x,\frac{1}{4}+z;\ \frac{1}{4}-z,\frac{1}{4}+x,\frac{1}{4}+x;\ \frac{1}{4}-x,\frac{1}{4}+z,\frac{1}{4}+x;$ $\frac{1}{4}+x,\frac{1}{4}-x,\frac{1}{4}+z;\ \frac{1}{4}+z,\frac{1}{4}-x,\frac{1}{4}+x;\ \frac{1}{4}+x,\frac{1}{4}-z,\frac{1}{4}+x;$ $\frac{1}{4}+x,\frac{1}{4}+x,\frac{1}{4}-z;\ \frac{1}{4}+z,\frac{1}{4}+x,\frac{1}{4}-x;\ \frac{1}{4}+x,\frac{1}{4}+z,\frac{1}{4}-x.$	
48	f	mm	$x,0,0;\ \bar{x},0,0;\ \frac{1}{4}+x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4}-x,\frac{1}{4},\frac{1}{4};$ $0,x,0;\ 0,\bar{x},0;\ \frac{1}{4},\frac{1}{4}+x,\frac{1}{4};\ \frac{1}{4},\frac{1}{4}-x,\frac{1}{4};$ $0,0,x;\ 0,0,\bar{x};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}+x;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}-x.$	hkl: $h+k+l=2n+1$ or $4n$
32	e	$3m$	$x,x,x;\ \frac{1}{4}-x,\frac{1}{4}-x,\frac{1}{4}-x;$ $x,\bar{x},\bar{x};\ \frac{1}{4}-x,\frac{1}{4}+x,\frac{1}{4}+x;$ $\bar{x},x,\bar{x};\ \frac{1}{4}+x,\frac{1}{4}-x,\frac{1}{4}+x;$ $\bar{x},\bar{x},x;\ \frac{1}{4}+x,\frac{1}{4}+x,\frac{1}{4}-x.$	no extra conditions
16	d	$\bar{3}m$	$\frac{5}{8},\frac{5}{8},\frac{5}{8};\ \frac{5}{8},\frac{7}{8},\frac{7}{8};\ \frac{7}{8},\frac{5}{8},\frac{7}{8};\ \frac{7}{8},\frac{7}{8},\frac{5}{8}.$	hkl: $h=2n+1$, $k=2n+1$, $l=2n+1$
16	c	$\bar{3}m$.	$\frac{1}{8},\frac{1}{8},\frac{1}{8};\ \frac{1}{8},\frac{3}{8},\frac{3}{8};\ \frac{3}{8},\frac{1}{8},\frac{3}{8};\ \frac{3}{8},\frac{3}{8},\frac{1}{8}.$	$4n+2$, or $4n+2$, $4n+2$ } or { $4n$, or $4n$, $4n$
8	b	$\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2};\ \frac{3}{4},\frac{3}{4},\frac{3}{4}.$	hkl: $h+k+l=2n+1$ or $4n$
8	a	$\bar{4}3m$	$0,0,0;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}.$	

Origin at centre ($\bar{3}m$), at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from $\bar{4}3m$ (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$				Conditions limiting possible reflections
							General:
192	i	1	x,y,z;	$x,\frac{1}{4}-y,\frac{1}{4}-z$;	$\frac{1}{4}-x,y,\frac{1}{4}-z$;	$\frac{1}{4}-x,\frac{1}{4}-y,z$;	hkl: $h+k,k+l,(l+h)=2n$
			z,x,y;	$z,\frac{1}{4}-x,\frac{1}{4}-y$;	$\frac{1}{4}-z,x,\frac{1}{4}-y$;	$\frac{1}{4}-z,\frac{1}{4}-x,y$;	hhl: $(l+h=2n)$; ↻
			y,z,x;	$y,\frac{1}{4}-z,\frac{1}{4}-x$;	$\frac{1}{4}-y,z,\frac{1}{4}-x$;	$\frac{1}{4}-y,\frac{1}{4}-z,x$;	$0kl$: $(k,l=2n)$; $k+l=4n$
			x,z,y;	$x,\frac{1}{4}-z,\frac{1}{4}-y$;	$\frac{1}{4}-x,z,\frac{1}{4}-y$;	$\frac{1}{4}-x,\frac{1}{4}-z,y$;	↻
			y,x,z;	$y,\frac{1}{4}-x,\frac{1}{4}-z$;	$\frac{1}{4}-y,x,\frac{1}{4}-z$;	$\frac{1}{4}-y,\frac{1}{4}-x,z$;	
			z,y,x;	$z,\frac{1}{4}-y,\frac{1}{4}-x$;	$\frac{1}{4}-z,y,\frac{1}{4}-x$;	$\frac{1}{4}-z,\frac{1}{4}-y,x$;	
			$\bar{x},\bar{y},\bar{z}$;	$\bar{x},\frac{3}{4}+y,\frac{3}{4}+z$;	$\frac{3}{4}+x,\bar{y},\frac{3}{4}+z$;	$\frac{3}{4}+x,\frac{3}{4}+y,\bar{z}$;	
			$\bar{z},\bar{x},\bar{y}$;	$\bar{z},\frac{3}{4}+x,\frac{3}{4}+y$;	$\frac{3}{4}+z,\bar{x},\frac{3}{4}+y$;	$\frac{3}{4}+z,\frac{3}{4}+x,\bar{y}$;	
			$\bar{y},\bar{z},\bar{x}$;	$\bar{y},\frac{3}{4}+z,\frac{3}{4}+x$;	$\frac{3}{4}+y,\bar{z},\frac{3}{4}+x$;	$\frac{3}{4}+y,\frac{3}{4}+z,\bar{x}$;	
			$\bar{x},\bar{z},\bar{y}$;	$\bar{x},\frac{3}{4}+z,\frac{3}{4}+y$;	$\frac{3}{4}+x,\bar{z},\frac{3}{4}+y$;	$\frac{3}{4}+x,\frac{3}{4}+z,\bar{y}$;	
			$\bar{y},\bar{x},\bar{z}$;	$\bar{y},\frac{3}{4}+x,\frac{3}{4}+z$;	$\frac{3}{4}+y,\bar{x},\frac{3}{4}+z$;	$\frac{3}{4}+y,\frac{3}{4}+x,\bar{z}$;	
			$\bar{z},\bar{y},\bar{x}$;	$\bar{z},\frac{3}{4}+y,\frac{3}{4}+x$;	$\frac{3}{4}+z,\bar{y},\frac{3}{4}+x$;	$\frac{3}{4}+z,\frac{3}{4}+y,\bar{x}$.	
							Special: as above, plus
96	h	2	$0,x,\bar{x}$;	$0,\frac{1}{4}-x,\frac{1}{4}+x$;	$\frac{1}{4},x,\frac{1}{4}+x$;	$\frac{1}{4},\frac{1}{4}-x,\bar{x}$;	
			$\bar{x},0,x$;	$\frac{1}{4}+x,0,\frac{1}{4}-x$;	$\frac{1}{4}+x,\frac{1}{4},x$;	$\bar{x},\frac{1}{4},\frac{1}{4}-x$;	
			$x,\bar{x},0$;	$\frac{1}{4}-x,\frac{1}{4}+x,0$;	$x,\frac{1}{4}+x,\frac{1}{4}$;	$\frac{1}{4}-x,\bar{x},\frac{1}{4}$;	
			$0,\bar{x},x$;	$0,\frac{3}{4}+x,\frac{3}{4}-x$;	$\frac{3}{4},\bar{x},\frac{3}{4}-x$;	$\frac{3}{4},\frac{3}{4}+x,x$;	
			$x,0,\bar{x}$;	$\frac{3}{4}-x,0,\frac{3}{4}+x$;	$\frac{3}{4}-x,\frac{3}{4},\bar{x}$;	$x,\frac{3}{4},\frac{3}{4}+x$;	
			$\bar{x},x,0$;	$\frac{3}{4}+x,\frac{3}{4}-x,0$;	$\bar{x},\frac{3}{4}-x,\frac{3}{4}$;	$\frac{3}{4}+x,x,\frac{3}{4}$.	
							no extra conditions
96	g	m	x,x,z;	$x,\frac{1}{4}-x,\frac{1}{4}-z$;	$\frac{1}{4}-x,x,\frac{1}{4}-z$;	$\frac{1}{4}-x,\frac{1}{4}-x,z$;	
			z,x,x;	$z,\frac{1}{4}-x,\frac{1}{4}-x$;	$\frac{1}{4}-z,x,\frac{1}{4}-x$;	$\frac{1}{4}-z,\frac{1}{4}-x,x$;	
			x,z,x;	$x,\frac{1}{4}-z,\frac{1}{4}-x$;	$\frac{1}{4}-x,z,\frac{1}{4}-x$;	$\frac{1}{4}-x,\frac{1}{4}-z,x$;	
			$\bar{x},\bar{x},\bar{z}$;	$\bar{x},\frac{3}{4}+x,\frac{3}{4}+z$;	$\frac{3}{4}+x,\bar{x},\frac{3}{4}+z$;	$\frac{3}{4}+x,\frac{3}{4}+x,\bar{z}$;	
			$\bar{z},\bar{x},\bar{x}$;	$\bar{z},\frac{3}{4}+x,\frac{3}{4}+x$;	$\frac{3}{4}+z,\bar{x},\frac{3}{4}+x$;	$\frac{3}{4}+z,\frac{3}{4}+x,\bar{x}$;	
			$\bar{x},\bar{z},\bar{x}$;	$\bar{x},\frac{3}{4}+z,\frac{3}{4}+x$;	$\frac{3}{4}+x,\bar{z},\frac{3}{4}+x$;	$\frac{3}{4}+x,\frac{3}{4}+z,\bar{x}$.	
48	f	mm	$x,\frac{1}{8},\frac{1}{8}$;	$\bar{x},\frac{7}{8},\frac{7}{8}$;	$\frac{1}{4}-x,\frac{1}{8},\frac{1}{8}$;	$\frac{3}{4}+x,\frac{7}{8},\frac{7}{8}$;	hkl: $h+k+l=2n+1$ or $4n$
			$\frac{1}{8},x,\frac{1}{8}$;	$\frac{7}{8},\bar{x},\frac{7}{8}$;	$\frac{1}{8},\frac{1}{4}-x,\frac{1}{8}$;	$\frac{7}{8},\frac{3}{4}+x,\frac{7}{8}$;	
			$\frac{1}{8},\frac{1}{8},x$;	$\frac{7}{8},\frac{7}{8},\bar{x}$;	$\frac{1}{8},\frac{1}{8},\frac{1}{4}-x$;	$\frac{7}{8},\frac{7}{8},\frac{3}{4}+x$.	
32	e	$3m$	x,x,x;	$x,\frac{1}{4}-x,\frac{1}{4}-x$;	$\frac{1}{4}-x,x,\frac{1}{4}-x$;	$\frac{1}{4}-x,\frac{1}{4}-x,x$;	no extra conditions
			$\bar{x},\bar{x},\bar{x}$;	$\bar{x},\frac{3}{4}+x,\frac{3}{4}+x$;	$\frac{3}{4}+x,\bar{x},\frac{3}{4}+x$;	$\frac{3}{4}+x,\frac{3}{4}+x,\bar{x}$.	
16	d	$\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$;	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$;	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$;	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$.	hkl: $h=2n+1$, $k=2n+1$, $l=2n+1$
16	c	$\bar{3}m$	$0,0,0$;	$0,\frac{1}{4},\frac{1}{4}$;	$\frac{1}{4},0,\frac{1}{4}$;	$\frac{1}{4},\frac{1}{4},0$.	$4n+2$ or $4n+2$ or $4n+2$; $4n$ or $4n$ or $4n$
8	b	$\bar{4}3m$	$\frac{3}{8},\frac{3}{8},\frac{3}{8}$;	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$.			hkl: $h+k+l=2n+1$ or $4n$
8	a	$\bar{4}3m$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$;	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$.			

$Fd3c$ O_h^8

No. 228 $F\,4_1/d\,\bar{3}\,2/c$ $m\,3\,m$ Cubic

Origin at 23, at $\frac{\bar{3}}{8},\frac{\bar{3}}{8},\frac{\bar{3}}{8}$ from centre ($\bar{3}$) (compare next page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
192	h	1	$x,y,z;\ \bar{x},y,\bar{z};\ x,z,\frac{1}{2}+y;\ \bar{x},z,\frac{1}{2}-y;$ $z,x,y;\ \bar{z},x,\bar{y};\ y,x,\frac{1}{2}+z;\ \bar{y},x,\frac{1}{2}-z;$ $y,z,x;\ \bar{y},z,\bar{x};\ z,y,\frac{1}{2}+x;\ \bar{z},y,\frac{1}{2}-x;$ $x,\bar{y},\bar{z};\ \bar{x},\bar{y},z;\ x,\bar{z},\frac{1}{2}-y;\ \bar{x},\bar{z},\frac{1}{2}+y;$ $z,\bar{x},\bar{y};\ \bar{z},\bar{x},y;\ y,\bar{x},\frac{1}{2}-z;\ \bar{y},\bar{x},\frac{1}{2}+z;$ $y,\bar{z},\bar{x};\ \bar{y},\bar{z},x;\ z,\bar{y},\frac{1}{2}-x;\ \bar{z},\bar{y},\frac{1}{2}+x;$ $\frac{1}{4}-x,\frac{1}{4}-z,\frac{1}{4}-y;\ \frac{1}{4}-y,\frac{1}{4}-x,\frac{1}{4}-z;\ \frac{1}{4}-z,\frac{1}{4}-y,\frac{1}{4}-x;$ $\frac{1}{4}-x,\frac{1}{4}+z,\frac{1}{4}+y;\ \frac{1}{4}-y,\frac{1}{4}+x,\frac{1}{4}+z;\ \frac{1}{4}-z,\frac{1}{4}+y,\frac{1}{4}+x;$ $\frac{1}{4}+x,\frac{1}{4}-z,\frac{1}{4}+y;\ \frac{1}{4}+y,\frac{1}{4}-x,\frac{1}{4}+z;\ \frac{1}{4}+z,\frac{1}{4}-y,\frac{1}{4}+x;$ $\frac{1}{4}+x,\frac{1}{4}+z,\frac{1}{4}-y;\ \frac{1}{4}+y,\frac{1}{4}+x,\frac{1}{4}-z;\ \frac{1}{4}+z,\frac{1}{4}+y,\frac{1}{4}-x;$ $\frac{1}{4}-x,\frac{1}{4}-y,\frac{3}{4}-z;\ \frac{1}{4}-z,\frac{1}{4}-x,\frac{3}{4}-y;\ \frac{1}{4}-y,\frac{1}{4}-z,\frac{3}{4}-x;$ $\frac{1}{4}-x,\frac{1}{4}+y,\frac{3}{4}+z;\ \frac{1}{4}-z,\frac{1}{4}+x,\frac{3}{4}+y;\ \frac{1}{4}-y,\frac{1}{4}+z,\frac{3}{4}+x;$ $\frac{1}{4}+x,\frac{1}{4}-y,\frac{3}{4}+z;\ \frac{1}{4}+z,\frac{1}{4}-x,\frac{3}{4}+y;\ \frac{1}{4}+y,\frac{1}{4}-z,\frac{3}{4}+x;$ $\frac{1}{4}+x,\frac{1}{4}+y,\frac{3}{4}-z;\ \frac{1}{4}+z,\frac{1}{4}+x,\frac{3}{4}-y;\ \frac{1}{4}+y,\frac{1}{4}+z,\frac{3}{4}-x.$	hkl: $h+k,k+l,(l+h)=2n$ hhl: $l,(h)=2n$; ↻ $0kl$: $(k,l=2n)$; $k+l=4n$ ↻
				Special: as above, plus
96	g	2	$\frac{1}{8},x,\frac{1}{4}-x;\ \frac{1}{8},\bar{x},\frac{3}{4}+x;\ \frac{3}{8},x,\frac{1}{4}+x;\ \frac{3}{8},\bar{x},\frac{3}{4}-x;$ $\frac{1}{4}-x,\frac{1}{8},x;\ \frac{3}{4}+x,\frac{1}{8},\bar{x};\ \frac{1}{4}+x,\frac{3}{8},x;\ \frac{3}{4}-x,\frac{3}{8},\bar{x};$ $x,\frac{1}{4}-x,\frac{1}{8};\ \bar{x},\frac{3}{4}+x,\frac{1}{8};\ x,\frac{1}{4}+x,\frac{3}{8};\ \bar{x},\frac{3}{4}-x,\frac{3}{8};$ $\frac{1}{8},\frac{3}{4}-x,x;\ \frac{1}{8},\frac{1}{4}+x,\bar{x};\ \frac{3}{8},\frac{3}{4}+x,x;\ \frac{3}{8},\frac{1}{4}-x,\bar{x};$ $x,\frac{1}{8},\frac{3}{4}-x;\ \bar{x},\frac{1}{8},\frac{1}{4}+x;\ x,\frac{3}{8},\frac{3}{4}+x;\ \bar{x},\frac{3}{8},\frac{1}{4}-x;$ $\frac{3}{4}-x,x,\frac{1}{8};\ \frac{1}{4}+x,\bar{x},\frac{1}{8};\ \frac{3}{4}+x,x,\frac{3}{8};\ \frac{1}{4}-x,\bar{x},\frac{3}{8}.$	no extra conditions
96	f	2	$x,0,0;\ x,0,\frac{1}{2};\ \frac{1}{4}+x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4}+x,\frac{1}{4},\frac{3}{4};$ $0,x,0;\ \frac{1}{2},x,0;\ \frac{1}{4},\frac{1}{4}+x,\frac{1}{4};\ \frac{3}{4},\frac{1}{4}+x,\frac{1}{4};$ $0,0,x;\ 0,\frac{1}{2},x;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}+x;\ \frac{1}{4},\frac{3}{4},\frac{1}{4}+x;$ $\bar{x},0,0;\ \bar{x},0,\frac{1}{2};\ \frac{1}{4}-x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4}-x,\frac{1}{4},\frac{3}{4};$ $0,\bar{x},0;\ \frac{1}{2},\bar{x},0;\ \frac{1}{4},\frac{1}{4}-x,\frac{1}{4};\ \frac{3}{4},\frac{1}{4}-x,\frac{1}{4};$ $0,0,\bar{x};\ 0,\frac{1}{2},\bar{x};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}-x;\ \frac{1}{4},\frac{3}{4},\frac{1}{4}-x.$	hkl: $h,(k,l)=2n$; $h+k+l=4n$
64	e	3	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x;$ $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2}+x;\ \frac{1}{4}-x,\frac{1}{4}-x,\frac{1}{4}-x;\ \frac{3}{4}-x,\frac{3}{4}-x,\frac{3}{4}-x;$ $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}-x;\ \frac{1}{4}-x,\frac{1}{4}+x,\frac{1}{4}+x;\ \frac{3}{4}-x,\frac{3}{4}+x,\frac{3}{4}+x;$ $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}-x;\ \frac{1}{4}+x,\frac{1}{4}-x,\frac{1}{4}+x;\ \frac{3}{4}+x,\frac{3}{4}-x,\frac{3}{4}+x;$ $\frac{1}{2}-x,\frac{1}{2}-x,\frac{1}{2}+x;\ \frac{1}{4}+x,\frac{1}{4}+x,\frac{1}{4}-x;\ \frac{3}{4}+x,\frac{3}{4}+x,\frac{3}{4}-x.$	hkl: $h,(k,l)=2n$
48	d	$\bar{4}$	$\frac{1}{4},0,0;\ 0,\frac{1}{4},0;\ 0,0,\frac{1}{4};\ \frac{3}{4},0,0;\ 0,\frac{3}{4},0;\ 0,0,\frac{3}{4}.$ $0,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},0;\ \frac{1}{2},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{2},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{2}.$	hkl: $h,(k,l)=2n$; $h+k+l=4n$
32	c	$\bar{3}$	$\frac{3}{8},\frac{3}{8},\frac{3}{8};\ \frac{3}{8},\frac{5}{8},\frac{5}{8};\ \frac{5}{8},\frac{3}{8},\frac{5}{8};\ \frac{5}{8},\frac{5}{8},\frac{3}{8};$ $\frac{7}{8},\frac{7}{8},\frac{7}{8};\ \frac{7}{8},\frac{1}{8},\frac{1}{8};\ \frac{1}{8},\frac{7}{8},\frac{1}{8};\ \frac{1}{8},\frac{1}{8},\frac{7}{8}.$	hkl: $h=4n+2$, $k=4n+2$, $l=4n+2$ or $4n$, $4n$, $4n$
32	b	32	$\frac{1}{8},\frac{1}{8},\frac{1}{8};\ \frac{1}{8},\frac{3}{8},\frac{3}{8};\ \frac{3}{8},\frac{1}{8},\frac{3}{8};\ \frac{3}{8},\frac{3}{8},\frac{1}{8};$ $\frac{5}{8},\frac{5}{8},\frac{5}{8};\ \frac{5}{8},\frac{7}{8},\frac{7}{8};\ \frac{7}{8},\frac{5}{8},\frac{7}{8};\ \frac{7}{8},\frac{7}{8},\frac{5}{8}.$	
16	a	23	$0,0,0;\ \frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{2},\frac{1}{2},\frac{1}{2};\ \frac{3}{4},\frac{3}{4},\frac{3}{4}.$	hkl: $h,(k,l)=2n$; $h+k+l=4n$

Origin at centre ($\bar{3}$), at $\frac{3}{8},\frac{3}{8},\frac{3}{8}$ from 23 (compare previous page for alternative origin)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
192	h	1	$x,y,z;\ x,\frac{1}{4}-y,\frac{1}{4}-z;\ \frac{1}{4}-x,y,\frac{1}{4}-z;\ \frac{1}{4}-x,\frac{1}{4}-y,z;$ $z,x,y;\ z,\frac{1}{4}-x,\frac{1}{4}-y;\ \frac{1}{4}-z,x,\frac{1}{4}-y;\ \frac{1}{4}-z,\frac{1}{4}-x,y;$ $y,z,x;\ y,\frac{1}{4}-z,\frac{1}{4}-x;\ \frac{1}{4}-y,z,\frac{1}{4}-x;\ \frac{1}{4}-y,\frac{1}{4}-z,x;$ $\bar{x},\bar{y},\bar{z};\ \bar{x},\frac{3}{4}+y,\frac{3}{4}+z;\ \frac{3}{4}+x,\bar{y},\frac{3}{4}+z;\ \frac{3}{4}+x,\frac{3}{4}+y,\bar{z};$ $\bar{z},\bar{x},\bar{y};\ \bar{z},\frac{3}{4}+x,\frac{3}{4}+y;\ \frac{3}{4}+z,\bar{x},\frac{3}{4}+y;\ \frac{3}{4}+z,\frac{3}{4}+x,\bar{y};$ $\bar{y},\bar{z},\bar{x};\ \bar{y},\frac{3}{4}+z,\frac{3}{4}+x;\ \frac{3}{4}+y,\bar{z},\frac{3}{4}+x;\ \frac{3}{4}+y,\frac{3}{4}+z,\bar{x};$ $x,z,\frac{1}{2}+y;\ x,\frac{1}{4}-z,\frac{3}{4}-y;\ \frac{3}{4}-x,z,\frac{1}{4}-y;\ \frac{1}{4}-x,\frac{3}{4}-z,y;$ $y,x,\frac{1}{2}+z;\ y,\frac{1}{4}-x,\frac{3}{4}-z;\ \frac{3}{4}-y,x,\frac{1}{4}-z;\ \frac{1}{4}-y,\frac{3}{4}-x,z;$ $z,y,\frac{1}{2}+x;\ z,\frac{1}{4}-y,\frac{3}{4}-x;\ \frac{3}{4}-z,y,\frac{1}{4}-x;\ \frac{1}{4}-z,\frac{3}{4}-y,x;$ $\bar{x},\bar{z},\frac{1}{2}-y;\ \bar{x},\frac{3}{4}+z,\frac{1}{4}+y;\ \frac{1}{4}+x,\bar{z},\frac{3}{4}+y;\ \frac{3}{4}+x,\frac{1}{4}+z,\bar{y};$ $\bar{y},\bar{x},\frac{1}{2}-z;\ \bar{y},\frac{3}{4}+x,\frac{1}{4}+z;\ \frac{1}{4}+y,\bar{x},\frac{3}{4}+z;\ \frac{3}{4}+y,\frac{1}{4}+x,\bar{z};$ $\bar{z},\bar{y},\frac{1}{2}-x;\ \bar{z},\frac{3}{4}+y,\frac{1}{4}+x;\ \frac{1}{4}+z,\bar{y},\frac{3}{4}+x;\ \frac{3}{4}+z,\frac{1}{4}+y,\bar{x}.$	hkl: $h+k,k+l,(l+h)=2n$ hhl: $l,(h)=2n$; ↻ $0kl$: $(k,l=2n)$; $k+l=4n$ ↻
				Special: as above, plus
96	g	2	$\frac{1}{4},x,\bar{x};\ \frac{1}{4},\frac{1}{4}-x,\frac{1}{4}+x;\ 0,x,\frac{1}{4}+x;\ 0,\frac{1}{4}-x,\bar{x};$ $\bar{x},\frac{1}{4},x;\ \frac{1}{4}+x,\frac{1}{4},\frac{1}{4}-x;\ \frac{1}{4}+x,0,x;\ \bar{x},0,\frac{1}{4}-x;$ $x,\bar{x},\frac{1}{4};\ \frac{1}{4}-x,\frac{1}{4}+x,\frac{1}{4};\ x,\frac{1}{4}+x,0;\ \frac{1}{4}-x,\bar{x},0;$ $\frac{3}{4},\bar{x},x;\ \frac{3}{4},\frac{3}{4}+x,\frac{3}{4}-x;\ 0,\bar{x},\frac{3}{4}-x;\ 0,\frac{3}{4}+x,x;$ $x,\frac{3}{4},\bar{x};\ \frac{3}{4}-x,\frac{3}{4},\frac{3}{4}+x;\ \frac{3}{4}-x,0,\bar{x};\ x,0,\frac{3}{4}+x;$ $\bar{x},x,\frac{3}{4};\ \frac{3}{4}+x,\frac{3}{4}-x,\frac{3}{4};\ \bar{x},\frac{3}{4}-x,0;\ \frac{3}{4}+x,x,0.$	no extra conditions
96	f	2	$x,\frac{1}{8},\frac{1}{8};\ x,\frac{1}{8},\frac{5}{8};\ \frac{1}{4}-x,\frac{1}{8},\frac{1}{8};\ \frac{1}{4}-x,\frac{1}{8},\frac{5}{8};$ $\frac{1}{8},x,\frac{1}{8};\ \frac{5}{8},x,\frac{1}{8};\ \frac{1}{8},\frac{1}{4}-x,\frac{1}{8};\ \frac{5}{8},\frac{1}{4}-x,\frac{1}{8};$ $\frac{1}{8},\frac{1}{8},x;\ \frac{1}{8},\frac{5}{8},x;\ \frac{1}{8},\frac{1}{8},\frac{1}{4}-x;\ \frac{1}{8},\frac{5}{8},\frac{1}{4}-x;$ $\bar{x},\frac{7}{8},\frac{7}{8};\ \bar{x},\frac{7}{8},\frac{3}{8};\ \frac{3}{4}+x,\frac{7}{8},\frac{7}{8};\ \frac{3}{4}+x,\frac{7}{8},\frac{3}{8};$ $\frac{7}{8},\bar{x},\frac{7}{8};\ \frac{3}{8},\bar{x},\frac{7}{8};\ \frac{7}{8},\frac{3}{4}+x,\frac{7}{8};\ \frac{3}{8},\frac{3}{4}+x,\frac{7}{8};$ $\frac{7}{8},\frac{7}{8},\bar{x};\ \frac{7}{8},\frac{3}{8},\bar{x};\ \frac{7}{8},\frac{7}{8},\frac{3}{4}+x;\ \frac{7}{8},\frac{3}{8},\frac{3}{4}+x.$	hkl: $h,(k,l)=2n$; $h+k+l=4n$
64	e	3	$x,x,x;\ x,\frac{1}{4}-x,\frac{1}{4}-x;\ \frac{1}{4}-x,x,\frac{1}{4}-x;\ \frac{1}{4}-x,\frac{1}{4}-x,x;$ $\bar{x},\bar{x},\bar{x};\ \bar{x},\frac{3}{4}+x,\frac{3}{4}+x;\ \frac{3}{4}+x,\bar{x},\frac{3}{4}+x;\ \frac{3}{4}+x,\frac{3}{4}+x,\bar{x};$ $x,x,\frac{1}{2}+x;\ x,\frac{1}{4}-x,\frac{3}{4}-x;\ \frac{3}{4}-x,x,\frac{1}{4}-x;\ \frac{1}{4}-x,\frac{3}{4}-x,x;$ $\bar{x},\bar{x},\frac{1}{2}-x;\ \bar{x},\frac{3}{4}+x,\frac{1}{4}+x;\ \frac{1}{4}+x,\bar{x},\frac{3}{4}+x;\ \frac{3}{4}+x,\frac{1}{4}+x,\bar{x}.$	hkl: $h,(k,l)=2n$
48	d	$\bar{4}$	$\frac{7}{8},\frac{1}{8},\frac{1}{8};\ \frac{3}{8},\frac{1}{8},\frac{1}{8};\ \frac{1}{8},\frac{3}{8},\frac{3}{8};\ \frac{5}{8},\frac{3}{8},\frac{3}{8};$ $\frac{1}{8},\frac{7}{8},\frac{1}{8};\ \frac{1}{8},\frac{3}{8},\frac{1}{8};\ \frac{3}{8},\frac{1}{8},\frac{3}{8};\ \frac{3}{8},\frac{5}{8},\frac{3}{8};$ $\frac{1}{8},\frac{1}{8},\frac{7}{8};\ \frac{1}{8},\frac{1}{8},\frac{3}{8};\ \frac{3}{8},\frac{3}{8},\frac{1}{8};\ \frac{3}{8},\frac{3}{8},\frac{5}{8}.$	hkl: $h,(k,l)=2n$; $h+k+l=4n$
32	c	$\bar{3}$	$0,0,0;\ 0,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},0;$ $0,0,\frac{1}{2};\ 0,\frac{1}{4},\frac{3}{4};\ \frac{3}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{3}{4},0.$	hkl: $\left.\begin{matrix} h=4n+2 \\ k=4n+2 \\ l=4n+2 \end{matrix}\right\}$ or $\left.\begin{matrix} 4n \\ 4n \\ 4n \end{matrix}\right\}$
32	b	32	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},0,0;\ 0,\frac{1}{4},0;\ 0,0,\frac{1}{4};$ $\frac{3}{4},\frac{3}{4},\frac{3}{4};\ \frac{3}{4},0,0;\ 0,\frac{3}{4},0;\ 0,0,\frac{3}{4}.$	
16	a	23	$\frac{1}{8},\frac{1}{8},\frac{1}{8};\ \frac{3}{8},\frac{3}{8},\frac{3}{8};\ \frac{5}{8},\frac{5}{8},\frac{5}{8};\ \frac{7}{8},\frac{7}{8},\frac{7}{8}.$	hkl: $h,(k,l)=2n$; $h+k+l=4n$

$Im3m$ O_h^9

No. 229 $I\,4/m\,\bar{3}\,2/m$ $m\,3\,m$ Cubic

Origin at centre ($m3m$)

Co-ordinates of equivalent positions

$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+$

Number of positions,	Wyckoff notation,	and point symmetry	Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
96	l	1	$x,y,z;\ z,x,y;\ y,z,x;\ x,z,y;\ y,x,z;\ z,y,x;$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ x,\bar{z},\bar{y};\ y,\bar{x},\bar{z};\ z,\bar{y},\bar{x};$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ \bar{x},z,\bar{y};\ \bar{y},x,\bar{z};\ \bar{z},y,\bar{x};$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ \bar{x},\bar{z},y;\ \bar{y},\bar{x},z;\ \bar{z},\bar{y},x;$ $\bar{x},\bar{y},\bar{z};\ \bar{z},\bar{x},\bar{y};\ \bar{y},\bar{z},\bar{x};\ \bar{x},\bar{z},\bar{y};\ \bar{y},\bar{x},\bar{z};\ \bar{z},\bar{y},\bar{x};$ $\bar{x},y,z;\ \bar{z},x,y;\ \bar{y},z,x;\ \bar{x},z,y;\ \bar{y},x,z;\ \bar{z},y,x;$ $x,\bar{y},z;\ z,\bar{x},y;\ y,\bar{z},x;\ x,\bar{z},y;\ y,\bar{x},z;\ z,\bar{y},x;$ $x,y,\bar{z};\ z,x,\bar{y};\ y,z,\bar{x};\ x,z,\bar{y};\ y,x,\bar{z};\ z,y,\bar{x}.$	hkl: $h+k+l=2n$ hhl: $(l=2n)$; ○ $0kl$: $(k+l=2n)$; ○
				Special: as above, plus
48	k	m	$x,x,z;\ z,x,x;\ x,z,x;\ \bar{x},\bar{x},\bar{z};\ \bar{z},\bar{x},\bar{x};\ \bar{x},\bar{z},\bar{x};$ $x,\bar{x},\bar{z};\ z,\bar{x},\bar{x};\ x,\bar{z},\bar{x};\ \bar{x},x,z;\ \bar{z},x,x;\ \bar{x},z,x;$ $\bar{x},x,\bar{z};\ \bar{z},x,\bar{x};\ \bar{x},z,\bar{x};\ x,\bar{x},z;\ z,\bar{x},x;\ x,\bar{z},x;$ $\bar{x},\bar{x},z;\ \bar{z},\bar{x},x;\ \bar{x},\bar{z},x;\ x,x,\bar{z};\ z,x,\bar{x};\ x,z,\bar{x}.$	
48	j	m	$0,y,z;\ z,0,y;\ y,z,0;\ 0,z,y;\ y,0,z;\ z,y,0;$ $0,\bar{y},\bar{z};\ \bar{z},0,\bar{y};\ \bar{y},\bar{z},0;\ 0,\bar{z},\bar{y};\ \bar{y},0,\bar{z};\ \bar{z},\bar{y},0;$ $0,y,\bar{z};\ \bar{z},0,y;\ y,\bar{z},0;\ 0,\bar{z},y;\ y,0,\bar{z};\ \bar{z},y,0;$ $0,\bar{y},z;\ z,0,\bar{y};\ \bar{y},z,0;\ 0,z,\bar{y};\ \bar{y},0,z;\ z,\bar{y},0.$	
48	i	2	$\tfrac{1}{4},x,\tfrac{1}{2}-x;\ \tfrac{1}{4},\bar{x},\tfrac{1}{2}+x;\ \tfrac{1}{4},x,\tfrac{1}{2}+x;\ \tfrac{1}{4},\bar{x},\tfrac{1}{2}-x;$ $\tfrac{1}{2}-x,\tfrac{1}{4},x;\ \tfrac{1}{2}+x,\tfrac{1}{4},\bar{x};\ \tfrac{1}{2}+x,\tfrac{1}{4},x;\ \tfrac{1}{2}-x,\tfrac{1}{4},\bar{x};$ $x,\tfrac{1}{2}-x,\tfrac{1}{4};\ \bar{x},\tfrac{1}{2}+x,\tfrac{1}{4};\ x,\tfrac{1}{2}+x,\tfrac{1}{4};\ \bar{x},\tfrac{1}{2}-x,\tfrac{1}{4};$ $\tfrac{1}{4},\tfrac{1}{2}-x,x;\ \tfrac{1}{4},\tfrac{1}{2}+x,\bar{x};\ \tfrac{1}{4},\tfrac{1}{2}+x,x;\ \tfrac{1}{4},\tfrac{1}{2}-x,\bar{x};$ $x,\tfrac{1}{4},\tfrac{1}{2}-x;\ \bar{x},\tfrac{1}{4},\tfrac{1}{2}+x;\ x,\tfrac{1}{4},\tfrac{1}{2}+x;\ \bar{x},\tfrac{1}{4},\tfrac{1}{2}-x;$ $\tfrac{1}{2}-x,x,\tfrac{1}{4};\ \tfrac{1}{2}+x,\bar{x},\tfrac{1}{4};\ \tfrac{1}{2}+x,x,\tfrac{1}{4};\ \tfrac{1}{2}-x,\bar{x},\tfrac{1}{4}.$	no extra conditions
24	h	mm	$0,x,x;\ x,0,x;\ x,x,0;\ 0,x,\bar{x};\ \bar{x},0,x;\ x,\bar{x},0;$ $0,\bar{x},\bar{x};\ \bar{x},0,\bar{x};\ \bar{x},\bar{x},0;\ 0,\bar{x},x;\ x,0,\bar{x};\ \bar{x},x,0.$	
24	g	mm	$x,0,\tfrac{1}{2};\ \tfrac{1}{2},x,0;\ 0,\tfrac{1}{2},x;\ x,\tfrac{1}{2},0;\ 0,x,\tfrac{1}{2};\ \tfrac{1}{2},0,x;$ $\bar{x},0,\tfrac{1}{2};\ \tfrac{1}{2},\bar{x},0;\ 0,\tfrac{1}{2},\bar{x};\ \bar{x},\tfrac{1}{2},0;\ 0,\bar{x},\tfrac{1}{2};\ \tfrac{1}{2},0,\bar{x}.$	
16	f	$3m$	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x;$ $\bar{x},\bar{x},\bar{x};\ \bar{x},x,x;\ x,\bar{x},x;\ x,x,\bar{x}.$	
12	e	$4mm$	$x,0,0;\ 0,x,0;\ 0,0,x;\ \bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x}.$	
12	d	$\bar{4}2m$	$\tfrac{1}{4},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{4},0;\ 0,\tfrac{1}{2},\tfrac{1}{4};\ \tfrac{3}{4},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{3}{4},0;\ 0,\tfrac{1}{2},\tfrac{3}{4}.$	
8	c	$\bar{3}m$	$\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{3}{4},\tfrac{3}{4};\ \tfrac{3}{4},\tfrac{1}{4},\tfrac{3}{4};\ \tfrac{3}{4},\tfrac{3}{4},\tfrac{1}{4}.$	hkl: $h,k,(l)=2n$
6	b	$4/mmm$	$0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0.$	no extra conditions
2	a	$m3m$	$0,0,0.$	

Origin at centre ($\bar{3}$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+$	
				General:
96	h	1	$x,y,z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,\bar{z};\ \bar{x},\tfrac{1}{2}+y,\tfrac{1}{2}-z;\ \tfrac{1}{2}-x,\bar{y},\tfrac{1}{2}+z;$ $z,x,y;\ \tfrac{1}{2}+z,\tfrac{1}{2}-x,\bar{y};\ \bar{z},\tfrac{1}{2}+x,\tfrac{1}{2}-y;\ \tfrac{1}{2}-z,\bar{x},\tfrac{1}{2}+y;$ $y,z,x;\ \tfrac{1}{2}+y,\tfrac{1}{2}-z,\bar{x};\ \bar{y},\tfrac{1}{2}+z,\tfrac{1}{2}-x;\ \tfrac{1}{2}-y,\bar{z},\tfrac{1}{2}+x;$ $\bar{x},\bar{y},\bar{z};\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,z;\ x,\tfrac{1}{2}-y,\tfrac{1}{2}+z;\ \tfrac{1}{2}+x,y,\tfrac{1}{2}-z;$ $\bar{z},\bar{x},\bar{y};\ \tfrac{1}{2}-z,\tfrac{1}{2}+x,y;\ z,\tfrac{1}{2}-x,\tfrac{1}{2}+y;\ \tfrac{1}{2}+z,x,\tfrac{1}{2}-y;$ $\bar{y},\bar{z},\bar{x};\ \tfrac{1}{2}-y,\tfrac{1}{2}+z,x;\ y,\tfrac{1}{2}-z,\tfrac{1}{2}+x;\ \tfrac{1}{2}+y,z,\tfrac{1}{2}-x;$ $\tfrac{1}{4}+x,\tfrac{1}{4}+z,\tfrac{1}{4}+y;\ \tfrac{1}{4}+y,\tfrac{1}{4}+x,\tfrac{1}{4}+z;\ \tfrac{1}{4}+z,\tfrac{1}{4}+y,\tfrac{1}{4}+x;$ $\tfrac{3}{4}+x,\tfrac{1}{4}-z,\tfrac{3}{4}-y;\ \tfrac{3}{4}+y,\tfrac{1}{4}-x,\tfrac{3}{4}-z;\ \tfrac{3}{4}+z,\tfrac{1}{4}-y,\tfrac{3}{4}-x;$ $\tfrac{3}{4}-x,\tfrac{3}{4}+z,\tfrac{1}{4}-y;\ \tfrac{3}{4}-y,\tfrac{3}{4}+x,\tfrac{1}{4}-z;\ \tfrac{3}{4}-z,\tfrac{3}{4}+y,\tfrac{1}{4}-x;$ $\tfrac{1}{4}-x,\tfrac{3}{4}-z,\tfrac{3}{4}+y;\ \tfrac{1}{4}-y,\tfrac{3}{4}-x,\tfrac{3}{4}+z;\ \tfrac{1}{4}-z,\tfrac{3}{4}-y,\tfrac{3}{4}+x;$ $\tfrac{1}{4}-x,\tfrac{1}{4}-z,\tfrac{1}{4}-y;\ \tfrac{1}{4}-y,\tfrac{1}{4}-x,\tfrac{1}{4}-z;\ \tfrac{1}{4}-z,\tfrac{1}{4}-y,\tfrac{1}{4}-x;$ $\tfrac{3}{4}-x,\tfrac{1}{4}+z,\tfrac{3}{4}+y;\ \tfrac{3}{4}-y,\tfrac{1}{4}+x,\tfrac{3}{4}+z;\ \tfrac{3}{4}-z,\tfrac{1}{4}+y,\tfrac{3}{4}+x;$ $\tfrac{3}{4}+x,\tfrac{3}{4}-z,\tfrac{1}{4}+y;\ \tfrac{3}{4}+y,\tfrac{3}{4}-x,\tfrac{1}{4}+z;\ \tfrac{3}{4}+z,\tfrac{3}{4}-y,\tfrac{1}{4}+x;$ $\tfrac{1}{4}+x,\tfrac{3}{4}+z,\tfrac{3}{4}-y;\ \tfrac{1}{4}+y,\tfrac{3}{4}+x,\tfrac{3}{4}-z;\ \tfrac{1}{4}+z,\tfrac{3}{4}+y,\tfrac{3}{4}-x.$	hkl: $h+k+l=2n$ hhl: $(l=2n)$; $2h+l=4n$; ↻ $0kl$: $k,(l)=2n$; ↻
				Special: as above, plus
48	g	2	$\tfrac{1}{8},x,\tfrac{1}{4}-x;\ \tfrac{3}{8},x,\tfrac{3}{4}+x;\ \tfrac{5}{8},\bar{x},\tfrac{1}{4}-x;\ \tfrac{7}{8},\bar{x},\tfrac{3}{4}+x;$ $\tfrac{1}{4}-x,\tfrac{1}{8},x;\ \tfrac{3}{4}+x,\tfrac{3}{8},x;\ \tfrac{1}{4}-x,\tfrac{5}{8},\bar{x};\ \tfrac{3}{4}+x,\tfrac{7}{8},\bar{x};$ $x,\tfrac{1}{4}-x,\tfrac{1}{8};\ x,\tfrac{3}{4}+x,\tfrac{3}{8};\ \bar{x},\tfrac{1}{4}-x,\tfrac{5}{8};\ \bar{x},\tfrac{3}{4}+x,\tfrac{7}{8};$ $\tfrac{1}{8},\bar{x},\tfrac{1}{4}+x;\ \tfrac{3}{8},\bar{x},\tfrac{3}{4}-x;\ \tfrac{5}{8},x,\tfrac{1}{4}+x;\ \tfrac{7}{8},x,\tfrac{3}{4}-x;$ $\tfrac{1}{4}+x,\tfrac{1}{8},\bar{x};\ \tfrac{3}{4}-x,\tfrac{3}{8},\bar{x};\ \tfrac{1}{4}+x,\tfrac{5}{8},x;\ \tfrac{3}{4}-x,\tfrac{7}{8},x;$ $\bar{x},\tfrac{1}{4}+x,\tfrac{1}{8};\ \bar{x},\tfrac{3}{4}-x,\tfrac{3}{8};\ x,\tfrac{1}{4}+x,\tfrac{5}{8};\ x,\tfrac{3}{4}-x,\tfrac{7}{8}.$	hkl: h or k or $l=2n+1$ or $4n$
48	f	2	$x,0,\tfrac{1}{4};\ \bar{x},\tfrac{1}{2},\tfrac{1}{4};\ \tfrac{1}{4}-x,0,\tfrac{1}{4};\ \tfrac{3}{4}+x,\tfrac{1}{2},\tfrac{1}{4};$ $\tfrac{1}{4},x,0;\ \tfrac{1}{4},\bar{x},\tfrac{1}{2};\ \tfrac{1}{4},\tfrac{1}{4}-x,0;\ \tfrac{1}{4},\tfrac{3}{4}+x,\tfrac{1}{2};$ $0,\tfrac{1}{4},x;\ \tfrac{1}{2},\tfrac{1}{4},\bar{x};\ 0,\tfrac{1}{4},\tfrac{1}{4}-x;\ \tfrac{1}{2},\tfrac{1}{4},\tfrac{3}{4}+x;$ $x,\tfrac{1}{2},\tfrac{3}{4};\ \bar{x},0,\tfrac{3}{4};\ \tfrac{1}{4}-x,\tfrac{1}{2},\tfrac{3}{4};\ \tfrac{3}{4}+x,0,\tfrac{3}{4};$ $\tfrac{3}{4},x,\tfrac{1}{2};\ \tfrac{3}{4},\bar{x},0;\ \tfrac{3}{4},\tfrac{1}{4}-x,\tfrac{1}{2};\ \tfrac{3}{4},\tfrac{3}{4}+x,0;$ $\tfrac{1}{2},\tfrac{3}{4},x;\ 0,\tfrac{3}{4},\bar{x};\ \tfrac{1}{2},\tfrac{3}{4},\tfrac{1}{4}-x;\ 0,\tfrac{3}{4},\tfrac{3}{4}+x.$	
32	e	3	$x,x,x;\ \tfrac{1}{2}+x,\tfrac{1}{2}-x,\bar{x};\ \bar{x},\tfrac{1}{2}+x,\tfrac{1}{2}-x;\ \tfrac{1}{2}-x,\bar{x},\tfrac{1}{2}+x;$ $\bar{x},\bar{x},\bar{x};\ \tfrac{1}{2}-x,\tfrac{1}{2}+x,x;\ x,\tfrac{1}{2}-x,\tfrac{1}{2}+x;\ \tfrac{1}{2}+x,x,\tfrac{1}{2}-x;$ $\tfrac{1}{4}+x,\tfrac{1}{4}+x,\tfrac{1}{4}+x;\ \tfrac{1}{4}-x,\tfrac{1}{4}-x,\tfrac{1}{4}-x;$ $\tfrac{3}{4}+x,\tfrac{1}{4}-x,\tfrac{3}{4}-x;\ \tfrac{3}{4}-x,\tfrac{1}{4}+x,\tfrac{3}{4}+x;$ $\tfrac{3}{4}-x,\tfrac{3}{4}+x,\tfrac{1}{4}-x;\ \tfrac{3}{4}+x,\tfrac{3}{4}-x,\tfrac{1}{4}+x;$ $\tfrac{1}{4}-x,\tfrac{3}{4}-x,\tfrac{3}{4}+x;\ \tfrac{1}{4}+x,\tfrac{3}{4}+x,\tfrac{3}{4}-x.$	hkl: If $h,k,(l)=2n$, then $h+k+l=4n$
24	d	$\bar{4}$	$\tfrac{3}{8},0,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{3}{8},0;\ 0,\tfrac{1}{4},\tfrac{3}{8};\ \tfrac{1}{8},0,\tfrac{3}{4};\ \tfrac{3}{4},\tfrac{1}{8},0;\ 0,\tfrac{3}{4},\tfrac{1}{8};$ $\tfrac{7}{8},0,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{7}{8},0;\ 0,\tfrac{1}{4},\tfrac{7}{8};\ \tfrac{5}{8},0,\tfrac{3}{4};\ \tfrac{3}{4},\tfrac{5}{8},0;\ 0,\tfrac{3}{4},\tfrac{5}{8}.$	hkl: $h=2n+1$, $k=2n+1$, $l=4n+2$ or $4n+2$, $4n+2$, $4n$
24	c	222	$\tfrac{1}{8},0,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{8},0;\ 0,\tfrac{1}{4},\tfrac{1}{8};\ \tfrac{3}{8},0,\tfrac{3}{4};\ \tfrac{3}{4},\tfrac{3}{8},0;\ 0,\tfrac{3}{4},\tfrac{3}{8};$ $\tfrac{5}{8},0,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{5}{8},0;\ 0,\tfrac{1}{4},\tfrac{5}{8};\ \tfrac{7}{8},0,\tfrac{3}{4};\ \tfrac{3}{4},\tfrac{7}{8},0;\ 0,\tfrac{3}{4},\tfrac{7}{8}.$	$8n$ or $8n+4$, $4n+2$; $4n$ or $4n$, $4n$ h,k,l permutable

(*continued on next page*)

16	b	32	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$; $\frac{5}{8},\frac{3}{8},\frac{7}{8}$; $\frac{7}{8},\frac{5}{8},\frac{3}{8}$; $\frac{3}{8},\frac{7}{8},\frac{5}{8}$; $\frac{7}{8},\frac{7}{8},\frac{7}{8}$; $\frac{3}{8},\frac{5}{8},\frac{1}{8}$; $\frac{1}{8},\frac{3}{8},\frac{5}{8}$; $\frac{5}{8},\frac{1}{8},\frac{3}{8}$.	hkl: $h=2n+1$, $k=2n+1$, $l=4n+2$ or $h=4n$, $k=4n$, $l=4n$; h,k,l permutable
16	a	$\bar{3}$	0,0,0; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$; $\frac{3}{4},\frac{1}{4},\frac{3}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$.	hkl: $h,k,(l)=2n$; $h+k+l=4n$

Notes on Symbols used in 4. Space-group Symmetry

It is important to emphasise that no special (official) significance should be attached to the conventions adopted in this section for the space-group setting of axes. Other possible space-group symbols are given in section 6. If these are used, appropriate changes must be made in diagrams, co-ordinates and conditions for reflection as listed in sections 4.2 and 4.3, and in the structure factor and electron density formula as listed in sections 4.6 and 4.7.

If the unit-cell vectors are chosen and named **a**, **b**, **c** in any particular order[1] *before* the diffraction symbol (section 4.1) is determined, it may be found that the extinctions do not correspond to any of those given in the following section 4.4. This is because, in formulating the diffraction symbols given there, certain arbitrary conventions have been followed. Thus if, in the orthorhombic system, one glide plane only is found, with a translation parallel to an axis, this has been called $P\ c\ .\ .$; but it could be written in the 6 ways given below, the corresponding space-group symbols being shown in parentheses:

$P\ b\ .\ .$ ($Pb2_1m$, $Pbm2$, $Pbmm$); $P\ c\ .\ .$ ($Pcm2_1$, $Pc2m$, $Pcmm$);

$P\ .\ a\ .$ ($P2_1am$, $Pma2$, $Pmam$); $P\ .\ c\ .$ ($Pmc2_1$, $P2cm$, $Pmcm$);

$P\ .\ .\ a$ ($P2_1ma$, $Pm2a$, $Pmma$); $P\ .\ .\ b$ ($Pm2_1b$, $P2mb$, $Pmmb$).

These correspond, of course, to the various orientations given in section 6.2.1 of the three space groups whose "standard" settings are $Pmc2_1$, $Pma2$ and $Pmma$. It is an easy matter to construct a complete list of all possible diffraction symbols in all possible settings of the unit cell by making use of Table 6.2.1, and by writing a dot in place of all symbols whose nature is not directly observable by diffraction methods (including those which are the consequence of lattice conditions or of other extinction effects). Such a table should be made if any real difficulty occurs in applying Table 4.4.3 as it stands. The example given on p. 549 shows, however, that Table 6.2.1 can easily be used directly for the determination of possible space groups from any diffraction symbol.

Note on Symmetry Determination outside the Friedel Rule

Friedel's Rule states that in general it is impossible, by X-ray diffraction, to determine whether a crystal is centrosymmetric or not. An exception must be made if some atoms in the crystal show sufficient anomalous scattering effect (phase shift) for the particular X-radiation used; in these circumstances two reflections are required to be equal in intensity only if they are related by a symmetry operation of the point group (pp. 26–27). Thus all point groups may be distinguished, and the orientation of the symmetry elements is revealed in those cases where alternate settings occur in the Laue class (i.e. $mm2$, $m2m$, $2mm$; $\bar{4}2m$, $\bar{4}m2$; $\bar{6}m2$, $\bar{6}2m$). The effect fails to distinguish point groups in each Laue class if all atoms have the same phase shift, regardless of its magnitude. Anomalous scattering has no effect on the rules for absent reflections.

This question is discussed in the following papers, and reference can be made to section 5.3.

Peterson, S. W. 1955, *Nature*, London, **176**, 395.
Peerdeman, A. F., and Bijvoet, J. N. *Acta Cryst.*, 1956, **9**, 1012.
Okaya, Y., and Pepinsky, R. in *Computing Methods and the Phase Problem in X-ray Analysis* (pp. 273–299), 1961 (Pergamon Press, New York), ed. Pepinsky, Robertson, and Speakman.
Zachariasen, W. H. *Acta Cryst.*, 1965, **18**, 714.
Coster, D., Knol, K. S., and Prins, J. 1930, *Z. f. Physik*, **63**, 345.
James, R. W. 1948, *Optical Principles of the Diffraction of X-rays*, p. 33 (G. Bell & Sons, London).
Peerdeman, A. F., van Bommel, A. J., and Bijvoet, J. M. 1951, "Determination of Absolute Configuration of Optically Active Compounds by means of X-rays," *Koninklijke Nederlandse Akademie van Wetenschappen, Proceedings*, Series B, **54**, 3; *Acta Crystallographica* (in preparation).

[1] No rules are given in this Volume for the naming of the unit-cell vectors in any particular order of length.

4.4. Diffraction Symbols of the Space Groups

Section 4.1 contains a discussion of the information that is obtainable about the lattice type and the symmetry elements of space groups from the observation of systematically-absent reflections. This information is most conveniently presented in the form of symbols, and these are tabulated in the present section. It should be noted that this section contains only information that can be obtained from possible reflections and from Laue symmetry, that is information lying within the Friedel rule which states that, in general, it is not possible, by means of X-ray diffraction data alone, to decide whether a particular crystal is centric or not. For a brief discussion of methods of obtaining information outside the Friedel rule, reference can be made to section 5.3. (See also Note on p. 346).

Two-dimensional Diffraction Symbols

In two-dimensions there are 10 point groups in 6 Laue classes (p. 30). For simplicity of tabulation here we can list the extinction symbols at the left side, an extinction symbol being a diffraction symbol without the Laue class part. There are 4 such extinction symbols; the first occurs in all 6 Laue classes; the second occurs in two Laue classes; the third and fourth each occur in only one Laue class; hence there are in all 10 diffraction symbols (p. 52), while 4 space groups (shown in bold type) are uniquely distinguishable.

TABLE 4.4.1. **Extinction Symbols for the 17 Two-dimensional Space Groups**

Extinction symbol	System	Oblique		Rectangular		Square		Hexagonal			
	Laue symmetry	2		2*mm*		4	4*mm*	6		6*mm*	
	Point group	1	2	*m*	2*mm*	4	4*mm*	3	6	3*m*	6*mm*
p . . .		*p*1	*p*2	*p*1*m*1	*p*2*mm*	***p*4**	***p*4*mm***	*p*3	*p*6	(*p*3*m*1 / *p*31*m*)	*p*6*mm*
p . *g* .		—	—	*p*1*g*1	*p*2*gm* ≡*p*2*mg*	—	***p*4*gm***	—	—	—	—
p . *g g*		—	—	—	***p*2*gg***	—	—	—	—	—	—
c . . .		—	—	*c*1*m*1	*c*2*mm*	—	—	—	—	—	—

NOTE. The symbol *p* . *g* . as applied to a rectangular space group implies the presence of one glide-line; as applied to the square space group it implies the presence of two equivalent glide-lines normal to each other.

Three-dimensional Diffractional Symbols

The diffraction symbol, as defined by Buerger (1942) [2] and (1969) [4] is a statement of the symmetry information that can be obtained by X-ray diffraction. It consists of the Laue-symmetry symbol followed by an extinction symbol, which is identical with the aspect symbol of Donnay and Harker (1940) [1]; this extinction symbol gives the lattice type and explicitly expresses the glide planes and screw axes that are not inherent in the lattice itself. Whereas the number of different extinction symbols is 97, distributed among the crystal systems as shown in Table 4.4.2, the number of diffraction symbols is 120 if the Laue symmetry is not oriented. Among these 120 there are 6 diffraction symbols for the Laue symmetry $\bar{3}$m, but X-ray diffraction enables a distinction to be made between $\bar{3}$ml and $\bar{3}$lm, with the result that each of two of the 6 are split into two, namely:

$$\bar{3}\mathrm{mP}\ldots\begin{cases}\bar{3}\mathrm{mlP}\ldots\\ \bar{3}\mathrm{lmP}\ldots\end{cases}\text{ and }\bar{3}\mathrm{mP3_1}\ldots\begin{cases}\bar{3}\mathrm{mlP3_1}\ldots\\ \bar{3}\mathrm{lmP3_1}\ldots\end{cases}$$

Since each of the other 4 correspond to both orientations of the Laue symmetry, the number of diffraction symbols is now 122, these being distributed among the Laue classes as shown in Table 4.4.2. Finally it can be observed that 50 space groups are uniquely identifiable, so that only 72 diffraction symbols are actually required. The set of condensed symbols proposed by Donnay and Kennard (1964) [3] is given in Table 4.4.3 together with Buerger's diffraction symbols. This table is now arranged in separate Laue classes unlike that in the previous printings of this volume.

TABLE 4.4.2. **Distribution of Space Groups and Diffraction Symbols among the Laue Classes**

Number of	$\bar{1}$	$2/m$	mmm	$4/m$	$4/mmm$	$\bar{3}$	$\bar{3}m1$	$\bar{3}1m$	$6/m$	$6/mmm$	$m3$	$m3m$	Total
Space groups	2	13	59	14	54	6	12	7	9	18	12	24	230
Donnay-Harker aspects	1	6	33	—	31	—	—	—	—	9	—	17	97
Buerger diffraction symbols	1	6	33	8	29	3	5	3	4	7	8	15	122
Donnay-Kennard symbols	1	5	18	4	14	3	5	3	4	6	3	6	72
Uniquely identifiable space groups	0	1	15	4	15	0	0	0	0	1	5	9	50

In practice, in order to determine the space group of a crystal, the following procedure may be used.

1. The cell dimensions are measured and the Laue symmetry is determined (and oriented in the case of $\bar{3}$m). The cell is chosen and set in accordance with conventions appropriate to the crystal system.
2. A sufficient number of reflections are indexed and tabulated. The lattice mode is determined from the general $(h\ k\ l)$ reflection, by means of Table 4.1.8. The systematic extinctions of the special reflections are then established and the resulting symmetry elements are inferred from them with the help of Table 4.1.9. The extinction symbol can thus be written down.
3. By combining the information obtained in 1 (Laue class) and in 2 (extinction symbol), the diffraction symbol is immediately obtained and can be looked up in the appropriate section of Table 4.4.3, where it appears in the first column. Alternately, if the space group is not uniquely determined by the extinction criteria, the condensed symbol can be found in the last column. Between these two are given the symbols of the possible space groups.

In some special cases where X-ray methods leave the choice of point groups open, it may be possible to make a decision by the introduction of chemical considerations. For instance, if experiment shows that there are 2 molecules of formula $A_\alpha B_\beta$ in a unit cell of space group either $P2_1$ or $P2_1/m$, and if the molecule $A_\alpha B_\beta$ cannot possibly have either mirror- or centro-symmetry, then the space group must be $P2_1$.

When the actual point group of the crystal is known by means of methods other than X-ray methods (see section 3.8), the number of space groups which cannot be uniquely determined becomes small. These comprise 22 space groups in 11 enantiomorphous pairs plus 4 in 2 special pairs. Of the remaining 204 space groups in the main tables, 12 have been grouped between parentheses in pairs belonging to the same point group (3 pairs in the orthorhombic system, 2 pairs in the Laue class $4/mmm$ and 1 pair in the Laue class $6/mmm$). In these cases the actual orientation of the point group relative to the lattice must be known before the two members of each pair can be distinguished.

Statistical and other methods referred to in section 5.3 allow further space groups to be distinguished in favourable cases, and a complete resolution may sometimes be possible from structural considerations.

It is sometimes possible from morphology, etching or piezoelectric tests to distinguish between the two ends of a polar axis without being able to determine the complete symmetry. J. ter Berg and F. M. Jaeger (Proc. Roy. Acad. Sci. Amsterdam, 1937, 40, 406) have pointed out that if crystals belonging to any of the 6 enantiomorphous pairs of space groups

$$\begin{array}{cccccc} P3_1 & P4_1 & P6_1 & P6_2 & P3_121 & P3_112 \\ P3_2 & P4_3 & P6_5 & P6_4 & P3_221 & P3_212 \end{array}$$

(1) *Naturaliste Canadien*, **67**, 33–69 (1940).
(2) *X-ray Crystallography* (John Wiley and Sons Inc., New York, 1942), Table 34, pp. 511–16. Note, however, a numerical error in that the number of 'isometric' diffraction symbols should be 23 and the total 120, and not 24 and 121 respectively, as given on p. 511.
(3) *Acta Cryst.* **17**, 1337–1340 (1964)
(4) Buerger, M. J. "Diffraction Symbols," Chapter 3 of *Physics of the Solid State*, edited by S. Balakrishna. (Academic Press, London, 1969) pp. 27–42.

can be so orientated that the X-ray beam travels in a known sense along the polar axis (the principal axis in the first four pairs; any diad axis in the last two pairs, point group 32), then crystals of one hand can be distinguished from those of the other by means of Laue photographs. This is also true for moving-film photographs, care being taken in either case that the photographs being compared are viewed either both towards or both away from the X-ray source.

Conversely if, from morphology or optical activity, the hand of crystals belonging to one of these 6 pairs is known, Laue or moving-film photographs would enable the polar axes of the crystals to be orientated in known sense relative to each other. The method does not give the absolute configuration of the structure of such crystals.

TABLE 4.4.3 **4.4. Diffraction Symbols of the Space Groups**

TRICLINIC. Laue Class $\bar{1}$

Diffraction symbol	Point groups		Condensed symbol
	1	$\bar{1}$	
$\bar{1}P$	$P1$	$P\bar{1}$	$\bar{1}P*$

ORTHORHOMBIC. Laue Class *mmm*

Diffraction symbol	Point groups (and settings)						Condensed symbol
	222	2mm	or	m2m	or	mm2	mmm	
$mmmP$ — — —	$P222$	$P2mm=Pmm2$		$Pm2m=Pmm2$		$Pmm2$	$Pmmm$	$P***$
$mmmP$ — — 2_1	$P222_1$							.....
$mmmP$ 2_1 2_1 —	$P2_12_12$							.....
$mmmP$ 2_1 2_1 2_1	$P2_12_12_1$							.....
$mmmP$ c — —				$Pc2m=Pma2$		$Pcm2_1=Pmc2_1$	$Pcmm=Pmma$	$Pc**$
$mmmP$ n — —				$Pn2_1m=Pmn2_1$		$Pnm2_1=Pmn2_1$	$Pnmm=Pmmn$	$Pn**$
$mmmP$ c c —						$Pcc2$	$Pccm$	$Pcc*$
$mmmP$ c a —						$Pca2_1$	$Pcam=Pbcm$	$Pca*$
$mmmP$ b a —						$Pba2$	$Pbam$	$Pba*$
$mmmP$ n c —						$Pnc2$	$Pncm=Pmna$	$Pnc*$
$mmmP$ n a —						$Pna2_1$	$Pnam=Pnma$	$Pna*$
$mmmP$ n n —						$Pnn2$	$Pnnm$	$Pnn*$
$mmmP$ c c a							$Pcca$	.....
$mmmP$ b c a							$Pbca$	.....
$mmmP$ c c n							$Pccn$	.....
$mmmP$ b a n							$Pban$	.....
$mmmP$ b c n							$Pncn$	.....
$mmmP$ n n a							$Pnna$	.....
$mmmP$ n n n							$Pnnn$	.....
$mmmC$ — — —	$C222$	$C2mm=Amm2$		$Cm2m=Amm2$		$Cmm2$	$Cmmm$	$C***$
$mmmC$ — — 2_1	$C222_1$							.....
$mmmC$ — c —		$C2cm=Ama2$				$Cmc2_1$	$Cmcm$	$C*c*$
$mmmC$ — — a		$C2ma=Abm2$		$Cm2a=Abm2$			$Cmma$	$C**a$
$mmmC$ — c a		$C2ca=Aba2$					$Cmca$	$C*ca$
$mmmC$ c c —						$Ccc2$	$Cccm$	$Ccc*$
$mmmC$ c c a							$Ccca$	.....
$mmmI$ — — —	$\begin{bmatrix} I222 \\ I2_12_12_1 \end{bmatrix}$	$I2mm=Imm2$		$Im2m=Imm2$		$Imm2$	$Immm$	$I***$
$mmmI$ — a —		$I2am=Ima2$				$Ima2$	$Imam=Imma$	$I*a*$
$mmmI$ b a —						$Iba2$	$Ibam$	$Iba*$
$mmmI$ b c a							$Ibca$	.....
$mmmF$ — — —	$F222$	$F2mm=Fmm2$		$Fm2m=Fmm2$		$Fmm2$	$Fmmm$	$F***$
$mmmF$ d d —						$Fdd2$		.....
$mmmF$ d d d							$Fddd$	.....

TABLE 4.4.3 (*continued*)

MONOCLINIC. Laue Class $2/m$

	Diffraction symbol	Point groups			Condensed symbol
		2	m	$2/m$	
First setting	$2/mP$ — — —	$P2$	Pm	$P2/m$	$P*/*$
	$2/mP$ — — b		Pb	$P2/b$	$P*/b$
	$2/mP$ — — 2_1	$P2_1$		$P2_1/m$	$P2_1/*$
	$2/mP$ — — $2_1/b$			$P2_1/b$	.....
	$2/mB$ — — —	$B2$	Bm	$B2/m$	$B*/*$
	$2/mB$ — — b		Bb	$B2/b$	$B*/b$
Second setting	$2/mP$ — —	$P2$	Pm	$P2/m$	$P*/*$
	$2/mP$ — c		Pc	$P2/c$	$P*/c$
	$2/mP$ — 2_1	$P2_1$		$P2_1/m$	$P2_1/*$
	$2/mP$ — $2_1/c$			$P2_1/c$	.....
	$2/mC$ — —	$C2$	Cm	$C2/m$	$C*/*$
	$2/mC$ — c		Cc	$C2/c$	$C*/c$

TETRAGONAL. Laue Class $4/mmm$

Diffraction symbol	Point groups					Condensed symbol
	422	$4mm$	$\bar{4}2m$ or	$\bar{4}m2$	$4/mmm$	
$4/mmmP$ — — —	$P422$	$P4mm$	$P42m$	$P\bar{4}m2$	$P4/mmm$	$P4/***$
$4/mmmP\ 4_1$ — —	$\{P4_122, P4_322\}$					$P4_{1,3}22$
$4/mmmP\ 4_2$ — —	$P4_222$					.....
$4/mmmP$ — 2_1 —	$P42_12$		$P\bar{4}2_1m$			$P42_1*$
$4/mmmP\ 4_1\ 2_1$ —	$\{P4_12_12, P4_32_12\}$					$P4_{1,3}2_12$
$4/mmmP\ 4_2\ 2_1$ —	$P4_22_12$					.....
$4/mmmP\ n$ — —					$P4/nmm$	.....
$4/mmmP$ — — c		$P4_2mc$	$P\bar{4}2c$		$P4_2/mmc$	$P4/**c$
$4/mmmP$ — $2_1\ c$			$P\bar{4}2_1c$			.....
$4/mmmP$ — b —		$P4bm$	$P\bar{4}b2$		$P4/mbm$	$P4/*b*$
$4/mmmP$ — $b\ c$		$P4_2bc$			$P4_2/mbc$	$P4/*bc$
$4/mmmP$ — c —		$P4_2cm$		$P\bar{4}c2$	$P4_2/mcm$	$P4/*c*$
$4/mmmP$ — $c\ c$		$P4cc$			$P4/mcc$	$P4/*cc$
$4/mmmP$ — n —		$P4_2nm$	$P\bar{4}n2$		$P4_2/mnm$	$P4/*n*$
$4/mmmP$ — $n\ c$		$P4nc$			$P4/mnc$	$P4/*nc$
$4/mmmP\ n$ — c					$P4_2/nmc$	.....
$4/mmmP\ n\ b$ —					$P4/nbm$	.....
$4/mmmP\ n\ b\ c$					$P4_2/nbc$	.....
$4/mmmP\ n\ c$ —					$P4/ncm$	.....
$4/mmmP\ n\ c\ c$					$P4/ncc$	.....
$4/mmmP\ n\ n$ —					$P4_2/nnm$	.....
$4/mmmP\ n\ n\ c$					$P4/nnc$	.....
$4/mmmI$ — — —	$I422$	$I4mm$	$I\bar{4}2m$	$I\bar{4}m2$	$I4/mmm$	$I4/***$
$4/mmmI\ 4_1$ — —	$I4_122$					.....
$4/mmmI$ — c —		$I4cm$		$I\bar{4}c2$	$I4/mcm$	$I4/*c*$
$4/mmmI$ — — d		$I4_1md$	$I\bar{4}2d$			$I4*d$
$4/mmmI$ — $c\ d$		$I4_1cd$				.....
$4/mmmI\ a$ — d					$I4_1/amd$	.....
$4/mmmI\ a\ c\ d$					$I4_1/acd$	.....

TABLE 4.4.3 (*continued*)

TETRAGONAL. Laue Class $4/m$

Diffraction symbol	Point groups			Condensed symbol
	4	$\bar{4}$	$4/m$	
$4/mP$ —	$P4$	$P\bar{4}$	$P4/m$	$P4/*$
$4/mP\ 4_1$	$\{P4_1, P4_3\}$			$P4_{1,3}$
$4/mP\ 4_2$	$P4_2$		$P4_2/m$	$P4_2/*$
$4/mP\ n$			$P4/n$	.....
$4/mP\ 4_2/n$			$P4_2/n$	.....
$4/mI$ —	$I4$	$I\bar{4}$	$I4/m$	$I4/*$
$4/mI\ 4_1$	$I4_1$			.....
$4/mI\ 4_1/a$			$I4_1/a$	.....

TRIGONAL. Laue Class $\bar{3}$

Diffraction symbol	Point groups		Condensed symbol
	3	$\bar{3}$	
$\bar{3}P$ —	$P3$	$P\bar{3}$	$\bar{3}P*$
$\bar{3}P\ 3_1$	$\{P3_1, P3_2\}$		$P3_{1,2}$
$\bar{3}R$ —	$R3$	$R\bar{3}$	$R*$

TRIGONAL. Laue Class $\bar{3}m1$ or $\bar{3}1m$

Diffraction symbol	Point groups (and settings)						Condensed symbol
	321	or 312	$3m1$	or $31m$	$\bar{3}m1$	or $\bar{3}1m$	
$\bar{3}m1P$ — — —	$P321$		$P3m1$		$P\bar{3}m1$		$P3*1$
$\bar{3}1mP$ — — —		$P312$		$P31m$		$P\bar{3}1m$	$P31*$
$\bar{3}m1P\ 3_1$ — —	$\{P3_121, P3_221\}$						$P3_{1,2}21$
$\bar{3}1mP\ 3_1$ — —		$\{P3_112, P3_212\}$					$P3_{1,2}12$
$\bar{3}m1P$ — c —			$P3c1$		$P\bar{3}c1$		$\bar{3}mP*c1$
$\bar{3}1mP$ — — c				$P31c$		$P\bar{3}1c$	$\bar{3}mP*1c$
$\bar{3}m1R$ — —	$R32$		$R3m$		$R\bar{3}m$		$R**$
$\bar{3}m1R$ — c			$R3c$		$R\bar{3}c$		$R*c$

HEXAGONAL. Laue Class $6/m$

Diffraction symbol	Point groups			Condensed symbol
	6	$\bar{6}$	$6/m$	
$6/mP$ —	$P6$	$P\bar{6}$	$P6/m$	$P6/*$
$6/mP\ 6_1$	$\{P6_1, P6_5\}$			$P6_{1,5}$
$6/mP\ 6_2$	$\{P6_2, P6_4\}$			$P6_{2,4}$
$6/mP\ 6_3$	$P6_3$		$P6_3/m$	$P6_3/*$

TABLE 4.4.3 (*continued*) (See notes on pp. 350–1)

HEXAGONAL. Laue Class $6/mmm$

Diffraction symbol	Point groups					Condensed symbol
	622	$6mm$	$\bar{6}m2$	or $\bar{6}2m$	$6/mmm$	
$6/mmmP$ — — —	$P622$	$P6mm$	$P\bar{6}m2$	$P\bar{6}2m$	$P6/mmm$	$P6/***$
$6/mmmP\ 6_1$ — —	$\{P6_122, P6_522\}$					$P6_{1,5}22$
$6/mmmP\ 6_2$ — —	$\{P6_222, P6_422\}$					$P6_{2,4}22$
$6/mmmP\ 6_3$ — —	$P6_322$					.....
$6/mmmP$ — c —		$P6_3cm$	$P\bar{6}c2$		$P6_3/mcm$	$P6/*c*$
$6/mmmP$ — — c		$P6_3mc$		$P\bar{6}2c$	$P6_3/mmc$	$P6/**c$
$6/mmmP$ — c c		$P6cc$			$P6/mcc$	$P6/*cc$

CUBIC. Laue Class $m3$

Diffraction symbol	Point groups		Condensed symbol
	23	$m3$	
$m3P$ — —	$P23$	$Pm3$	$P*3$
$m3P\ 2_1$ —	$P2_13$		.....
$m3P\ n$ —		$Pn3$	.....
$m3P\ a$ —		$Pa3$	.....
$m3I$ — —	$[I23, I2_13]$	$Im3$	$I*3$
$m3I\ a$ —		$Ia3$	.....
$m3F$ — —	$F23$	$Fm3$	$F*3$
$m3F\ d$ —		$Fd3$	.....

CUBIC. Laue Class $m3m$

Diffraction symbol	Point groups			Condensed symbol
	432	$\bar{4}3m$	$m3m$	
$m3mP$ — — —	$P432$	$P\bar{4}3m$	$Pm3m$	$P*3*$
$m3mP\ 4_1$ — —	$\{P4_132, P4_332\}$			$P4_{1,3}32$
$m3mP\ 4_2$ — —	$P4_232$			.....
$m3mP\ n$ — —			$Pn3m$	.....
$m3mP$ — — n		$P\bar{4}3n$	$Pm3n$	$P*3n$
$m3mP\ n$ — n			$Pn3n$	.....
$m3mI$ — — —	$I432$	$I\bar{4}3m$	$Im3m$	$I*3*$
$m3mI\ 4_1$ — —	$I4_132$			.....
$m3mI$ — — d		$I\bar{4}3d$		.....
$m3mI\ a$ — d			$Ia3d$	.....
$m3mF$ — — —	$F432$	$F\bar{4}3m$	$Fm3m$	$F*3*$
$m3mF\ 4_1$ — —	$F4_132$			.....
$m3mF\ d$ — —			$Fd3m$	.....
$m3mF$ — — c		$F\bar{4}3c$	$Fm3c$	$F*3c$
$m3mF\ d$ — c			$Fd3c$	.....

4.5. Introduction to Structure Factor Tables

In every expression for the intensity of the beam of X-rays diffracted in any given direction from a crystal of any shape or size a factor F occurs, the *structure factor*, which is a measure of the composite wave due to the combined scattering of all the atoms in the unit cell in the given direction. It depends

(1) on the nature of the scattering material,

(2) on the arrangement of the scattering material,

(3) on the direction of scattering.

1. The scattering power of a single atom is dependent on its electronic structure and on the direction of scattering (which determines $(\sin\theta)/\lambda$). It is independent of the space group to which the symmetry of the crystal as a whole conforms, except in so far as the electronic structure is influenced by the arrangement of neighbouring atoms. It is also modified in the neighbourhood of an X-ray absorption edge. Following W. L. Bragg and others, we call this *atomic scattering factor* f_0, and make it a pure number by taking as unit the scattering power of a single electron under corresponding conditions. Tables of values of f_0, together with references to original papers giving methods of computation or of observation, will be found in a succeeding volume of these *International Tables*. In general f_0 will be modified by thermal vibration to a value $f = f_0 e^{-B}$, where B is dependent on $(\sin\theta)/\lambda$ and on temperature T, as well as on the nature of the atom and the forces to surrounding atoms.

2. The arrangement of the scattering material determines the space group. If one asymmetric scattering unit in the cell has co-ordinates x_r, y_r, z_r (expressed, for convenience, as fractions of the crystallographic unit axes a, b, c), then the co-ordinates of a definite number of similar units are rigidly fixed by the crystal symmetry. For example, in the unit cell of a crystal belonging to the $P2_12_12_1$ space group there may be different sets of scattering units A, B, C, etc. These must lie in the positions

$$\begin{array}{llllll} \text{A} & x_1,y_1,z_1; & \frac{1}{2}-x_1,\bar{y}_1,\frac{1}{2}+z_1; & \frac{1}{2}+x_1,\frac{1}{2}-y_1,\bar{z}_1; & \bar{x}_1,\frac{1}{2}+y_1,\frac{1}{2}-z_1; \\ \text{B} & x_2,y_2,z_2; & \frac{1}{2}-x_2,\bar{y}_2,\frac{1}{2}+z_2; & \frac{1}{2}+x_2,\frac{1}{2}-y_2,\bar{z}_2; & \bar{x}_2,\frac{1}{2}+y_2,\frac{1}{2}-z_2; \\ \text{C} & x_3,y_3,z_3; & \frac{1}{2}-x_3,\bar{y}_3,\frac{1}{2}+z_3; & \frac{1}{2}+x_3,\frac{1}{2}-y_3,\bar{z}_3; & \bar{x}_3,\frac{1}{2}+y_3,\frac{1}{2}-z_3; \end{array}$$

and so on.

The co-ordinates of the general positions in which the asymmetric scattering units lie (four in the above case) are known as the *co-ordinates of equivalent positions* of point symmetry 1, or sometimes as *general co-ordinates of equivalent positions*. They will vary according to the origin adopted. The agreed origins have always been taken on symmetry elements, if possible. The co-ordinates of equivalent positions were originally tabulated by R. W. G. Wyckoff, but the origins, crystallographic-axis orientations and therefore the co-ordinates, used in the following Tables are not necessarily the same as those adopted by Wyckoff and other writers.

3. The direction in which scattering occurs is defined by the indices (hkl) of the scattering set of planes, since for a given crystal each set of planes (hkl) corresponds to a definite value of $(\sin\theta)/\lambda$, as governed by the Bragg relation. $f_r(hkl)$ means f for the atom r and the planes (hkl).

The structure factor $F(hkl)$ may be expressed in exponential form by the formula

$$F(hkl) = \sum_r f_r(hkl) e^{2\pi i\,(hx_r + ky_r + lz_r)} \quad \text{I}$$

and it is therefore a complex quantity, introducing both the absolute value and the phase of the scattered wave. By taking the *positive* sign of the exponential function there is a phase *advance* with respect to the origin.

The electron density ρ at any point X, Y, Z in the unit cell can also be expressed as an exponential function.

$$\rho(XYZ) = \frac{1}{V_c} \sum_{-\infty}^{\infty} h \sum_{-\infty}^{\infty} k \sum_{-\infty}^{\infty} l\, F(hkl) e^{-2\pi i\,(hX + kY + lZ)} \quad \text{II}$$

where V_c is the volume of the unit cell. The co-ordinates X, Y, Z, which also represent fractions of the crystallographic axes, must not be confused with x_r, y_r, z_r, the co-ordinates of a scattering unit.

X, Y, Z will usually be taken as successive integral multiples of a sub-unit of the axial lengths, say $a/60$ or $a/120$, $b/30$, etc.

The exponential terms in the expressions for F and ρ are opposite in sign because these quantities are Fourier transforms of each other. It would have been equally correct to use the expressions $F=\sum f\,.\,e^{-i\phi}$ and $\rho=\frac{1}{V}\sum F\,.\,e^{i\theta}$; this has been done by some writers and leads to the same final results as are given here. It simply means that the scattered wave has a phase-lag relative to the origin, instead of a phase-*advance* as in I. It is *not* correct to use the *same* signs for the exponential functions in both expressions.

Friedel's law, which only breaks down in the neighbourhood of an absorption edge (*The Crystalline State*, vol. I, p. 94 (1933); vol. II, p. 33 (1948)) states that $F(hkl)$ and $F(\bar{h}\bar{k}\bar{l})$ are conjugate, the moduli $|F(hkl)|$ and $|F(\bar{h}\bar{k}\bar{l})|$ being, in general, indistinguishable.

The value of $|F(hkl)|$, which is the amplitude of the scattered wave, can be determined experimentally, but for the purpose of a Fourier analysis the value of the phase angle $\alpha(hkl)$, relative to the agreed origin, must also be known as accurately as possible. This quantity, $\alpha(hkl)$, which also depends on the nature and arrangement of the scattering material and on the direction of scattering, cannot be directly determined by experiment except in certain limited circumstances. It can, however, be calculated for any given structure, as follows:

Let $F(hkl)=A'+iB'$; $F(\bar{h}\bar{k}\bar{l})=A'-iB'$; $2\pi(hX+kY+lZ)=\theta$.

$$\text{Then}\quad \rho(XYZ)=\frac{1}{2V_c}\sum_{-\infty}^{\infty}h\sum_{-\infty}^{\infty}k\sum_{-\infty}^{\infty}l\,\{[A'+iB']e^{-i\theta}+[A'-iB']e^{i\theta}\}$$

$$=\frac{1}{V_c}\sum_{-\infty}^{\infty}h\sum_{-\infty}^{\infty}k\sum_{-\infty}^{\infty}l\left\{A'\frac{e^{i\theta}+e^{-i\theta}}{2}-iB'\frac{e^{i\theta}-e^{-i\theta}}{2}\right\}$$

$$=\frac{1}{V_c}\sum_{-\infty}^{\infty}h\sum_{-\infty}^{\infty}k\sum_{-\infty}^{\infty}l\,(A'\cos\theta+B'\sin\theta)\quad\text{IIa}$$

Hence the electron density is everywhere real; and

$$\rho(-X,-Y,-Z)=\frac{1}{V_c}\sum_{-\infty}^{\infty}h\sum_{-\infty}^{\infty}k\sum_{-\infty}^{\infty}l\,(A'\cos\theta-B'\sin\theta)\quad\text{IIb}$$

which means that the electron densities at (X,Y,Z) and at $(-X,-Y,-Z)$ will differ unless B' is zero.

We can write

$$A'=|F(hkl)|\cos\alpha(hkl)$$
$$B'=|F(hkl)|\sin\alpha(hkl)$$

$$\text{Then}\quad \rho(XYZ)=\frac{1}{V_c}\sum_{-\infty}^{\infty}h\sum_{-\infty}^{\infty}k\sum_{-\infty}^{\infty}l\,|F(hkl)|\{\cos\theta\cos\alpha(hkl)+\sin\theta\sin\alpha(hkl)\}$$

$$=\frac{1}{V_c}\sum_{-\infty}^{\infty}h\cdot\sum_{-\infty}^{\infty}k\sum_{-\infty}^{\infty}l\,|F(hkl)|\cos[\theta-\alpha(hkl)]\quad\text{III}$$

where $|F(hkl)|^2=A'^2+B'^2$
and $\alpha(hkl)=\tan^{-1}(B'/A')$

Summing over all the different kinds of atoms in a unit cell, we have

$$A'=\sum\sum f_r\cos 2\pi(hx_r+ky_r+lz_r)$$
$$B'=\sum\sum f_r\sin 2\pi(hx_r+ky_r+lz_r)$$

the summations being taken over all the different kinds of atoms and all the different equivalent positions of those atoms in the unit cell. Here f_r is the atomic scattering factor, corrected for thermal vibration, appropriate to the set of planes (hkl), for any one of the scattering units in the unit cell, and x_r, y_r, z_r are the co-ordinates of *any one* of the equivalent positions at which that particular scattering unit is placed.

Now let

$$\left.\begin{aligned}A&=\sum\cos 2\pi(hx+ky+lz)\\B&=\sum\sin 2\pi(hx+ky+lz)\end{aligned}\right\}\quad\text{IV}$$

the summation extending over all the equivalent positions in a unit cell. Then

$$|F(hkl)| = \left\{\left[\sum_r f_r A_r\right]^2 + \left[\sum_r f_r B_r\right]^2\right\}^{\frac{1}{2}} \quad \text{V}$$

$$\alpha(hkl) = \tan^{-1}\left\{\left[\sum_r f_r B_r\right] \Big/ \left[\sum_r f_r A_r\right]\right\} \quad \text{VI}$$

the summations in V and VI being taken over all the different kinds of scattering units (atoms or ions, or sub-multiples of these) in the unit cell. Thus, in general:

$$\alpha(hkl) = \tan^{-1}\{[f_1B_1+f_2B_2+f_3B_3 \ldots f_rB_r \ldots]/[f_1A_1+f_2A_2+f_3A_3 \ldots f_rA_r \ldots]\}$$

The value of $\alpha(hkl)$ will depend not only on the values but also on the *signs* of $\sum fB$ and of $\sum fA$.

$\sum fB$ positive, $\sum fA$ positive: $\frac{\pi}{2} > \alpha(hkl) > 0$

$\sum fB$ positive, $\sum fA$ negative: $\pi > \alpha(hkl) > \frac{\pi}{2}$

$\sum fB$ negative, $\sum fA$ negative: $\frac{3\pi}{2} > \alpha(hkl) > \pi$

$\sum fB$ negative, $\sum fA$ positive: $2\pi > \alpha(hkl) > \frac{3\pi}{2}$

A and B are characteristic of the space group, being dependent entirely on the co-ordinates of equivalent positions. One object of the following tables is to give the simplest forms of A and B, for purposes of computation. An example will illustrate the process of simplification: detailed examples are given later (pp. 361, 364).

In the space group $P222$ the co-ordinates of equivalent positions, four in number, relative to an origin at the 222 symmetry position, are $|x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z|$.

$A = \sum \cos 2\pi(hx+ky+lz)$

$= \cos 2\pi(hx+ky+lz) + \cos 2\pi(hx-ky-lz) + \cos 2\pi(-hx+ky-lz) + \cos 2\pi(-hx-ky+lz)$

$= 2\cos 2\pi lz[\cos 2\pi(hx+ky) + \cos 2\pi(hx-ky)]$

$= 4\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz$

Similarly, $B = -4 \sin 2\pi hx \sin 2\pi ky \sin 2\pi lz$.

In the space group $Pba2$ the co-ordinates are $|x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}+y,z;\ \frac{1}{2}+x,\frac{1}{2}-y,z|$.

$$A = \cos 2\pi(hx+ky+lz) + \cos 2\pi(-hx-ky+lz) + \cos 2\pi\left(-hx+ky+lz+\frac{h+k}{2}\right) + \cos 2\pi\left(hx-ky+lz+\frac{h+k}{2}\right)$$

$$= 2\left[\cos 2\pi(hx+ky) + \cos 2\pi\left(hx-ky-\frac{h+k}{2}\right)\right]\cos 2\pi lz$$

$$A = 4\cos 2\pi\left(hx-\frac{h+k}{4}\right)\cos 2\pi\left(ky+\frac{h+k}{4}\right)\cos 2\pi lz$$

$$B = 4\cos 2\pi\left(hx-\frac{h+k}{4}\right)\cos 2\pi\left(ky+\frac{h+k}{4}\right)\sin 2\pi lz$$

Note that since h and k are integers, $\cos 2\pi\left(\phi+\frac{h+k}{2}\right) = \cos 2\pi\left(\phi-\frac{h+k}{2}\right)$.

It is essential to realise that the final form of A and B depends on the choice of origin and co-ordinate system, because these in turn will decide the co-ordinates of equivalent positions. If another origin is taken, or the co-ordinate system differently orientated, the co-ordinates of equivalent positions should be redetermined and the simplified forms of A and B obtained from first principles. Any attempts at short cuts are likely to be regretted. On the other hand, the co-ordinates themselves contain all the information required to determine what origin and co-ordinate axes have been assumed and what symmetry elements are present. For instance, the co-ordinates $|x,y,z;\ \bar{x},\bar{y},\bar{z};\ x,\frac{1}{2}-y,\frac{1}{2}+z;\ \bar{x},\frac{1}{2}+y,\frac{1}{2}-z|$ tell us that the origin is at a centre of symmetry, and that there is a diad screw-axis parallel to the y-axis, and a glide-plane (glide $c/2$) parallel to (010): space-group $P2_1/c$.

The corresponding values of A and B are

$$A=2\left[\cos 2\pi(hx+ky+lz)+\cos 2\pi\left(hx-ky+lz+\frac{k+l}{2}\right)\right]=4\cos 2\pi\left(hx+lz+\frac{k+l}{4}\right)\cos 2\pi\left(ky-\frac{k+l}{4}\right)$$

$B=0$ (as always when the origin is at a centre of symmetry).

If the diad screw-axis had been taken along z and the glide-plane parallel to (001), with a glide of $a/2$, the co-ordinates would have been $|x,y,z;\ \bar{x},\bar{y},\bar{z};\ \frac{1}{2}+x,y,\frac{1}{2}-z;\ \frac{1}{2}-x,\bar{y},\frac{1}{2}+z|$ . . . space group $P2_1/a$

$$A=4\cos 2\pi\left(hx+ky+\frac{h+l}{4}\right)\cos 2\pi\left(lz-\frac{h+l}{4}\right)$$

The usual procedure in a crystal structure analysis is to determine experimentally the values of $|F(hkl)|$ for as many planes as possible, especially for planes in the principal zones. Knowing the kinds and numbers of atoms or ions in the unit cell, all the peculiarities of intensity distribution are next used (including, if necessary, Patterson syntheses as outlined on p. 526 and described in succeeding volumes) in order to decide the most probable distribution of scattering material in the cell, that is, the most probable values of x,y,z for each atom or ion. Details of this procedure are given in such papers as

"A Technique for the X-ray Examination of Crystal Structures with Many Parameters." W. L. Bragg and J. West, *Z. f. Kristallog.*, **69**, 118–48 (1928).

Various structure analyses by J. M. Robertson *et al.*, in *Proc. Roy. Soc.*, London, and *J. Chem. Soc.*, from 1932 onwards.

"Crystal Structure of Melamine." E. W. Hughes, *J. Am. Chem. Soc.*, **63**, 1737 (1941).

The approximate values of x,y,z so obtained, when substituted in equations IV and V, should give values of $|F(hkl)|$ not far from the observed values for all the observed reflections. In other words, the value of the quantity $\Sigma\big||F_{\text{obs}}|-|F_{\text{calc}}|\big|/\Sigma|F_{\text{obs}}|$ should be small ($<0{\cdot}25$ to $0{\cdot}15$, say).

Experimental observation alone cannot, in general, determine the phase angle $\alpha(hkl)$, but if this can be estimated with sufficient accuracy from the approximate structure by means of equation VI, then equation III can be used to carry out a Fourier analysis in one, two or three dimensions, the distribution of electron density thus being determined accurately and uniquely. If, on completion of the Fourier analysis, it is found that the approximate structure was not sufficiently exact, it may be necessary to repeat the analysis, using as an "approximate" structure the result of the previous analysis, thus arriving at a final structure by a series of successive approximations. In order to perform the calculations involved in equation III it is necessary to know not only the phase of $F(hkl)$ but also how the absolute value and the phase of $F(hkl)$ change when h, k and/or l change sign.

(i) *If the origin of co-ordinates is taken at a centre of symmetry*, then B (and therefore B') is zero for all planes. In this case $\tan\alpha(hkl)=0$, and α is 0 or π, according to whether A is positive or negative for the plane considered. Equations II*a* and II*b* reduce, if $B'=0$, to

$$\rho(XYZ)=\rho(-X,-Y,-Z)=\frac{1}{V_c}\sum_{-\infty}^{\infty}h\sum_{-\infty}^{\infty}k\sum_{-\infty}^{\infty}l\,A'\cos 2\pi(hX+kY+lZ)$$

where $A'=\Sigma fA=F(hkl)$, and is positive or negative according to the relative positions of the various atoms or ions. The absolute value of $F(hkl)$ is that determined experimentally and the sign is deduced from the approximate structure determined by trial and error. Since $B'=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})$; $F(\bar{h}kl)=F(h\bar{k}\bar{l})$; etc., for all values of h, k and l; but, in general, $F(hkl)\neq F(\bar{h}kl)\neq F(h\bar{k}l)\neq F(hk\bar{l})$.

The exceptions to this generalisation are, however, most important, for they affect the very zones in which preliminary Fourier analyses are usually carried out.

For example, in space-group $P2_1/b$, with co-ordinates $|x,y,z;\ \bar{x},\bar{y},\bar{z};\ x,\frac{1}{2}+y,\frac{1}{2}-z;\ \bar{x},\frac{1}{2}-y,\frac{1}{2}+z|$ (monoclinic, unique axis c, glide-plane (001) with glide $b/2$)

$$A=4\cos 2\pi\left(hx+ky+\frac{k+l}{4}\right)\cos 2\pi\left(lz-\frac{k+l}{4}\right)$$

$B=0$

The expression for A can be simplified still further as follows:

If $k+l=2n$ (that is, an even integer)

$A=4\cos 2\pi(hx+ky)\cos 2\pi lz$; $B=0$

$F(hkl)=F(hk\bar{l})$; $F(\bar{h}kl)=F(h\bar{k}l)$; $F(hkl)\neq\pm F(\bar{h}kl)$

If $k+l=2n+1$ (that is, an odd integer)

$A=-4\sin 2\pi(hx+ky)\sin 2\pi lz$; $B=0$

$F(hkl)=-F(hk\bar{l})$; $F(\bar{h}kl)=-F(h\bar{k}l)$; $F(hkl)\neq\pm F(\bar{h}kl)$

If $l=0$ and k is odd, or if $h=k=0$ and l is odd, then $A=B=0$. That is, all reflections are missing for planes $(hk0)$ having k odd, and for planes $(00l)$ having l odd.

In actual practice it is often simplest to write down A and B for the particular set of planes under immediate investigation. In the case considered above ($P2_1/b$) the structure factors for the axial planes and for planes in the axial zones assume the still more simplified forms:

$(h00)$	$A=4\cos 2\pi hx$, h even or odd.
$(0k0)$	$A=4\cos 2\pi ky$ if k is even; $A=0$ if k is odd.
$(00l)$	$A=4\cos 2\pi lz$ if l is even; $A=0$ if l is odd.
$(0kl)$	$A=4\cos 2\pi ky\cos 2\pi lz$; $F(0kl)=F(0k\bar{l})$; if $k+l$ is even.
	$A=-4\sin 2\pi ky\sin 2\pi lz$; $F(0kl)=-F(0k\bar{l})$; if $k+l$ is odd.
$(h0l)$	$A=4\cos 2\pi hx\cos 2\pi lz$; $F(h0l)=F(\bar{h}0l)$; if l is even.
	$A=-4\sin 2\pi hx\sin 2\pi lz$; $F(h0l)=-F(\bar{h}0l)$; if l is odd.
$(hk0)$	$A=4\cos 2\pi(hx+ky)$; $F(hk0)\neq\pm F(\bar{h}k0)$; if k is even.
	$A=0$ if k is odd.

When the atoms occupy not general but special co-ordinate positions, further simplification is sometimes possible. If, for example, the atoms themselves, in space group $P2_1/b$, occupy centres of symmetry, their co-ordinates will be

$$|0,0,0;\quad 0,\tfrac{1}{2},\tfrac{1}{2}| \text{ or } |\tfrac{1}{2},0,0;\quad \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}| \text{ or } |0,\tfrac{1}{2},0;\quad 0,0,\tfrac{1}{2}| \text{ or } |\tfrac{1}{2},\tfrac{1}{2},0;\quad \tfrac{1}{2},0,\tfrac{1}{2}|$$

Different atoms may, of course, occupy any or all of these pairs of positions.

The expression for A then becomes

$A=4\cos^2\pi\dfrac{k+l}{2}$; which is 4 if $k+l$ is even, 0 if $k+l$ is odd:

or $4\cos\pi h\cos^2\pi\dfrac{k+l}{2}$; which is $4\cos\pi h$ if $k+l$ is even, 0 if $k+l$ is odd:

or $4\cos\pi k\cos^2\pi\dfrac{k+l}{2}$; which is $4\cos\pi k$ if $k+l$ is even, 0 if $k+l$ is odd:

or $4\cos\pi(h+k)\cos^2\pi\dfrac{k+l}{2}$; which is $4\cos\pi(h+k)$ if $k+l$ is even, 0 if $k+l$ is odd

in the four respective cases.

The tabulation of A and B for all special values of h,k,l and of x,y,z would take up a very large amount of space if attempted systematically here, but should be undertaken for any particular space group whenever the number of any kind of atom in the unit cell is less than the number of general equivalent positions, or when there is any reason to suspect that atoms occupy special positions in the unit cell.

(ii) *If the structure is centro-symmetrical, but the origin of co-ordinates is not taken at a centre of symmetry,* it will be found from the following tables that the choice of origin is always such that either

$$A=0\ldots\ldots\ldots\ldots\ldots\alpha(hkl)=\frac{\pi}{2}\quad(B'+\text{ve})\quad\text{or}\quad\frac{3\pi}{2}\quad(B'-\text{ve});$$

$$\text{or } B=0\ldots\ldots\ldots\ldots\ldots\alpha(hkl)=0\quad(A'+\text{ve})\quad\text{or}\quad\pi\quad(A'-\text{ve});$$

$$\text{or } A=B\ldots\ldots\ldots\ldots\ldots\alpha(hkl)=\frac{\pi}{4}\quad(A'+\text{ve})\quad\text{or}\quad\frac{5\pi}{4}\quad(A'-\text{ve});$$

$$\text{or } A=-B\ldots\ldots\ldots\ldots\alpha(hkl)=\frac{3\pi}{4}\quad(B'+\text{ve})\quad\text{or}\quad\frac{7\pi}{4}\quad(B'-\text{ve});$$

for the various (hkl) planes.

The Fourier analysis may be slightly more laborious in such a case, but it is no less exact. The expressions for A and B are sometimes simpler.

(iii) *If the structure has no centre of symmetry* the Fourier analysis is much more difficult and is likely to be less exact, but it is still possible. The phase angles must be calculated, separately for each observed reflection, from the approximate "trial and error" structure and substituted, together with the measured values of $|F(hkl)|$, in equation III, or in the modified form of equation III appropriate to a one-dimensional or to a two-dimensional analysis. A knowledge of the way in which $\alpha(hkl)$ and $F(hkl)$ vary with changes in sign of h, k and l enables us to simplify equation III to such an extent that only *positive* values of h, k and l need be considered. As an example we may take space group $P222$:

$A'=\sum fA$ where $A=4\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz$

$B'=\sum fB$ where $B=-4\sin 2\pi hx \sin 2\pi ky \sin 2\pi lz$

Since $|F(hkl)|=(A'^2+B'^2)^{\frac{1}{2}}$, it follows that

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(hk\bar{l})|=|F(h\bar{k}l)|=|F(\bar{h}k\bar{l})|=$ etc.

and $\tan^{-1}(B'/A')=\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=$ etc.

Equation III gives, on substitution:

$$\rho(XYZ)=\frac{2}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\{\cos[2\pi(hX+kY+lZ)-\alpha(hkl)]+\cos[2\pi(hX-kY-lZ)-\alpha(hkl)]+$$
$$\cos[2\pi(-hX+kY-lZ)-\alpha(hkl)]+\cos[2\pi(-hX-kY+lZ)-\alpha(hkl)]\}$$
$$=\frac{8}{abc}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\{\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-$$
$$\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)\}$$

This equation, however, is misleading, as a closer examination will show that the contributions from (000), (h00), (hk0) and, in general, from any planes having h, k or l zero, have been counted too many times. The complete and correct formula should take account of the fact that $F(000)$ occurs only once, $|F(h00)|$ etc. only twice (to include (h00) and ($\bar{h}$00)), $|F(hk0)|$ etc. only four times (to include (hk0), ($\bar{h}k$0), ($h\bar{k}$0) and ($\bar{h}\bar{k}$0)), and $|F(hkl)|$ with no zero index eight times, to include (hkl), ($\bar{h}kl$), ($h\bar{k}l$), ($hk\bar{l}$), ($h\bar{k}\bar{l}$), ($\bar{h}k\bar{l}$), ($\bar{h}\bar{k}l$) and ($\bar{h}\bar{k}\bar{l}$). Thus

$$\rho(XYZ)=\frac{1}{V_c}\Big[F(000)+2\Big\{\sum_1^\infty h|F(h00)|\cos 2\pi hX\cos\alpha(h00)+\sum_1^\infty k|F(0k0)|\cos 2\pi kY\cos\alpha(0k0)+$$
$$\sum_1^\infty l|F(00l)|\cos 2\pi lZ\cos\alpha(00l)\Big\}+4\Big\{\sum_1^\infty k\sum_1^\infty l|F(0kl)|\cos 2\pi kY\cos 2\pi lZ\cos\alpha(0kl)+$$
$$\sum_1^\infty l\sum_1^\infty h|F(h0l)|\cos 2\pi hX\cos 2\pi lZ\cos\alpha(h0l)+\sum_1^\infty h\sum_1^\infty k|F(hk0)|\cos 2\pi hX\cos 2\pi kY\cos\alpha(hk0)\Big\}+$$
$$8\sum_1^\infty h\sum_1^\infty k\sum_1^\infty l|F(hkl)|\{\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-$$
$$\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)\}\Big]$$

If a two-dimensional analysis is all that is required, V_c, the volume of the unit cell, must be replaced by S, the area of the projection over which the analysis is to be performed, and the number of terms in the formula will be reduced.

In order to economise space, only the last (general) term of the above equation is given in the tables for each space group; the terms corresponding to zero values of h, k and/or l may easily be derived from the general term, and some of these will be found to take simplified forms (as above), or even to disappear in certain space groups, owing to the absence of reflections from corresponding planes (for which $A=B=0$). Detailed examples are given later (pp. 361, 364).

A little trigonometrical manipulation soon shows that in the more complicated space-groups the general structure factor expressions, A and B, can be given in a variety of ways which, although equivalent, look very different. For example, in space group $Fddd$, origin at 222, page 412,

$$A=G\cos 2\pi\frac{h+k+l}{8}\quad B=G\sin 2\pi\frac{h+k+l}{8},$$

$$\text{where } G=16\cos 2\pi\frac{h+k}{4}\cos 2\pi\frac{k+l}{4}\left\{\cos 2\pi\left[hx+\frac{h+k-3l}{8}\right]\cos 2\pi(ky+lz)+\right.$$
$$\left.\cos 2\pi\left[hx+\frac{3h-k-l}{8}\right]\cos 2\pi(ky-lz)\right\}$$
$$=32\cos 2\pi\frac{h-k}{4}\cos 2\pi\frac{k-l}{4}\cos 2\pi\frac{l-h}{4}\left\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz\cos 2\pi\frac{h+k+l}{8}-\right.$$
$$\left.\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz\sin 2\pi\frac{h+k+l}{8}\right\}$$
$$=32\cos 2\pi\frac{h+k}{4}\cos 2\pi\frac{k+l}{4}\cos 2\pi\frac{l+h}{4}\left\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz\cos 2\pi\frac{h+k+l}{8}-\right.$$
$$\left.\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz\sin 2\pi\frac{h+k+l}{8}\right\}$$

The particular expressions of the general formulae given in the tables which follow have been chosen, as far as possible, on account of the ease with which further simplification for special values of h, k, l could be carried out for those formulations.

In determining the $F(hkl)$ or $|F(hkl)|$ relationships, and the resulting form of the $\rho(XYZ)$ equation in the more complicated space groups, it is essential to go back to the general formula. For example, in space group $Fd3$, with the origin at 23, page 495, the general formula is

$$A=32\cos 2\pi\frac{h+k}{4}\cos 2\pi\frac{k+l}{4}\cos 2\pi\frac{h+k+l}{8}\,.\,G$$
$$B=32\cos 2\pi\frac{h+k}{4}\cos 2\pi\frac{k+l}{4}\sin 2\pi\frac{h+k+l}{8}\,.\,G,$$
$$\text{where } G=\cos 2\pi\frac{h+k+l}{8}\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+$$
$$\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz\}-$$
$$\sin 2\pi\frac{h+k+l}{8}\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+$$
$$\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz+\sin 2\pi lx\sin 2\pi hy\sin 2\pi kz\}$$

which simplifies to $\qquad A=B=16\{ccc+ccc+ccc-sss-sss-sss\}$

when $(h+k)$ and $(k+l)$ are even and $h+k+l=4n+1$ (using an obvious form of abbreviation).

Now substitution of $\bar{h}$ for h would apparently change this formula to

$$A=B=16\{ccc+ccc+ccc+sss+sss+sss\}$$

but in fact the change of sign of h has altered the conditions: $\bar{h}+k+l=4n+3$ if $(h+k)$ and $(k+l)$ are even. Substitution in the general formula shows that in both cases

$$A=16\{ccc+ccc+ccc-sss-sss-sss\}$$

but that for (hkl) $B=A$, whereas for $(\bar{h}kl)$ $B=-A$.
Hence $|F(hkl)|=|F(\bar{h}kl)|$; but $\alpha(hkl)=-\alpha(\bar{h}kl)$.

Similarly, in space group 230 ($Ia3d$, origin at $\bar{3}$), the simplified formula for $h+k+l=4n$, $h=2n$, $k=2n+1$ is

$$A=-16\{\sin 2\pi hx[\cos 2\pi ky\sin 2\pi lz+\cos 2\pi ly\sin 2\pi kz]+$$
$$\sin 2\pi hy[\cos 2\pi kz\sin 2\pi lx+\cos 2\pi lz\sin 2\pi kx]+$$
$$\sin 2\pi hz[\cos 2\pi kx\sin 2\pi ly+\cos 2\pi lx\sin 2\pi ky]\}$$
$$B=0.$$

For $(h\bar{k}l)$ the second terms in the brackets would apparently change sign, giving a different expression, but again the conditions have been changed. Substitution in the general formula

$$A=16\cos 2\pi\frac{h+k+l}{4}\Big\{\cos 2\pi\Big(hx+\frac{l}{4}\Big)\cos 2\pi\Big(ky+\frac{h}{4}\Big)\cos 2\pi\Big(lz+\frac{k}{4}\Big)+\cos 2\pi\Big(hz+\frac{l}{4}\Big)\cos 2\pi\Big(kx+\frac{h}{4}\Big)\times$$
$$\cos 2\pi\Big(ly+\frac{k}{4}\Big)+\cos 2\pi\Big(hy+\frac{l}{4}\Big)\cos 2\pi\Big(kz+\frac{h}{4}\Big)\cos 2\pi\Big(lx+\frac{k}{4}\Big)+\cos 2\pi\Big(h+k+\frac{l}{4}\Big)\Big[\cos 2\pi\Big(hx+\frac{k}{4}\Big)\times$$
$$\cos 2\pi\Big(ly+\frac{h}{4}\Big)\cos 2\pi\Big(kz+\frac{l}{4}\Big)+\cos 2\pi\Big(hy+\frac{k}{4}\Big)\cos 2\pi\Big(lz+\frac{h}{4}\Big)\cos 2\pi\Big(kx+\frac{l}{4}\Big)+\cos 2\pi\Big(hz+\frac{k}{4}\Big)\times$$
$$\cos 2\pi\Big(lx+\frac{h}{4}\Big)\cos 2\pi\Big(ky+\frac{l}{4}\Big)\Big]\Big\}$$

although tedious, does show clearly that there is no change: $F(hkl)=F(h\bar{k}l)$.

In certain cases in the following tables alternative sets of co-ordinates have been given, together with the corresponding formulae. In particular, if a centre of symmetry exists in the space group, one set of co-ordinates is always chosen using the centre as origin.

Some of the trigonometrical formulae used in the calculation of simplified factors are given below:

$$\cos A+\cos B=2\cos\frac{A+B}{2}\cos\frac{A-B}{2} \qquad \sin A+\sin B=2\sin\frac{A+B}{2}\cos\frac{A-B}{2}$$

$$\cos A-\cos B=-2\sin\frac{A+B}{2}\sin\frac{A-B}{2} \qquad \sin A-\sin B=2\cos\frac{A+B}{2}\sin\frac{A-B}{2}$$

$$\cos A+\cos B+\cos C+\cos(A+B+C)=4\cos\frac{A+B}{2}\cos\frac{B+C}{2}\cos\frac{C+A}{2}$$

$$\cos A+\cos B+\cos C+\cos(A+B-C)=4\cos\frac{A+B}{2}\cos\frac{C-A}{2}\cos\frac{C-B}{2}$$

$$\sin A+\sin B+\sin C+\sin(-A-B-C)=4\sin\frac{A+B}{2}\sin\frac{B+C}{2}\sin\frac{C+A}{2}$$

$$\sin A+\sin B+\sin C+\sin(A+B-C)=4\sin\frac{A+B}{2}\cos\frac{C-A}{2}\cos\frac{C-B}{2}$$

For any *integral* values of h, k, and l (including zero)

$$\cos 2\pi\frac{h+k+l}{4}\cos\Big(A\pm 2\pi\frac{h+k+l}{4}\Big)=\cos^2 2\pi\frac{h+k+l}{4}\cos A$$

$$\cos 2\pi\frac{h+k+l}{4}\sin\Big(A\pm 2\pi\frac{h+k+l}{4}\Big)=\cos^2 2\pi\frac{h+k+l}{4}\sin A$$

$$\sin 2\pi\frac{h+k+l}{4}\cos\Big(A\pm 2\pi\frac{h+k+l}{4}\Big)=\mp\sin^2 2\pi\frac{h+k+l}{4}\sin A$$

$$\sin 2\pi\frac{h+k+l}{4}\sin\Big(A\pm 2\pi\frac{h+k+l}{4}\Big)=\pm\sin^2 2\pi\frac{h+k+l}{4}\cos A$$

$$\cos\Big(A+\frac{\pi m}{2}\Big)=\begin{cases}\cos A & \text{if } m=4n\\ -\sin A & \text{if } m=4n+1\\ -\cos A & \text{if } m=4n+2\\ \sin A & \text{if } m=4n+3\end{cases} \qquad \sin\Big(A+\frac{\pi m}{2}\Big)=\begin{cases}\sin A & \text{if } m=4n\\ \cos A & \text{if } m=4n+1\\ -\sin A & \text{if } m=4n+2\\ -\cos A & \text{if } m=4n+3\end{cases}$$

Note also that if h, k, l are integers and $h+k=2n$, $k+l=2n$ then $h+l=2n$, $k-l=2n$, $l-h=2n$, etc. Relationships such as these have been extensively used in compiling these tables.

$$\text{If } h=2n: \quad \cos 2\pi\left(\theta\pm\frac{h}{4}\right)\cos 2\pi\left(\phi\pm\frac{h}{4}\right)=\cos 2\pi\theta\cos 2\pi\phi$$

$$\cos 2\pi\left(\theta\pm\frac{h}{4}\right)\sin 2\pi\left(\phi\pm\frac{h}{4}\right)=\cos 2\pi\theta\sin 2\pi\phi$$

$$\sin 2\pi\left(\theta\pm\frac{h}{4}\right)\sin 2\pi\left(\phi\pm\frac{h}{4}\right)=\sin 2\pi\theta\sin 2\pi\phi$$

$$\text{If } h=2n+1: \quad \sin 2\pi\left(\theta\pm\frac{h}{4}\right)\sin 2\pi\left(\phi\pm\frac{h}{4}\right)=\cos 2\pi\theta\cos 2\pi\phi$$

$$\sin 2\pi\left(\theta+\frac{h}{4}\right)\sin 2\pi\left(\phi-\frac{h}{4}\right)=-\cos 2\pi\theta\cos 2\pi\phi$$

$$\sin 2\pi\left(\theta+\frac{h}{4}\right)\cos 2\pi\left(\phi\pm\frac{h}{4}\right)=\mp\cos 2\pi\theta\sin 2\pi\phi$$

$$\cos 2\pi\left(\theta\pm\frac{h}{4}\right)\cos 2\pi\left(\phi\pm\frac{h}{4}\right)=\sin 2\pi\theta\sin 2\pi\phi$$

$$\cos 2\pi\left(\theta+\frac{h}{4}\right)\cos 2\pi\left(\phi-\frac{h}{4}\right)=-\sin 2\pi\theta\sin 2\pi\phi$$

$$\cos 2\pi\left(\theta\pm\frac{h}{4}\right)\sin 2\pi\left(\phi-\frac{h}{4}\right)=\pm\sin 2\pi\theta\cos 2\pi\phi$$

Detailed Examples

Example I. $Pmn2_1$

Bravais lattice: simple orthorhombic.
Mirror plane parallel to (100) at $0yz$.
Glide plane (n) parallel to (010) at $x0z$.
Screw 2_1-axis parallel to [001] at $\frac{1}{4}0z$.
General co-ordinates of equivalent points:
x,y,z; $\bar{x},y,z$; $\frac{1}{2}+x,\bar{y},\frac{1}{2}+z$; $\frac{1}{2}-x,\bar{y},\frac{1}{2}+z$.

$$A=\left[\cos 2\pi(hx+ky+lz)+\cos 2\pi\left(-hx-ky+lz+\frac{h+l}{2}\right)\right]+\left[\cos 2\pi(-hx+ky+lz)+\cos 2\pi\left(hx-ky+lz+\frac{h+l}{2}\right)\right]$$

$$=2\cos 2\pi\left(hx+ky-\frac{h+l}{4}\right)\cos 2\pi\left(lz+\frac{h+l}{4}\right)+2\cos 2\pi\left(-hx+ky-\frac{h+l}{4}\right)\cos 2\pi\left(lz+\frac{h+l}{4}\right)$$

$$=4\cos 2\pi hx\cos 2\pi\left(ky-\frac{h+l}{4}\right)\cos 2\pi\left(lz+\frac{h+l}{4}\right)$$

$$B=\left[\sin 2\pi(hx+ky+lz)+\sin 2\pi\left(-hx-ky+lz+\frac{h+l}{2}\right)\right]+\left[\sin 2\pi(-hx+ky+lz)+\sin 2\pi\left(hx-ky+lz+\frac{h+l}{2}\right)\right]$$

$$=2\cos 2\pi\left(hx+ky-\frac{h+l}{4}\right)\sin 2\pi\left(lz+\frac{h+l}{4}\right)+2\cos 2\pi\left(-hx+ky-\frac{h+l}{4}\right)\sin 2\pi\left(lz+\frac{h+l}{4}\right)$$

$$=4\cos 2\pi hx\cos 2\pi\left(ky-\frac{h+l}{4}\right)\sin 2\pi\left(lz+\frac{h+l}{4}\right)$$

It is best *at this stage* to separate the equations for $(h+l)$ even or odd, and to consider the variation of $|F|$ and of α with change of sign of h, k and/or l, for each case in turn.

$h+l=2n$ $\quad A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$
$\quad B=4\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$

Since $|F|=[(\sum fA)^2+(\sum fB)^2]^{\frac{1}{2}}$, $|F|$ cannot be affected by a change of sign in either A or B, but only by a change of value, if any. There is no such change of value on changing h into $\bar{h}$, etc. Therefore

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|= \text{ etc.}$$

Since $\alpha=\tan^{-1}(\sum fB/\sum fA)$, α *is* affected by a change of sign in B or A, even if there is no change of absolute value of either. In this example, changing the sign of h or k does not affect either A or B; but changing the sign of l makes B negative, leaving A positive, and brings $\alpha(hk\bar{l})$ into the fourth quadrant relative to $\alpha(hkl)$.

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})= \text{ etc.}$$

$h+l=2n+1 \quad A=-4\cos 2\pi hx \sin 2\pi ky \sin 2\pi lz$

$\qquad\qquad B=4\cos 2\pi hx \sin 2\pi ky \cos 2\pi lz$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|= \text{ etc.}$

Changing the sign of k only, makes both A and B negative and brings α into the third quadrant. That is:

$$\alpha(h\bar{k}l)=\pi+\alpha(hkl)$$

Changing the sign of l only, makes A negative, B positive, and brings α into the second quadrant.

$$\alpha(hk\bar{l})=\pi-\alpha(hkl)$$

Considering all possible changes:

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)-\pi=\pi-\alpha(hk\bar{l})= \text{ etc.}$$

This enables us to determine the "general term" of the electron density formula, which is

$$\sum_{-\infty}^{\infty}h\sum_{-\infty}^{\infty}k\sum_{-\infty}^{\infty}l\{|F(hkl)|\cos[2\pi(hX+kY+lZ)-\alpha(hkl)]+|F(\bar{h}\bar{k}\bar{l})|\cos[2\pi(-hX-kY-lZ)-\alpha(\bar{h}\bar{k}\bar{l})]+$$
$$|F(\bar{h}kl)|\cos[2\pi(-hX+kY+lZ)-\alpha(\bar{h}kl)]+ \text{ terms in } (h\bar{k}l)\ (hk\bar{l})\ (h\bar{k}\bar{l})\ (\bar{h}k\bar{l}) \text{ and } (\bar{h}\bar{k}l)\}$$

Now $|F(\bar{h}\bar{k}\bar{l})|=|F(hkl)|$ and $\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hkl)$ always.

Therefore $|F(\bar{h}\bar{k}\bar{l})|\cos[2\pi(-hX-kY-lZ)-\alpha(\bar{h}\bar{k}\bar{l})]=|F(hkl)|\cos[2\pi(hX+kY+lZ)-\alpha(hkl)]$

Hence the "general term" may be written as

$$2\sum_{0}^{\infty}h\sum_{0}^{\infty}k\sum_{0}^{\infty}l\{|F(hkl)|\cos[2\pi(hX+kY+lZ)-\alpha(hkl)]+|F(\bar{h}kl)|\cos[2\pi(-hX+kY+lZ)-\alpha(\bar{h}kl)]+ \text{ etc.}\}$$

At this point it is again necessary to separate $(h+l)$ even from $(h+l)$ odd, since the α relations differ. But we can put $|F(\bar{h}kl)|= \text{ etc.} =|F(hkl)|$ in both. The "general term" then becomes

$$2\Big\{\sum_{0}^{\infty}h\sum_{0}^{\infty}k\sum_{0}^{\infty}l\,{}^{h+l\text{ even}}|F(hkl)|\{\cos[2\pi(hX+kY+lZ)-\alpha(hkl)]+\cos[2\pi(-hX+kY+lZ)-\alpha(hkl)]+$$
$$\cos[2\pi(hX-kY+lZ)-\alpha(hkl)]+\cos[2\pi(hX+kY-lZ)+\alpha(hkl)]\}+$$
$$\sum_{0}^{\infty}h\sum_{0}^{\infty}k\sum_{0}^{\infty}l\,{}^{h+l\text{ odd}}|F(hkl)|\{\cos[2\pi(hX+kY+lZ)-\alpha(hkl)]+\cos[2\pi(-hX+kY+lZ)-\alpha(hkl)]+$$
$$\cos[2\pi(hX-kY+lZ)-(\pi+\alpha(hkl))]+\cos[2\pi(hX+kY-lZ)-(\pi-\alpha(hkl))]\}\Big\}$$

Simplifying this in the usual way, we obtain

$$8\Big\{\sum_{0}^{\infty}h\sum_{0}^{\infty}k\sum_{0}^{\infty}l\,{}^{h+l\text{ even}}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-$$
$$\sum_{0}^{\infty}h\sum_{0}^{\infty}k\sum_{0}^{\infty}l\,{}^{h+l\text{ odd}}|F(hkl)|\cos 2\pi hX\sin 2\pi kY\sin[2\pi lZ-\alpha(hkl)]\Big\}$$

To obtain the form of the terms with one or more zero index, it is best to go back to the equations:

$h+l=2n \quad A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$

$\qquad\qquad B=4\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$

$h+l=2n+1 \quad A=-4\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$

$\qquad\qquad B=4\cos 2\pi hx\sin 2\pi ky\cos 2\pi lz$

$h00$: h even: $A=4\cos 2\pi hx$, $B=0$

Since $B=0$, $\alpha(h00)=0$ or π according as A is +ve or −ve; and $|F(h00)|=|A(h00)|$. It is better, in practice, to omit α, and to allow the phase to be indicated by giving $F(h00)$ the sign of A.

$h00$: h odd: $A=B=0$

$0k0$: $h+l=0$: $A=4\cos 2\pi ky$, $B=0$

$F(0k0)$ takes the sign of A, α being omitted.

$00l$: l even: $A=4\cos 2\pi lz$, $B=4\sin 2\pi lz$

Note that since $\alpha=\tan^{-1}(\sum fB/\sum fA)$ and *not* B/A, the trigonometrical relationships between B and A cannot be used to simplify the α (or the $|F|$) expression unless there is only one kind of atom in the unit cell.

$00l$: l odd: $A=B=0$

$0kl$: l even: $A=4\cos 2\pi ky\cos 2\pi lz$

$B=4\cos 2\pi ky\sin 2\pi lz$

$\alpha(0kl)=-\alpha(0\bar{k}\bar{l})=\alpha(0\bar{k}l)=-\alpha(0k\bar{l})$

l odd: $A=-4\sin 2\pi ky\sin 2\pi lz$

$B=4\sin 2\pi ky\cos 2\pi lz$

$\alpha(0kl)=-\alpha(0\bar{k}\bar{l})=\alpha(0\bar{k}l)-\pi=\pi-\alpha(0k\bar{l})$

$h0l$: $h+l$ even: $A=4\cos 2\pi hx\cos 2\pi lz$

$B=4\cos 2\pi hx\sin 2\pi lz$

$\alpha(h0l)=-\alpha(\bar{h}0\bar{l})=\alpha(\bar{h}0l)=-\alpha(h0\bar{l})$

$h+l$ odd: $A=B=0$

$hk0$: h even: $A=4\cos 2\pi hx\cos 2\pi ky$

$B=0$

$F(hk0)$ takes the sign of A; $F(hk0)=F(h\bar{k}0)$

h odd: $A=0$

$B=4\cos 2\pi hx\sin 2\pi ky$

$\alpha(hk0)=\frac{\pi}{2}$ or $\frac{3\pi}{2}$ according as B is +ve or −ve.

This is indicated by giving $F(hk0)$ the sign of B, but substituting $\alpha=\frac{\pi}{2}$ in either case.

$F(hk0)=-F(\bar{h}\bar{k}0)=F(\bar{h}k0)=-(F\bar{h}\bar{k}0)$

Using all these relationships, we find that

$$\begin{aligned}\rho(XYZ)=\frac{1}{V_c}\Big\{&F(000)+2\sum_{2}^{\infty}{}^{h\ even}_{h}F(h00)\cos 2\pi hX+\\
&2\sum_{1}^{\infty}{}_{k}F(0k0)\cos 2\pi kY+2\sum_{2}^{\infty}{}^{l\ even}_{l}|F(00l)|\cos[2\pi lZ-\alpha(00l)]+\\
&4\sum_{1}^{\infty}{}_{k}\sum_{2}^{\infty}{}^{l\ even}_{l}|F(0kl)|\cos 2\pi kY\cos[2\pi lZ-\alpha(0kl)]-\\
&4\sum_{1}^{\infty}{}_{k}\sum_{1}^{\infty}{}^{l\ odd}_{l}|F(0kl)|\sin 2\pi kY\sin[2\pi lZ-\alpha(0kl)]+\\
&4\sum_{1}^{\infty}{}_{h}\sum_{1}^{\infty}{}^{h+l\ even}_{l}|F(h0l)|\cos 2\pi hX\cos[2\pi lZ-\alpha(h0l)]+\\
&4\sum_{2}^{\infty}{}_{h}\sum_{1}^{\infty}{}^{h\ even}_{k}F(hk0)\cos 2\pi hX\cos 2\pi kY-4\sum_{1}^{\infty}{}_{h}\sum_{1}^{\infty}{}^{h\ odd}_{k}F(hk0)\cos 2\pi hX\sin 2\pi kY+\\
&8\sum_{1}^{\infty}{}_{h}\sum_{1}^{\infty}{}_{k}\sum_{1}^{\infty}{}^{h+l\ even}_{l}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\\
&8\sum_{1}^{\infty}{}_{h}\sum_{1}^{\infty}{}_{k}\sum_{1}^{\infty}{}^{h+l\ odd}_{l}|F(hkl)|\cos 2\pi hX\sin 2\pi kY\sin[2\pi lZ-\alpha(hkl)]\Big\}\end{aligned}$$

The expressions simplify somewhat for special points with symmetry m: $0,y,z$; $\frac{1}{2},\bar{y},\frac{1}{2}+z$.
Substituting $x=0$, we find for this special case:

$h+l=2n$ $\quad A=2\cos 2\pi ky\cos 2\pi lz$
$\quad B=2\cos 2\pi ky\sin 2\pi lz$
$h+l=2n+1$ $\quad A=-2\sin 2\pi ky\sin 2\pi lz$
$\quad B=2\sin 2\pi ky\cos 2\pi lz$

Note, however, that we cannot just substitute $x=0$ in the electron density formula, since here X has a different meaning. The structure factor formulae are in some cases simplified for special co-ordinates, but *the electron density formulae are unchanged.*

$h00$: h even: $A=2$, $B=0$
h odd: $A=B=0$
$h0l$: $h+l$ even: $A=2\cos 2\pi lz$
$B=2\sin 2\pi lz$
$h+l$ odd: $A=B=0$
$hk0$: h even: $A=2\cos 2\pi ky$, $B=0$
h odd: $A=0$, $B=2\sin 2\pi ky$

All the other structure factor formulae are simply halved.

Example II. $C222_1$
Bravais lattice: (001)—face-centred orthorhombic.
Twofold rotation axis parallel to [100] at $x00$.
Twofold rotation axis parallel to [010] at $0y\frac{1}{4}$.
Twofold screw axis parallel to [001] at $00z$.
Co-ordinates of general positions are:

$$x,y,z;\quad \bar{x},\bar{y},\tfrac{1}{2}+z;\quad \tfrac{1}{2}+x,\tfrac{1}{2}+y,z;\quad \tfrac{1}{2}-x,\tfrac{1}{2}-y,\tfrac{1}{2}+z;$$
$$x,\bar{y},\bar{z};\quad \bar{x},y,\tfrac{1}{2}-z;\quad \tfrac{1}{2}+x,\tfrac{1}{2}-y,\bar{z};\quad \tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{2}-z.$$

This may be written

$$(0,0,0;\quad \tfrac{1}{2},\tfrac{1}{2},0)+\ |\ x,y,z;\quad x,\bar{y},\bar{z};\quad \bar{x},y,\tfrac{1}{2}-z;\quad \bar{x},\bar{y},\tfrac{1}{2}+z\ |$$

$$\text{Now}\ \begin{matrix}\sin\\ \cos\end{matrix}\theta+\begin{matrix}\sin\\ \cos\end{matrix}\left(\theta+n\pi\right)=2\cos n\frac{\pi}{2}\begin{matrix}\sin\\ \cos\end{matrix}\left(\theta+n\frac{\pi}{2}\right)=2\cos^2 n\frac{\pi}{2}\begin{matrix}\sin\\ \cos\end{matrix}\theta$$

Hence the effect of a Bravais lattice other than P (simple type) can always be introduced by a term or terms of the type $S\cos^2 n\frac{\pi}{2}$ where $n=h+k$ for a C lattice, $n=h+k+l$ for an I lattice and so on, S being the number of Bravais points in the unit cell.

For our present example:

$$A=2\cos^2 2\pi\frac{h+k}{4}\Big[\cos 2\pi(hx+ky+lz)+\cos 2\pi\left(-hx-ky+lz+\frac{l}{2}\right)+\cos 2\pi(hx-ky-lz)+$$
$$\cos 2\pi\left(-hx+ky-lz+\frac{l}{2}\right)\Big]$$

Changing $+\frac{l}{2}$ into $-\frac{l}{2}$ in the last term (this is always permissible, since it only means changing the angle by $2\pi l$):

$$A=4\cos^2 2\pi\frac{h+k}{4}\left[\cos 2\pi\left(hx+ky-\frac{l}{4}\right)\cos 2\pi\left(lz+\frac{l}{4}\right)+\cos 2\pi\left(hx-ky+\frac{l}{4}\right)\cos 2\pi\left(-lz-\frac{l}{4}\right)\right]$$
$$=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi\left(ky-\frac{l}{4}\right)\cos 2\pi\left(lz+\frac{l}{4}\right)$$
$$B=-8\cos^2 2\pi\frac{h+k}{4}\sin 2\pi hx\sin 2\pi\left(ky-\frac{l}{4}\right)\sin 2\pi\left(lz+\frac{l}{4}\right)$$

$\left\{\begin{array}{l} h+k \text{ even} \\ \quad l \text{ even} \end{array}\right.$ $A=8\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz$

$B=-8\sin 2\pi hx \sin 2\pi ky \sin 2\pi lz$

$B=0$ if h or k or $l=0$

$|F(hkl)|$ is unchanged by any changes of sign of h, k or l.

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$\left\{\begin{array}{l} h+k \text{ even} \\ \quad l \text{ odd} \end{array}\right.$ $A=-8\cos 2\pi hx \sin 2\pi ky \sin 2\pi lz=0$ if $k=0$

$B=8\sin 2\pi hx \cos 2\pi ky \cos 2\pi lz=0$ if $h=0$

$|F(hkl)|$ is again unchanged by changes of sign of h, k or l.

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$

$h+k$ odd $A=B=0$

The general term in the electron density formula is:

$$\begin{aligned}
\rho(XYZ)=\frac{2}{V_c}\Big\{&\sum\sum\sum^{h+k \text{ even}, l \text{ even}} |F(hkl)|\{\cos[2\pi(hX+kY+lZ)-\alpha(hkl)]+\cos[2\pi(-hX+kY+lZ)+\alpha(hkl)]+\\
&\cos[2\pi(hX-kY+lZ)+\alpha(hkl)]+\cos[2\pi(hX+kY-lZ)+\alpha(hkl)]\}+\\
&\sum\sum\sum^{h+k \text{ even}, l \text{ odd}} |F(hkl)|\{\cos[2\pi(hX+kY+lZ)-\alpha(hkl)]+\cos[2\pi(-hX+kY+lZ)+\alpha(hkl)]+\\
&\cos[2\pi(hX-kY+lZ)-\pi+\alpha(hkl)]+\cos[2\pi(hX+kY-lZ)-\pi+\alpha(hkl)\}]\Big\}\\
=\frac{4}{V_c}\Big\{&\sum\sum\sum^{h+k \text{ even}, l \text{ even}} |F(hkl)|\{\cos(2\pi hX-\alpha)\cos 2\pi(kY+lZ)+\cos(2\pi hX+\alpha)\cos 2\pi(kY-lZ)\}+\\
&\sum\sum\sum^{h+k \text{ even}, l \text{ odd}} |F(hkl)|\{\cos(2\pi hX-\alpha)\cos 2\pi(kY+lZ)-\cos(2\pi hX+\alpha)\cos 2\pi(kY-lZ)\}\Big\}\\
=\frac{4}{V_c}\Big\{&\sum\sum\sum^{h+k \text{ even}, l \text{ even}} |F|\{(\cos 2\pi hX\cos\alpha+\sin 2\pi hX\sin\alpha)(\cos 2\pi kY\cos 2\pi lZ-\sin 2\pi kY\sin 2\pi lZ)+\\
&(\cos 2\pi hX\cos\alpha-\sin 2\pi hX\sin\alpha)(\cos 2\pi kY\cos 2\pi lZ+\sin 2\pi kY\sin 2\pi lZ)\}+\\
&\sum\sum\sum^{h+k \text{ even}, l \text{ odd}} |F|\{(\cos 2\pi hX\cos\alpha+\sin 2\pi hX\sin\alpha)(\cos 2\pi kY\cos 2\pi lZ-\sin 2\pi kY\sin 2\pi lZ)-\\
&(\cos 2\pi hX\cos\alpha-\sin 2\pi hX\sin\alpha)(\cos 2\pi kY\cos 2\pi lZ+\sin 2\pi kY\sin 2\pi lZ)\}\Big\}\\
=\frac{8}{V_c}\Big\{&\sum\sum\sum^{h+k \text{ even}, l \text{ even}} |F|\{\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha\}-\\
&\sum\sum\sum^{h+k \text{ even}, l \text{ odd}} |F|\{\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos\alpha-\sin 2\pi hX\cos 2\pi kY\cos 2\pi lZ\sin\alpha\}\Big\}
\end{aligned}$$

In order to obtain the zero index terms in their simplest forms we consider the α values for each term.

$h00$: h even: $A=8\cos 2\pi hx$, $B=0$
$F(h00)$ takes the sign of $A(h00)$.

h odd: $A=B=0$

$0k0$: k even: $A=8\cos 2\pi ky$, $B=0$
$F(0k0)$ takes the sign of $A(0k0)$.

k odd: $A=B=0$

$00l$: l even: $A=8\cos 2\pi lz$, $B=0$
$F(00l)$ takes the sign of $A(00l)$.

l odd: $A=B=0$

$0kl$: k, l even: $A=8\cos 2\pi ky\cos 2\pi lz$, $B=0$
$F(0kl)$ takes the sign of $A(0kl)$; $F(0kl)=F(0\bar{k}l)$.

k even, l odd: $A=-8\sin 2\pi ky\sin 2\pi lz$, $B=0$
$F(0kl)$ takes the sign of $A(0kl)$; $F(0kl)=-F(0\bar{k}l)$.

$h0l$: h, l even: $A=8\cos 2\pi hx\cos 2\pi lz$, $B=0$
$F(h0l)$ takes the sign of $A(h0l)$; $F(h0l)=F(\bar{h}0l)$.

h even, l odd: $A=0,\quad B=8\sin 2\pi hx\cos 2\pi lz$

$\alpha(h0l)=\pm\frac{\pi}{2}$ as B is +ve or −ve.

$\alpha(hol)=-\alpha(\bar{h}0\bar{l})=-\alpha(\bar{h}0l)=\alpha(h0\bar{l})$

$hk0$: $h+k$ even: $A=8\cos 2\pi hx\cos 2\pi ky,\quad B=0$

$F(hk0)$ takes the sign of $A(hk0)$

$h+k$ odd: $A=B=0$

$$\begin{aligned}\rho(XYZ)=\frac{1}{V_c}\Big\{&F(000)+2\sum_{2}^{\infty}{}_{h}^{h=2n}F(h00)\cos 2\pi hX+\\
&2\sum_{2}^{\infty}{}_{k}^{k=2n}F(0k0)\cos 2\pi kY+2\sum_{2}^{\infty}{}_{l}^{l=2n}F(00l)\cos 2\pi lZ+\\
&4\sum_{2}^{\infty}{}_{k}\sum_{2}^{\infty}{}_{l}^{k=2n,\ l=2n}F(0kl)\cos 2\pi kY\cos 2\pi lZ-4\sum_{2}^{\infty}{}_{k}\sum_{1}^{\infty}{}_{l}^{k=2n,\ l=2n+1}F(0kl)\sin 2\pi kY\sin 2\pi lZ+\\
&4\sum_{2}^{\infty}{}_{h}\sum_{2}^{\infty}{}_{l}^{h=2n,\ l=2n}F(h0l)\cos 2\pi hX\cos 2\pi lZ+4\sum_{2}^{\infty}{}_{h}\sum_{1}^{\infty}{}_{l}^{h=2n,\ l=2n+1}F(h0l)\sin 2\pi hX\cos 2\pi lZ+\\
&4\sum_{1}^{\infty}{}_{h}\sum_{1}^{\infty}{}_{k}^{h+k=2n}F(hk0)\cos 2\pi hX\cos 2\pi kY+\\
&8\sum_{1}^{\infty}{}_{h}\sum_{1}^{\infty}{}_{k}\sum_{2}^{\infty}{}_{l}^{h+k=2n,\ l=2n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha]-\\
&8\sum_{1}^{\infty}{}_{h}\sum_{1}^{\infty}{}_{k}\sum_{1}^{\infty}{}_{l}^{h+k=2n,\ l=2n+1}|F(hkl)|[\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos\alpha-\sin 2\pi hX\cos 2\pi kY\cos 2\pi lZ\sin\alpha]\Big\}\end{aligned}$$

Note that although the origin of the $(h0l)$ projection in this space group is not at a point of apparent centrosymmetry, the electron density formula for that projection is no more complicated than that of the $(0kl)$ projection, where there is an apparent centre of symmetry at the origin.

4.6. GEOMETRICAL STRUCTURE FACTORS AND ELECTRON DENSITY FORMULAE FOR THE TWO-DIMENSIONAL SPACE GROUPS

$p1$ No. 1 Origin on 1 Co-ordinates: $|x,y|$

$A = \cos 2\pi(hx+ky)$ $\qquad |F(hk)| = |F(\bar{h}\bar{k})| \neq |F(\bar{h}k)|$

$B = \sin 2\pi(hx+ky)$ $\qquad \alpha(hk) = -\alpha(\bar{h}\bar{k}) \neq \alpha(\bar{h}k)$

$$\rho(XY) = \frac{1}{A_c}\Big[F(00) + 2\sum_1^\infty h\,|F(h0)| \cos[2\pi hX - \alpha(h0)] + 2\sum_1^\infty k\,|F(0k)| \cos[2\pi kY - \alpha(0k)] + 2\sum_1^\infty h \sum_1^\infty k \Big\{|F(hk)| \cos[2\pi(hX+kY) - \alpha(hk)] + |F(\bar{h}k)| \cos[2\pi(-hX+kY) - \alpha(\bar{h}k)]\Big\}\Big]$$

$p2$ No. 2 Origin at 2 $\pm|x,y|$

$A = 2\cos 2\pi(hx+ky)$ $\qquad F(hk) = F(\bar{h}\bar{k}) \neq F(\bar{h}k)$

$B = 0$

$$\rho(XY) = \frac{1}{A_c}\Big[F(00) + 2\sum_1^\infty h\,F(h0) \cos 2\pi hX + 2\sum_1^\infty k\,F(0k) \cos 2\pi kY + 2\sum_1^\infty h \sum_1^\infty k \Big\{F(hk) \cos 2\pi(hX+kY) + F(\bar{h}k) \cos 2\pi(-hX+kY)\Big\}\Big]$$

pm No. 3 Origin on m $|x,y;\ \bar{x},y|$

$A = 2\cos 2\pi hx \cos 2\pi ky$ $\qquad |F(hk)| = |F(\bar{h}\bar{k})| = |F(\bar{h}k)|$

$B = 2\cos 2\pi hx \sin 2\pi ky \quad = 0$ if $k = 0$ $\qquad \alpha(hk) = -\alpha(\bar{h}\bar{k}) = \alpha(\bar{h}k) = -\alpha(h\bar{k})$

$$\rho(XY) = \frac{1}{A_c}\Big[F(00) + 2\sum_1^\infty h\,|F(h0)| \cos 2\pi hX + 2\sum_1^\infty k\,|F(0k)| \cos[2\pi kY - \alpha(0k)] + 4\sum_1^\infty h \sum_1^\infty k\,|F(hk)| \cos 2\pi hX \cos[2\pi kY - \alpha(hk)]\Big]$$

Origin on g Co-ordinates: $|\ x,y;\ \bar{x},\tfrac{1}{2}+y\ |$ No. 4 pg

$$A=2\cos 2\pi\left(hx-\frac{k}{4}\right)\cos 2\pi\left(ky+\frac{k}{4}\right)$$
$$B=2\cos 2\pi\left(hx-\frac{k}{4}\right)\sin 2\pi\left(ky+\frac{k}{4}\right)$$

$|F(hk)|=|F(\bar{h}\bar{k})|=|F(\bar{h}k)|$

$k=2n$ $A=2\cos 2\pi hx\cos 2\pi ky$ $\alpha(hk)=-\alpha(\bar{h}\bar{k})=\alpha(\bar{h}k)=-\alpha(h\bar{k})$

$B=2\cos 2\pi hx\sin 2\pi ky$ $=0$ if $k=0$

$k=2n+1$ $A=-2\sin 2\pi hx\sin 2\pi ky$ $\alpha(hk)=-\alpha(\bar{h}\bar{k})=\pi+\alpha(\bar{h}k)=\pi-\alpha(h\bar{k})$

$B=2\sin 2\pi hx\cos 2\pi ky;$ $A=B=0$ if $h=0$

$$\rho(XY)=\frac{1}{A_c}\Big[F(00)+2\Big\{\sum_1^\infty h|F(h0)|\cos 2\pi hX+\sum_2^\infty k|F(0k)|\cos[2\pi kY-\alpha(0k)]\Big\}+$$
$$4\Big\{\sum_1^\infty h\sum_2^\infty k|F(hk)|\cos 2\pi hX\cos[2\pi kY-\alpha(hk)]-\sum_1^\infty h\sum_1^\infty k|F(hk)|\sin 2\pi hX\sin[2\pi kY-\alpha(hk)]\Big\}\Big]$$

Origin on m $(0,0;\ \tfrac{1}{2},\tfrac{1}{2})\ +\ |\ x,y;\ \bar{x},y\ |$ No. 5 cm

$$A=4\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi ky$$
$$B=4\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\sin 2\pi ky$$

$h+k=2n$ $A=4\cos 2\pi hx\cos 2\pi ky$ $|F(hk)|=|F(\bar{h}\bar{k})|=|F(\bar{h}k)|=|F(h\bar{k})|$

$B=4\cos 2\pi hx\sin 2\pi ky$ $=0$ if $k=0$ $\alpha(hk)=-\alpha(\bar{h}\bar{k})=\alpha(\bar{h}k)=-\alpha(h\bar{k})$

$h+k=2n+1$ $A=B=0$

$$\rho(XY)=\frac{1}{A_c}\Big[F(00)+2\Big\{\sum_2^\infty h|F(h0)|\cos 2\pi hX+\sum_2^\infty k|F(0k)|\cos[2\pi kY-\alpha(0k)]\Big\}+$$
$$4\sum_1^\infty h\sum_1^\infty k|F(hk)|\cos 2\pi hX\cos[2\pi kY-\alpha(hk)]\Big]$$

Origin at $2mm$ $\pm\ |\ x,y;\ \bar{x},y\ |$ No. 6 pmm

$A=4\cos 2\pi hx\cos 2\pi ky$ $F(hk)=F(\bar{h}\bar{k})=F(\bar{h}k)$

$B=0$

$$\rho(XY)=\frac{1}{A_c}\Big[F(00)+2\Big\{\sum_1^\infty hF(h0)\cos 2\pi hX+\sum_1^\infty kF(0k)\cos 2\pi kY\Big\}+4\sum_1^\infty h\sum_1^\infty kF(hk)\cos 2\pi hX\cos 2\pi kY\Big]$$

pmg No. 7 Origin at 2 Co-ordinates: $\pm\,|\,x,y;\ \frac{1}{2}+x,\bar{y}\,|$

$$A=4\cos 2\pi\left(hx+\frac{h}{4}\right)\cos 2\pi\left(ky-\frac{h}{4}\right)$$
$$B=0$$

$h=2n$	$A=4\cos 2\pi hx\cos 2\pi ky;\quad B=0$	$F(hk)=F(\bar{h}\bar{k})=F(\bar{h}k)$
$h=2n+1$	$A=-4\sin 2\pi hx\sin 2\pi ky;\quad A=B=0$ if $k=0$	$F(hk)=F(\bar{h}\bar{k})=-F(\bar{h}k)$

$$\rho(XY)=\frac{1}{A_c}\Big[F(00)+2\Big\{\sum_2^{\infty}{}^{h=2n}_{h}F(h0)\cos 2\pi hX+\sum_1^{\infty}{}_{k}F(0k)\cos 2\pi kY\Big\}+$$
$$4\Big\{\sum_2^{\infty}{}_{h}\sum_1^{\infty}{}^{h=2n}_{k}F(hk)\cos 2\pi hX\cos 2\pi kY-\sum_1^{\infty}{}_{h}\sum_1^{\infty}{}^{h=2n+1}_{k}F(hk)\sin 2\pi hX\sin 2\pi kY\Big\}\Big]$$

pgg No. 8 Origin at 2 $\pm\,|\,x,y;\ \frac{1}{2}+x,\frac{1}{2}-y\,|$

$$A=4\cos 2\pi\left(hx+\frac{h+k}{4}\right)\cos 2\pi\left(ky-\frac{h+k}{4}\right)$$
$$B=0$$

$h+k=2n$	$A=4\cos 2\pi hx\cos 2\pi ky;\quad B=0$	$F(hk)=F(\bar{h}\bar{k})=F(\bar{h}k)$
$h+k=2n+1$	$A=-4\sin 2\pi hx\sin 2\pi ky$	$F(hk)=F(\bar{h}\bar{k})=-F(\bar{h}k)$
	$A=B=0$ if $h=0$ or $k=0$	

$$\rho(XY)=\frac{1}{A_c}\Big[F(00)+2\Big\{\sum_2^{\infty}{}^{h=2n}_{h}F(h0)\cos 2\pi hX+\sum_2^{\infty}{}^{k=2n}_{k}F(0k)\cos 2\pi kY\Big\}+$$
$$4\Big\{\sum_1^{\infty}{}_{h}\sum_1^{\infty}{}^{h+k=2n}_{k}F(hk)\cos 2\pi hX\cos 2\pi kY-\sum_1^{\infty}{}_{h}\sum_1^{\infty}{}^{h+k=2n+1}_{k}F(hk)\sin 2\pi hX\sin 2\pi kY\Big\}\Big]$$

cmm No. 9 Origin at 2*mm* $(0,0;\ \frac{1}{2},\frac{1}{2})\pm\,|\,x,y;\ \bar{x},y\,|$

$$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi ky;\quad B=0$$

$h+k=2n$	$A=8\cos 2\pi hx\cos 2\pi ky;\quad B=0$	$F(hk)=F(\bar{h}\bar{k})=F(\bar{h}k)$
$h+k=2n+1$	$A=B=0$	

$$\rho(XY)=\frac{1}{A_c}\Big[F(00)+2\cdot\Big\{\sum_2^{\infty}{}^{h=2n}_{h}F(h0)\cos 2\pi hX+\sum_2^{\infty}{}^{k=2n}_{k}F(0k)\cos 2\pi kY\Big\}+4\sum_1^{\infty}{}_{h}\sum_1^{\infty}{}^{h+k=2n}_{k}F(hk)\cos 2\pi hX\cos 2\pi kY\Big]$$

Origin at 4 | Co-ordinates: $\pm\,|\,x,y;\ \bar{y},x\,|$ | No. 10 | $p4$

$A=4\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]$ $\qquad F(hk)=F(\bar{h}\bar{k})\neq F(\bar{h}k)$

$B=0$

$$\rho(XY)=\frac{1}{A_c}\Big[F(00)+2\Big\{\sum_1^\infty h\,F(h0)\cos 2\pi hX+\sum_1^\infty k\,F(0k)\cos 2\pi kY\Big\}+$$
$$2\Big\{\sum_1^\infty h\sum_1^\infty k\,F(hk)\cos 2\pi(hX+kY)+\sum_1^\infty h\sum_1^\infty k\,F(\bar{h}k)\cos 2\pi(hX-kY)\Big\}\Big]$$

Origin at $4mm$ | $\pm\,|\,x,y;\ \bar{x},y;\ y,x;\ \bar{y},x\,|$ | No. 11 | $p4m$

$A=4[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$ $\qquad F(hk)=F(\bar{h}\bar{k})=F(\bar{h}k)$

$B=0$

$$\rho(XY)=\frac{1}{A_c}\Big[F(00)+2\Big\{\sum_1^\infty h\,F(h0)\cos 2\pi hX+\sum_1^\infty k\,F(0k)\cos 2\pi kY\Big\}+4\sum_1^\infty h\sum_1^\infty k\,F(hk)\cos 2\pi hX\cos 2\pi kY\Big]$$

Origin at 4 | $\pm\,|\,x,y;\ \frac{1}{2}-x,\frac{1}{2}+y;\ \bar{y},x;\ \frac{1}{2}+y,\frac{1}{2}+x\,|$ | No. 12 | $p4g$

$$A=4\Big[\cos 2\pi\Big(hx-\frac{h+k}{4}\Big)\cos 2\pi\Big(ky+\frac{h+k}{4}\Big)+\cos 2\pi\Big(kx+\frac{h+k}{4}\Big)\cos 2\pi\Big(hy+\frac{h+k}{4}\Big)\Big]$$

$B=0$

$h+k=2n$ $\qquad A=4[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$ $\qquad F(hk)=F(\bar{h}\bar{k})=F(\bar{h}k)$

$h+k=2n+1$ $\qquad A=-4[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$ $\qquad F(hk)=F(\bar{h}\bar{k})=-F(\bar{h}k)$

$A=B=0$ if $h=0$ or $k=0$

$$\rho(XY)=\frac{1}{A_c}\Big[F(00)+2\Big\{\sum_2^\infty h\,F(h0)^{h=2n}\cos 2\pi hX+\sum_2^\infty k\,F(0k)^{k=2n}\cos 2\pi kY\Big\}+$$
$$4\Big\{\sum_1^\infty h\sum_1^\infty k\,F(hk)^{h+k=2n}\cos 2\pi hX\cos 2\pi kY-\sum_1^\infty h\sum_1^\infty k\,F(hk)^{h+k=2n+1}\sin 2\pi hX\sin 2\pi kY\Big\}\Big]$$

Origin at 3 | $|\,x,y;\ \bar{y},x-y;\ y-x,\bar{x}\,|$ | No. 13 | $p3$

$A=\cos 2\pi(hx+ky)+\cos 2\pi(kx-(h+k)y)+\cos 2\pi(hy-(h+k)x)$

$B=\sin 2\pi(hx+ky)+\sin 2\pi(kx-(h+k)y)+\sin 2\pi(hy-(h+k)x)$

$|F(hk)|=|F(\bar{h}\bar{k})|\neq|F(\bar{h}k)|;\quad |F(\bar{h}k)|=|F(h\bar{k})|$ $\qquad \alpha(hk)=-\alpha(\bar{h}\bar{k})\neq\alpha(\bar{h}k);\quad \alpha(\bar{h}k)=-\alpha(h\bar{k})$

$$\rho(XY)=\frac{1}{A_c}\Big[F(00)+2\Big\{\sum_1^\infty h\,|F(h0)|\cos[2\pi hX-\alpha(h0)]+\sum_1^\infty k\,|F(0k)|\cos[2\pi kY-\alpha(0k)]\Big\}+$$
$$2\Big\{\sum_1^\infty h\sum_1^\infty k\,|F(hk)|\cos[2\pi(hX+kY)-\alpha(hk)]+\sum_1^\infty h\sum_1^\infty k\,|F(\bar{h}k)|\cos[2\pi(-hX+kY)-\alpha(\bar{h}k)]\Big\}\Big]$$

$p3m1$ No. 14 Origin at $3m1$ Co-ordinates: $|\ x,y;\ \bar{y},x-y;\ y-x,\bar{x};\ \bar{y},\bar{x};\ x,x-y;\ y-x,y\ |$

$A=2\{\cos\pi(h-k)(x-y)\cos\pi(h+k)(x+y)+\cos\pi(h+2k)(x-y)\cos\pi h(x+y)+\cos\pi(2h+k)(x-y)\cos\pi k(x+y)\}$

$B=2\{\sin\pi(h-k)(x-y)\cos\pi(h+k)(x+y)+\sin\pi(h+2k)(x-y)\cos\pi h(x+y)-\sin\pi(2h+k)(x-y)\cos\pi k(x+y)\}$

$B=0$ if $h=k$ (or if $-2k=h$ or if $-2h=k$)

$|F(hk)|$, $\alpha(hk)$ relationships as for No. 13; $\rho(XY)$ as for No. 13.

$p31m$ No. 15 Origin at $31m$ $|\ x,y;\ \bar{y},x-y;\ y-x,\bar{x};\ y,x;\ \bar{x},y-x;\ x-y,\bar{y}\ |$

$A=2\{\cos\pi(h-k)(x-y)\cos\pi(h+k)(x+y)+\cos\pi(h+2k)(x-y)\cos\pi h(x+y)+\cos\pi(2h+k)(x-y)\cos\pi k(x+y)\}$

$B=2\{\cos\pi(h-k)(x-y)\sin\pi(h+k)(x+y)-\cos\pi(h+2k)(x-y)\sin\pi h(x+y)-\cos\pi(2h+k)(x-y)\sin\pi k(x+y)\}$

$B=0$ if $h=-k$ (or if $h=0$ or if $k=0$)

$|F(hk)|$, $\alpha(hk)$ relationships as for No. 13; $\rho(XY)$ as for No. 13.

$p6$ No. 16 Origin at 6 $\pm\ |\ x,y;\ \bar{y},x-y;\ y-x,\bar{x}\ |$

$A=2\{\cos 2\pi(hx+ky)+\cos 2\pi(kx-(h+k)y)+\cos 2\pi(hy-(h+k)x)\}$ $F(hk)=F(\bar{h}\bar{k})\neq F(\bar{h}k)$

$B=0$

$$\rho(XY)=\frac{1}{A_c}\left[F(00)+2\left\{\sum_1^\infty h\,F(h0)\cos 2\pi hX+\sum_1^\infty k\,F(0k)\cos 2\pi kY\right\}+\right.$$
$$\left.2\left\{\sum_1^\infty h\sum_1^\infty k\,F(hk)\cos 2\pi(hX+kY)+\sum_1^\infty h\sum_1^\infty k\,F(\bar{h}k)\cos 2\pi(hX-kY)\right\}\right]$$

$p6m$ No. 17 Origin at $6mm$ $\pm\ |\ x,y;\ \bar{y},x-y;\ y-x,\bar{x};\ y,x;\ \bar{x},y-x;\ x-y,\bar{y}\ |$

$A=4\{\cos\pi(h-k)(x-y)\cos\pi(h+k)(x+y)+\cos\pi(h+2k)(x-y)\cos\pi h(x+y)+\cos\pi(2h+k)(x-y)\cos\pi k(x+y)\}$

$B=0$ $F(hk)=F(\bar{h}\bar{k})\neq F(\bar{h}k)$

$\rho(XY)$ as for No. 16.

4.7. GEOMETRICAL STRUCTURE FACTORS AND ELECTRON DENSITY FORMULAE FOR THE THREE-DIMENSIONAL SPACE GROUPS

$P1$ C_1^1

No. 1

Origin on 1. Co-ordinates: $|\ x,y,z\ |$

$A = \cos 2\pi(hx+ky+lz)$ $|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|\neq|F(\bar{h}kl)|\neq|F(h\bar{k}l)|\neq|F(hk\bar{l})|$

$B = \sin 2\pi(hx+ky+lz)$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})$

$$\rho(XYZ)=\frac{2}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos[2\pi(hX+kY+lZ)-\alpha(hkl)]+|F(\bar{h}kl)|\cos[2\pi(-hX+kY+lZ)-\alpha(\bar{h}kl)]+$$
$$|F(h\bar{k}l)|\cos[2\pi(hX-kY+lZ)-\alpha(h\bar{k}l)]+|F(hk\bar{l})|\cos[2\pi(hX+kY-lZ)-\alpha(hk\bar{l})]\}$$

$P\bar{1}$ C_i^1

No. 2

Origin at $\bar{1}$. $\pm\ |\ x,y,z\ |$

$A=2\cos 2\pi(hx+ky+lz)$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})\neq F(\bar{h}kl)\neq F(h\bar{k}l)\neq F(hk\bar{l})$

$B=0$

$$\rho(XYZ)=\frac{2}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{F(hkl)\cos 2\pi(hX+kY+lZ)+F(\bar{h}kl)\cos 2\pi(-hX+kY+lZ)+$$
$$F(h\bar{k}l)\cos 2\pi(hX-kY+lZ)+F(hk\bar{l})\cos 2\pi(hX+kY-lZ)\}$$

$P2$ C_2^1

No. 3

Origin on 2. c as unique axis: $|\ x,y,z;\ \bar{x},\bar{y},z\ |$

$A=2\cos 2\pi(hx+ky)\cos 2\pi lz$ $|F(hkl)|=F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|$

$B=2\cos 2\pi(hx+ky)\sin 2\pi lz\ \ =0$ if $l=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(-hX+kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\}$$

Origin on 2. b as unique axis: $|\ x,y,z;\ \bar{x},y,\bar{z}\ |$

$A=2\cos 2\pi(hx+lz)\cos 2\pi ky$ $|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(h\bar{k}l)|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(hk\bar{l})|$

$B=2\cos 2\pi(hx+lz)\sin 2\pi ky\ \ =0$ if $k=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(h\bar{k}l)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(hk\bar{l})$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+lZ)\cos[2\pi kY-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(-hX+lZ)\cos[2\pi kY-\alpha(\bar{h}kl)]\}$$

Origin on 2_1. c as unique axis: $|\ x,y,z;\ \bar{x},\bar{y},\frac{1}{2}+z\ |$

$A=2\cos 2\pi\left(hx+ky+\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{l}{4}\right)$ $\quad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|$

$B=2\cos 2\pi\left(hx+ky+\frac{l}{4}\right)\sin 2\pi\left(lz-\frac{l}{4}\right)$

$l=2n$ $\quad A=2\cos 2\pi(hx+ky)\cos 2\pi lz$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$B=2\cos 2\pi(hx+ky)\sin 2\pi lz\ \ =0$ if $l=0$

$l=2n+1$ $\quad A=-2\sin 2\pi(hx+ky)\sin 2\pi lz$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})\neq\alpha(\bar{h}kl)$

$B=2\sin 2\pi(hx+ky)\cos 2\pi lz$ $\quad \alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$

$A=B=0$ if $h=k=0$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(-hX+kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\}^{l=2n}-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\sin 2\pi(hX+kY)\sin[2\pi lZ-\alpha(hkl)]+|F(\bar{h}kl)|\sin 2\pi(-hX+kY)\sin[2\pi lZ-\alpha(\bar{h}kl)]\}^{l=2n+1}\right\}$$

Origin on 2_1. b as unique axis: $|\ x,y,z;\ \bar{x},\frac{1}{2}+y,\bar{z}\ |$

$A=2\cos 2\pi\left(hx+lz+\frac{k}{4}\right)\cos 2\pi\left(ky-\frac{k}{4}\right)$ $\quad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(h\bar{k}l)|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(hk\bar{l})|$

$B=2\cos 2\pi\left(hx+lz+\frac{k}{4}\right)\sin 2\pi\left(ky-\frac{k}{4}\right)$

$k=2n$ $\quad A=2\cos 2\pi(hx+lz)\cos 2\pi ky$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(h\bar{k}l)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(hk\bar{l})$

$B=2\cos 2\pi(hx+lz)\sin 2\pi ky\ \ =0$ if $k=0$

$k=2n+1$ $\quad A=-2\sin 2\pi(hx+lz)\sin 2\pi ky$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(h\bar{k}l)\neq\alpha(\bar{h}kl)$

$B=2\sin 2\pi(hx+lz)\cos 2\pi ky$ $\quad \alpha(\bar{h}kl)=\pi+\alpha(hk\bar{l})$

$A=B=0$ if $h=l=0$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+lZ)\cos[2\pi kY-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(-hX+lZ)\cos[2\pi kY-\alpha(\bar{h}kl)]\}^{k=2n}-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\sin 2\pi(hX+lZ)\sin[2\pi kY-\alpha(hkl)]+|F(\bar{h}kl)|\sin 2\pi(-hX+lZ)\sin[2\pi kY-\alpha(\bar{h}kl)]\}^{k=2n+1}\right\}$$

$B2$ C_2^3 No. 5

Origin on 2. c as unique axis: $(0,0,0;\ \frac{1}{2},0,\frac{1}{2})\ +\ |\ x,y,z;\ \bar{x},\bar{y},z\ |$

$A=4\cos^2 2\pi\frac{h+l}{4}\cos 2\pi(hx+ky)\cos 2\pi lz$ $\quad |F(hkl)|=|F(\bar{h}k\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|$

$B=4\cos^2 2\pi\frac{h+l}{4}\cos 2\pi(hx+ky)\sin 2\pi lz\ =0$ if $l=0$ $\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|$

$h+l=2n$ $\quad A=4\cos 2\pi(hx+ky)\cos 2\pi lz$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(hk\bar{l})\neq\alpha(\bar{h}kl)$

$B=4\cos 2\pi(hx+ky)\sin 2\pi lz$ $\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$h+l=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(-hX+kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\}$$

$C2$ C_2^3 No. 5

Origin on 2. b as unique axis: $(0,0,0;\ \frac{1}{2},\frac{1}{2},0)\ +\ |\ x,y,z;\ \bar{x},y,\bar{z}\ |$

$A=4\cos^2 2\pi\frac{h+k}{4}\cos 2\pi(hx+lz)\cos 2\pi ky$ $\quad |F(hkl)|=|F(\bar{h}k\bar{l})|=|F(h\bar{k}l)|\neq|F(\bar{h}kl)|$

$B=4\cos^2 2\pi\frac{h+k}{4}\cos 2\pi(hx+lz)\sin 2\pi ky\ =0$ if $k=0$ $\quad |F(\bar{h}kl)|=|F(hk\bar{l})|$

$h+k=2n$ $\quad A=4\cos 2\pi(hx+lz)\cos 2\pi ky$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(h\bar{k}l)\neq\alpha(\bar{h}kl)$

$B=4\cos 2\pi(hx+lz)\sin 2\pi ky$ $\quad \alpha(\bar{h}kl)=\alpha(hk\bar{l})$

$h+k=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+lZ)\cos[2\pi kY-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(-hX+lZ)\cos[2\pi kY-\alpha(\bar{h}kl)]\}$$

No. 6

Pm C_s^1

Origin on m. c as unique ($\bar{2}$) axis: $|\ x,y,z;\ x,y,\bar{z}\ |$

$A=2\cos 2\pi(hx+ky)\cos 2\pi lz$ $\quad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|$

$B=2\sin 2\pi(hx+ky)\cos 2\pi lz\ =0$ if $h=k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(hk\bar{l})\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=-\alpha(h\bar{k}l)$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos[2\pi(hX+kY)-\alpha(hkl)]+|F(\bar{h}kl)|\cos[2\pi(-hX+kY)-\alpha(\bar{h}kl)]\}\cos 2\pi lz$$

Origin on m. b as unique ($\bar{2}$) axis: $|\ x,y,z;\ x,\bar{y},z\ |$

$A=2\cos 2\pi(hx+lz)\cos 2\pi ky$ $\quad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(h\bar{k}l)|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(hk\bar{l})|$

$B=2\sin 2\pi(hx+lz)\cos 2\pi ky\ =0$ if $h=l=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(h\bar{k}l)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=-\alpha(hk\bar{l})$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos[2\pi(hX+lZ)-\alpha(hkl)]+|F(\bar{h}kl)|\cos[2\pi(-hX+lZ)-\alpha(\bar{h}kl)]\}\cos 2\pi kY$$

No. 7

Pb C_s^2

Origin on glide-plane (glide $b/2$). c as unique ($\bar{2}$) axis: $|\ x,y,z;\ x,\frac{1}{2}+y,\bar{z}\ |$

$A=2\cos 2\pi\left(hx+ky+\frac{k}{4}\right)\cos 2\pi\left(lz-\frac{k}{4}\right)$ $\quad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|$

$B=2\sin 2\pi\left(hx+ky+\frac{k}{4}\right)\cos 2\pi\left(lz-\frac{k}{4}\right)\ =0$ if $h=k=0$

$k=2n$ $\quad A=2\cos 2\pi(hx+ky)\cos 2\pi lz$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(hk\bar{l})\neq\alpha(\bar{h}kl)$

$B=2\sin 2\pi(hx+ky)\cos 2\pi lz$ $\quad \alpha(\bar{h}kl)=-\alpha(h\bar{k}l)$

$k=2n+1$ $\quad A=-2\sin 2\pi(hx+ky)\sin 2\pi lz$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(hk\bar{l})\neq\alpha(\bar{h}kl)$

$B=2\cos 2\pi(hx+ky)\sin 2\pi lz$ $\quad \alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)$

$A=B=0$ if $l=0$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|\overset{k=2n}{F(hkl)}|\cos[2\pi(hX+kY)-\alpha(hkl)]+|F(\bar{h}kl)|\cos[2\pi(-hX+kY)-\alpha(\bar{h}kl)]\}\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|\overset{k=2n+1}{F(hkl)}|\sin[2\pi(hX+kY)-\alpha(hkl)]+|F(\bar{h}kl)|\sin[2\pi(-hX+kY)-\alpha(\bar{h}kl)]\}\sin 2\pi lZ\right\}$$

Pc C_s^2 No. 7

Origin on glide-plane (glide $c/2$). b as unique ($\bar{2}$) axis: $|\ x,y,z;\ x,\bar{y},\frac{1}{2}+z\ |$

$A=2\cos 2\pi\left(hx+lz+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)$ $\quad |F(hkl)|=|F(\bar{h}k\bar{l})|=|F(h\bar{k}l)|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(hk\bar{l})|$

$B=2\sin 2\pi\left(hx+lz+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)$ $=0$ if $h=l=0$

$l=2n$ $\quad A=2\cos 2\pi(hx+lz)\cos 2\pi ky$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(h\bar{k}l)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=-\alpha(hk\bar{l})$

$B=2\sin 2\pi(hx+lz)\cos 2\pi ky$

$l=2n+1$ $\quad A=-2\sin 2\pi(hx+lz)\sin 2\pi ky$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(h\bar{k}l)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\pi-\alpha(hk\bar{l})$

$B=2\cos 2\pi(hx+lz)\sin 2\pi ky$

$A=B=0$ if $k=0$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty\overset{l=2n}{}\{|F(hkl)|\cos[2\pi(hX+lZ)-\alpha(hkl)]+|F(\bar{h}kl)|\cos[2\pi(-hX+lZ)-\alpha(\bar{h}kl)]\}\cos 2\pi kY-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty\overset{l=2n+1}{}\{|F(hkl)|\sin[2\pi(hX+lZ)-\alpha(hkl)]+|F(\bar{h}kl)|\sin[2\pi(-hX+lZ)-\alpha(\bar{h}kl)]\}\sin 2\pi kY\right\}$$

Bm C_s^3 No. 8

Origin on m. c as unique ($\bar{2}$) axis: $(0,0,0;\ \frac{1}{2},0,\frac{1}{2})+\ |\ x,y,z;\ x,y,\bar{z}\ |$

$A=4\cos^2 2\pi\frac{h+l}{4}\cos 2\pi(hx+ky)\cos 2\pi lz$ $\quad |F(hkl)|=|F(\bar{h}k\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|$

$B=4\cos^2 2\pi\frac{h+l}{4}\sin 2\pi(hx+ky)\cos 2\pi lz$ $\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|$

$h+l=2n$ $\quad A=4\cos 2\pi(hx+ky)\cos 2\pi lz$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(hk\bar{l})\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=-\alpha(h\bar{k}l)$

$B=4\sin 2\pi(hx+ky)\cos 2\pi lz$ $=0$ if $h=k=0$

$h+l=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos[2\pi(hX+kY)-\alpha(hkl)]+|F(\bar{h}kl)|\cos[2\pi(-hX+kY)-\alpha(\bar{h}kl)]\}\cos 2\pi lZ$$

No. 8 Cm C_s^3

Origin on m. b as unique ($\bar{2}$) axis: $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) + |\ x,y,z;\ x,\bar{y},z\ |$

$A=4\cos^2 2\pi\frac{h+k}{4}\cos 2\pi(hx+lz)\cos 2\pi ky$ $\quad |F(hkl)|=|F(\bar{h}k\bar{l})|=|F(h\bar{k}l)|\neq|F(\bar{h}kl)|$

$B=4\cos^2 2\pi\frac{h+k}{4}\sin 2\pi(hx+lz)\cos 2\pi ky$ $\quad |F(\bar{h}kl|=|F(hk\bar{l})|$

$h+k=2n$ $\quad A=4\cos 2\pi(hx+lz)\cos 2\pi ky$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(h\bar{k}l)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=-\alpha(hk\bar{l})$

$B=4\sin 2\pi(hx+lz)\cos 2\pi ky$ $=0$ if $h=l=0$

$h+k=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos[2\pi(hX+lZ)-\alpha(hkl)]+|F(\bar{h}kl)|\cos[2\pi(-hX+lZ)-\alpha(\bar{h}kl)]\}\cos 2\pi kY$$

No. 9 Bb C_s^4

Origin on glide-plane (glide $b/2$). c as unique ($\bar{2}$) axis: $(0,0,0;\ \frac{1}{2},0,\frac{1}{2}) + |\ x,y,z;\ x,\frac{1}{2}+y,\bar{z}\ |$

$A=4\cos^2 2\pi\frac{h+l}{4}\cos 2\pi\left(hx+ky+\frac{k}{4}\right)\cos 2\pi\left(lz-\frac{k}{4}\right)$ $\quad |F(hkl)|=|F(\bar{h}k\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|$

$B=4\cos^2 2\pi\frac{h+l}{4}\sin 2\pi\left(hx+ky+\frac{k}{4}\right)\cos 2\pi\left(lz-\frac{k}{4}\right)$ $\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|$

$\begin{cases} h+l=2n \\ k=2n \end{cases}$ $\quad A=4\cos 2\pi(hx+ky)\cos 2\pi lz$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(hk\bar{l})\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=-\alpha(h\bar{k}l)$

$B=4\sin 2\pi(hx+ky)\cos 2\pi lz$ $=0$ if $h=k=0$

$\begin{cases} h+l=2n \\ k=2n+1 \end{cases}$ $\quad A=-4\sin 2\pi(hx+ky)\sin 2\pi lz$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(hk\bar{l})\neq\alpha(\bar{h}kl)$

$B=4\cos 2\pi(hx+ky)\sin 2\pi lz$ $\quad \alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)$

$A=B=0$ if $l=0$

$h+l=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty\overset{k=2n}{\{}|F(hkl)|\cos[2\pi(hX+kY)-\alpha(hkl)]+|F(\bar{h}kl)|\cos[2\pi(-hX+kY)-\alpha(\bar{h}kl)]\}\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty\overset{k=2n+1}{\{}|F(hkl)|\sin[2\pi(hX+kY)-\alpha(hkl)]+|F(\bar{h}kl)|\sin[2\pi(-hX+kY)-\alpha(\bar{h}kl)]\}\sin 2\pi lZ\}\right\}$$

Cc C_s^4

No. 9

Origin on glide-plane (glide $c/2$). b as unique ($\bar{2}$) axis: $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) + \mid x,y,z;\ x,\bar{y},\frac{1}{2}+z \mid$

$A=4\cos^2 2\pi\frac{h+k}{4}\cos 2\pi\left(hx+lz+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)$ $\quad |F(hkl)|=|F(\bar{h}k\bar{l})|=|F(h\bar{k}l)|\neq|F(\bar{h}kl)|$

$B=4\cos^2 2\pi\frac{h+k}{4}\sin 2\pi\left(hx+lz+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)$ $\quad |F(\bar{h}kl)|=|F(hk\bar{l})|$

$\begin{cases} h+k=2n \\ l=2n \end{cases}$ $\quad A=4\cos 2\pi(hx+lz)\cos 2\pi ky$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(h\bar{k}l)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=-\alpha(hk\bar{l})$

$B=4\sin 2\pi(hx+lz)\cos 2\pi ky$ $\quad =0$ if $h=l=0$

$\begin{cases} h+k=2n \\ l=2n+1 \end{cases}$ $\quad A=-4\sin 2\pi(hx+lz)\sin 2\pi ky$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(h\bar{k}l)\neq\alpha(\bar{h}kl)$

$B=4\cos 2\pi(hx+lz)\sin 2\pi ky$ $\quad \alpha(\bar{h}kl)=\pi-\alpha(hk\bar{l})$

$A=B=0$ if $k=0$

$h+k=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos[2\pi(hX+lZ)-\alpha(hkl)]+|F(\bar{h}kl)|\cos[2\pi(-hX+lZ)-\alpha(\bar{h}kl)]\}\cos 2\pi kY-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\sin[2\pi(hX+lZ)-\alpha(hkl)]+|F(\bar{h}kl)|\sin[2\pi(-hX+lZ)-\alpha(\bar{h}kl)]\}\sin 2\pi kY\right\}$$

$P2/m$ C_{2h}^1

No. 10

Origin at centre ($2/m$) $\quad c$ as unique axis: $\quad \pm \mid x,y,z;\ x,y,\bar{z} \mid$

$A=4\cos 2\pi(hx+ky)\cos 2\pi lz$ $\quad F(hkl)=F(\bar{h}k\bar{l})=F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(h\bar{k}l)$

$B=0$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(-hX+kY)\}\cos 2\pi lZ$$

Origin at centre ($2/m$) $\quad b$ as unique axis: $\quad \pm \mid x,y,z;\ x,\bar{y},z \mid$

$A=4\cos 2\pi(hx+lz)\cos 2\pi ky$ $\quad F(hkl)=F(\bar{h}k\bar{l})=F(h\bar{k}l)\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(hk\bar{l})$

$B=0$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{F(hkl)\cos 2\pi(hX+lZ)+F(\bar{h}kl)\cos 2\pi(-hX+lZ)\}\cos 2\pi kY$$

No. 11 $P2_1/m$ C_{2h}^2

Origin at $\bar{1}$. c as unique axis: $\pm\ |\ x,y,z;\ x,y,\frac{1}{2}-z\ |$

$A=4\cos 2\pi\left(hx+ky+\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{l}{4}\right)$ $F(hkl)=F(\bar{h}k\bar{l})$

$B=0$

$l=2n$	$A=4\cos 2\pi(hx+ky)\cos 2\pi lz;\ B=0$	$F(hkl)=F(hk\bar{l})\neq F(\bar{h}kl);\ F(\bar{h}kl)=F(h\bar{k}l)$
$l=2n+1$	$A=-4\sin 2\pi(hx+ky)\sin 2\pi lz;\ B=0$	$F(hkl)=-F(hk\bar{l})\neq F(\bar{h}kl);\ F(\bar{h}kl)=-F(h\bar{k}l)$
	$A=B=0$ if $h=k=0$	

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^{l=2n}[F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(-hX+kY)]\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^{l=2n+1}[F(hkl)\sin 2\pi(hX+kY)+F(\bar{h}kl)\sin 2\pi(-hX+kY)]\sin 2\pi lZ\right\}$$

Origin at $\bar{1}$. b as unique axis: $\pm\ |\ x,y,z;\ x,\frac{1}{2}-y,z\ |$

$A=4\cos 2\pi\left(hx+lz+\frac{k}{4}\right)\cos 2\pi\left(ky-\frac{k}{4}\right)$ $F(hkl)=F(\bar{h}k\bar{l})$

$B=0$

$k=2n$	$A=4\cos 2\pi(hx+lz)\cos 2\pi ky;\ B=0$	$F(hkl)=F(h\bar{k}l)\neq F(\bar{h}kl);\ F(\bar{h}kl)=F(hk\bar{l})$
$k=2n+1$	$A=-4\sin 2\pi(hx+lz)\sin 2\pi ky;\ B=0$	$F(hkl)=-F(h\bar{k}l)\neq F(\bar{h}kl);\ F(\bar{h}kl)=-F(hk\bar{l})$
	$A=B=0$ if $h=l=0$	

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^{k=2n}[F(hkl)\cos 2\pi(hX+lZ)+F(\bar{h}kl)\cos 2\pi(-hX+lZ)]\cos 2\pi kY-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^{k=2n+1}[F(hkl)\sin 2\pi(hX+lZ)+F(\bar{h}kl)\sin 2\pi(-hX+lZ)]\sin 2\pi kY\right\}$$

No. 12 $B2/m$ C_{2h}^3

Origin at centre $(2/m)$ c as unique axis: $(0,0,0;\ \frac{1}{2},0,\frac{1}{2})\ \pm\ |\ x,y,z;\ x,y,\bar{z}\ |$

$A=8\cos^2 2\pi\frac{h+l}{4}\cos 2\pi(hx+ky)\cos 2\pi lz$ $F(hkl)=F(\bar{h}k\bar{l})$

$B=0$

$h+l=2n$	$A=8\cos 2\pi(hx+ky)\cos 2\pi lz;\ B=0$	$F(hkl)=F(hk\bar{l})\neq F(\bar{h}kl);\ F(\bar{h}kl)=F(h\bar{k}l)$
$h+l=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(-hX+kY)\}\cos 2\pi lZ$$

$C2/m$
C_{2h}^3

No. 12

Origin at centre $(2/m)$ — b as unique axis: — $(0,0,0;\ \frac{1}{2},\frac{1}{2},0)\ \pm\ |\ x,y,z;\ x,\bar{y},z\ |$

$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi(hx+lz)\cos 2\pi ky$ — $F(hkl)=F(\bar{h}\bar{k}\bar{l})$

$B=0$

$h+k=2n$	$A=8\cos 2\pi(hx+lz)\cos 2\pi ky;\quad B=0$	$F(hkl)=F(h\bar{k}l)\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(hk\bar{l})$
$h+k=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{F(hkl)\cos 2\pi(hX+lZ)+F(\bar{h}kl)\cos 2\pi(-hX+lZ)\}\cos 2\pi kY$$

$P2/b$
C_{2h}^4

No. 13

Origin at $\bar{1}$. — c as unique axis: — $\pm\ |\ x,y,z;\ x,\frac{1}{2}+y,\bar{z}\ |$

$A=4\cos 2\pi\left(hx+ky+\frac{k}{4}\right)\cos 2\pi\left(lz-\frac{k}{4}\right);\quad B=0$ — $F(hkl)=F(\bar{h}\bar{k}\bar{l})$

$k=2n$	$A=4\cos 2\pi(hx+ky)\cos 2\pi lz;\quad B=0$	$F(hkl)=F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(h\bar{k}l)$
$k=2n+1$	$A=-4\sin 2\pi(hx+ky)\sin 2\pi lz;\quad B=0$	$F(hkl)=-F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(h\bar{k}l)$
	$A=B=0$ if $l=0$	

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n}[F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(-hX+kY)]\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n+1}[F(hkl)\sin 2\pi(hX+kY)+F(\bar{h}kl)\sin 2\pi(-hX+kY)]\sin 2\pi lZ\right\}$$

$P2/c$
C_{2h}^4

No. 13

Origin at $\bar{1}$. — b as unique axis: — $\pm\ |\ x,y,z;\ x,\bar{y},\frac{1}{2}+z\ |$

$A=4\cos 2\pi\left(hx+lz+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right);\quad B=0$ — $F(hkl)=F(\bar{h}\bar{k}\bar{l})$

$l=2n$	$A=4\cos 2\pi(hx+lz)\cos 2\pi ky;\quad B=0$	$F(hkl)=F(h\bar{k}l)\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(hk\bar{l})$
$l=2n+1$	$A=-4\sin 2\pi(hx+lz)\sin 2\pi ky;\quad B=0$	$F(hkl)=-F(h\bar{k}l)\neq F(\bar{h}kl);\quad F(\bar{h}kl)=-F(hk\bar{l})$
	$A=B=0$ if $k=0$	

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}[F(hkl)\cos 2\pi(hX+lZ)+F(\bar{h}kl)\cos 2\pi(-hX+lZ)]\cos 2\pi kY-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}[F(hk\bar{l})\sin 2\pi(hX+lZ)+F(\bar{h}kl)\sin 2\pi(-hX+lZ)]\sin 2\pi kY\right\}$$

No. 14 $P2_1/b$ C_{2h}^5

Origin at $\bar{1}$. c as unique axis: $\pm\ |x,y,z;\ x,\frac{1}{2}+y,\frac{1}{2}-z|$

$A=4\cos 2\pi\left(hx+ky+\frac{k+l}{4}\right)\cos 2\pi\left(lz-\frac{k+l}{4}\right);\quad B=0$ $\qquad F(hkl)=F(\bar{h}k\bar{l})$

$k+l=2n$	$A=4\cos 2\pi(hx+ky)\cos 2\pi lz;\quad B=0$	$F(hkl)=F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(h\bar{k}l)$
$k+l=2n+1$	$A=-4\sin 2\pi(hx+ky)\sin 2\pi lz;\quad B=0$	$F(hkl)=-F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=-F(h\bar{k}l)$
	$A=B=0$ if $h=k=0$ or if $l=0$	

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k+l=2n}[F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(-hX+kY)]\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k+l=2n+1}[F(hkl)\sin 2\pi(hX+kY)+F(\bar{h}kl)\sin 2\pi(-hX+kY)]\sin 2\pi lZ\right\}$$

No. 14 $P2_1/c$ C_{2h}^5

Origin at $\bar{1}$. b as unique axis: $\pm\ |x,y,z;\ x,\frac{1}{2}-y,\frac{1}{2}+z|$

$A=4\cos 2\pi\left(hx+lz+\frac{k+l}{4}\right)\cos 2\pi\left(ky-\frac{k+l}{4}\right);\quad B=0$ $\qquad F(hkl)=F(\bar{h}k\bar{l})$

$k+l=2n$	$A=4\cos 2\pi(hx+lz)\cos 2\pi ky;\quad B=0$	$F(hkl)=F(h\bar{k}l)\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(hk\bar{l})$
$k+l=2n+1$	$A=-4\sin 2\pi(hx+lz)\sin 2\pi ky;\quad B=0$	$F(hkl)=-F(h\bar{k}l)\neq F(\bar{h}kl);\quad F(\bar{h}kl)=-F(hk\bar{l})$
	$A=B=0$ if $h=l=0$ or if $k=0$	

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k+l=2n}[F(hkl)\cos 2\pi(hX+lZ)+F(\bar{h}kl)\cos 2\pi(-hX+lZ)]\cos 2\pi kY-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k+l=2n+1}[F(hkl)\sin 2\pi(hX+lZ)+F(\bar{h}kl)\sin 2\pi(-hX+lZ)]\sin 2\pi kY\right\}$$

No. 15 $\bar{B}2/b$ C_{2h}^6

Origin at $\bar{1}$ on glide-plane b. c as unique axis: $(0,0,0;\ \frac{1}{2},0,\frac{1}{2})\ \pm\ |x,y,z;\ x,\frac{1}{2}+y,\bar{z}|$

$A=8\cos^2 2\pi\frac{h+l}{4}\cos 2\pi\left(hx+ky+\frac{k}{4}\right)\cos 2\pi\left(lz-\frac{k}{4}\right);\quad B=0$ $\qquad F(hkl)=F(\bar{h}k\bar{l})$

$h+l=2n$	$A=8\cos 2\pi(hx+ky)\cos 2\pi lz$	$F(hkl)=F(hk\bar{l})\neq F(\bar{h}kl)$
$k=2n$	$B=0$	$F(\bar{h}kl)=F(h\bar{k}l)$
$h+l=2n$	$A=-8\sin 2\pi(hx+ky)\sin 2\pi lz;\quad B=0$	$F(hkl)=-F(hk\bar{l})\neq F(\bar{h}kl)$
$k=2n+1$	$A=B=0$ if $l=0$	$F(\bar{h}kl)=-F(h\bar{k}l)$
$h+l=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n}[F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(-hX+kY)]\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n+1}[F(hkl)\sin 2\pi(hX+kY)+F(\bar{h}kl)\sin 2\pi(-hX+kY)]\sin 2\pi lZ\right\}$$

$C2/c$ C_{2h}^{6}

No. 15

Origin at $\bar{1}$ on glide-plane c. b as unique axis: $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) \pm \ |\ x,y,z;\ x,\bar{y},\frac{1}{2}+z\ |$

$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi\left(hx+lz+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right);\quad B=0$ $\qquad F(hkl)=F(\bar{h}\bar{k}\bar{l})$

$\begin{cases} h+k=2n \\ \quad l=2n \end{cases}$ $\quad A=8\cos 2\pi(hx+lz)\cos 2\pi ky$, $\quad B=0$ $\qquad F(hkl)=F(h\bar{k}l)\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(hk\bar{l})$

$\begin{cases} h+k=2n \\ \quad l=2n+1 \end{cases}$ $\quad A=-8\sin 2\pi(hx+lz)\sin 2\pi ky;\quad B=0$ $\qquad F(hkl)=-F(h\bar{k}l)\neq F(\bar{h}kl);\quad F(\bar{h}kl)=-F(hk\bar{l})$

$h+k=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^{l=2n}[F(hkl)\cos 2\pi(hX+lZ)+F(\bar{h}kl)\cos 2\pi(-hX+lZ)]\cos 2\pi kY-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^{l=2n+1}[F(hkl)\sin 2\pi(hX+lZ)+F(\bar{h}kl)\sin 2\pi(-hX+lZ)]\sin 2\pi kY\right\}$$

$P222$ D_2^1

No. 16

Origin at 222. $\qquad |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z\ |$

$A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $\qquad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$B=-4\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $\qquad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$B=0$ if $h=0$ or $k=0$ or $l=0$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\{\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)\}$$

$P222_1$ D_2^2

No. 17

Origin at 212_1. $\qquad |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\frac{1}{2}-z;\ \bar{x},\bar{y},\frac{1}{2}+z\ |$

$A=4\cos 2\pi hx\cos 2\pi\left(ky+\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{l}{4}\right)$ $\qquad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$B=-4\sin 2\pi hx\sin 2\pi\left(ky+\frac{l}{4}\right)\sin 2\pi\left(lz-\frac{l}{4}\right)=0$ if $h=0$ or $l=0$

$l=2n$	$A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=-4\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $k=0$	
$l=2n+1$	$A=-4\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $k=0$	
	$B=4\sin 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}|F(hkl)|[\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\cos 2\pi kY\cos 2\pi lZ\sin\alpha(hkl)]\right\}$$

No. 18 $P2_12_12$ D_2^3

Origin at 112, in plane of 2_12_1. | $x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}+x,\frac{1}{2}-y,\bar{z};\ \frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$ |

$$A=4\cos 2\pi\left(hx+\frac{h+k}{4}\right)\cos 2\pi\left(ky-\frac{h+k}{4}\right)\cos 2\pi lz \qquad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$$B=-4\sin 2\pi\left(hx+\frac{h+k}{4}\right)\sin 2\pi\left(ky-\frac{h+k}{4}\right)\sin 2\pi lz \quad =0 \text{ if } l=0$$

$h+k=2n$	$A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=-4\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $h=0$ or $k=0$	
$h+k=2n+1$	$A=-4\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$ $=0$ if $h=0$ or $k=0$	
	$B=4\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|[\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]\right\}$$

No. 19 $P2_12_12_1$ D_2^4

Origin midway between 3 pairs of non-intersecting screw axes.

| $x,y,z;\ \frac{1}{2}-x,\bar{y},\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}-y,\bar{z};\ \bar{x},\frac{1}{2}+y,\frac{1}{2}-z$ |

$$A=4\cos 2\pi\left(hx-\frac{h-k}{4}\right)\cos 2\pi\left(ky-\frac{k-l}{4}\right)\cos 2\pi\left(lz-\frac{l-h}{4}\right) \qquad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$$B=-4\sin 2\pi\left(hx-\frac{h-k}{4}\right)\sin 2\pi\left(ky-\frac{k-l}{4}\right)\sin 2\pi\left(lz-\frac{l-h}{4}\right)$$

$\begin{cases} h+k=2n \\ k+l=2n \end{cases}$	$A=4\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz$ $B=-4\sin 2\pi hx \sin 2\pi ky \sin 2\pi lz$ $=0$ if $h=0$ or $k=0$ or $l=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$\begin{cases} h+k=2n \\ k+l=2n+1 \end{cases}$	$A=-4\cos 2\pi hx \sin 2\pi ky \sin 2\pi lz$ $=0$ if $k=0$ or $l=0$ $B=4\sin 2\pi hx \cos 2\pi ky \cos 2\pi lz$ $=0$ if $h=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$
$\begin{cases} h+k=2n+1 \\ k+l=2n \end{cases}$	$A=-4\sin 2\pi hx \cos 2\pi ky \sin 2\pi lz$ $=0$ if $h=0$ or $l=0$ $B=4\cos 2\pi hx \sin 2\pi ky \cos 2\pi lz$ $=0$ if $k=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$
$\begin{cases} h+k=2n+1 \\ k+l=2n+1 \end{cases}$	$A=-4\sin 2\pi hx \sin 2\pi ky \cos 2\pi lz$ $=0$ if $h=0$ or $k=0$ $B=4\cos 2\pi hx \cos 2\pi ky \sin 2\pi lz$ $=0$ if $l=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n+1}|F(hkl)|[\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\cos 2\pi kY\cos 2\pi lZ\sin\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n}|F(hkl)|[\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\cos\alpha(hkl)-\cos 2\pi hX\sin 2\pi kY\cos 2\pi lZ\sin\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n+1}|F(hkl)|[\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]\Big\}$$

$C222_1$
D_2^5

No. 20

Origin at 212_1. $(0,0,0;\ \frac{1}{2},\frac{1}{2},0)+\ |\ x,y,z;\ \ x,\bar{y},\bar{z};\ \ \bar{x},y,\frac{1}{2}-z;\ \ \bar{x},\bar{y},\frac{1}{2}+z\ |$

$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi\left(ky+\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{l}{4}\right)$ $\quad |F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$B=-8\cos^2 2\pi\frac{h+k}{4}\sin 2\pi hx\sin 2\pi\left(ky+\frac{l}{4}\right)\sin 2\pi\left(lz-\frac{l}{4}\right)$ $=0$ if $h=0$ or $l=0$

$\begin{cases} h+k=2n \\ l=2n \end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $k=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$\begin{cases} h+k=2n \\ l=2n+1 \end{cases}$	$A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $k=0$ $B=8\sin 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$
$h+k=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}|F(hkl)|[\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\cos 2\pi kY\cos 2\pi lZ\sin\alpha(hkl)]\Big\}$$

No. 21 $C222$ D_2^6

Origin at 222. $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) +\ |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z\ |$

$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $\quad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|\bar{F}(hk\bar{l})|=|F(hk\bar{l})|$

$B=-8\cos^2 2\pi\frac{h+k}{4}\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $h=0$ or $k=0$ or $l=0$

$h+k=2n$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$	
$h+k=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\{\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cdot\sin\alpha(hkl)\}$$

No. 22 $F222$ D_2^7

Origin at 222. $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0) +\ |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z\ |$

$A=16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $\quad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$B=-16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $h=0$ or $k=0$ or $l=0$

$\begin{cases} h+k=2n \text{ and} \\ k+l=2n \end{cases}$	$A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=-16\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$	(indices all even or all odd)
$h+k=2n+1$ or $k+l=2n+1$	$A=B=0$	(indices mixed even and odd)

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\{\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)\}$$

No. 23 $I222$ D_2^8

Origin at 222. $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) +\ |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z\ |$

$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $\quad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$B=-8\cos^2 2\pi\frac{h+k+l}{4}\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $h=0$ or $k=0$ or $l=0$

$h+k+l=2n$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$	
$h+k+l=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\{\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)\}$$

$I2_12_12_1$ D_2^9

No. 24

Origin midway between 3 pairs of non-intersecting rotation axes.

$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) + \ |\ x,y,z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,\bar{z};\ \bar{x},\tfrac{1}{2}+y,\tfrac{1}{2}-z;\ \tfrac{1}{2}-x,\bar{y},\tfrac{1}{2}+z\ |$

$$A=8\cos 2\pi\frac{h+k+l}{4}\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{h}{4}\right)\cos 2\pi\left(lz-\frac{k}{4}\right)$$

$$B=-8\cos 2\pi\frac{h+k+l}{4}\sin 2\pi\left(hx-\frac{l}{4}\right)\sin 2\pi\left(ky-\frac{h}{4}\right)\sin 2\pi\left(lz-\frac{k}{4}\right)$$

[Note that the first term is not squared.]

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

h, k, l all even	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $h=0$ or $k=0$ or $l=0$	
$h+k+l=2n+1$	$A=B=0$	
h even, k and l odd	$A=-8\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz$ $=0$ if $h=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$
	$B=8\cos 2\pi hx\sin 2\pi ky\cos 2\pi lz$	
k even, l and h odd	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$ $=0$ if $k=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=8\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	
l even, h and k odd	$A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $l=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$
	$B=8\sin 2\pi hx\cos 2\pi ky\cos 2\pi lz$	

$$\rho(XYZ)=\frac{8}{V_0}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n,\,l=2n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n+1,\,l=2n+1}|F(hkl)|[\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\cos\alpha(hkl)-\cos 2\pi hX\sin 2\pi kY\cos 2\pi lZ\sin\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n,\,l=2n+1}|F(hkl)|[\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n+1,\,l=2n}|F(hkl)|[\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\cos 2\pi kY\cos 2\pi lZ\sin\alpha(hkl)]\Big\}$$

$Pmm2$ C_{2v}^1

No. 25

Origin on $mm2$.

$|\ x,y,z;\ \bar{x},y,z;\ x,\bar{y},z;\ \bar{x},\bar{y},z\ |$

$A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$

$B=4\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$ $=0$ if $l=0$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_0}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]$$

No. 26 $Pmc2_1$ C_{2v}^{2}

Origin on 2_1. | $x,y,z;\ \bar{x},y,z;\ x,\bar{y},\frac{1}{2}+z;\ \bar{x},\bar{y},\frac{1}{2}+z$ |

$A=4\cos 2\pi hx\cos 2\pi\left(ky-\frac{l}{4}\right)\cos 2\pi\left(lz+\frac{l}{4}\right)$ $\quad |F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$B=4\cos 2\pi hx\cos 2\pi\left(ky-\frac{l}{4}\right)\sin 2\pi\left(lz+\frac{l}{4}\right)$ $=0$ if $l=0$

$l=2n$	$A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=4\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	
$l=2n+1$	$A=-4\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$
	$B=4\cos 2\pi hx\sin 2\pi ky\cos 2\pi lz$	
	$A=B=0$ if $k=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}|F(hkl)|\cos 2\pi hX\sin 2\pi kY\sin[2\pi lZ-\alpha(hkl)]\right\}$$

No. 27 $Pcc2$ C_{2v}^{3}

Origin on 2. | $x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z$ |

$A=4\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)\cos 2\pi lz$ $\quad |F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$B=4\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)\sin 2\pi lz$ $=0$ if $l=0$

$l=2n$	$A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=4\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	
$l=2n+1$	$A=-4\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=-4\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$	
	$A=B=0$ if $h=0$ or $k=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

$Pma2$ C_{2v}^{4}

No. 28

Origin on 2. | $x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,y,z;\ \frac{1}{2}+x,\bar{y},z$ |

$A=4\cos 2\pi\left(hx-\frac{h}{4}\right)\cos 2\pi\left(ky+\frac{h}{4}\right)\cos 2\pi lz$ $\quad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$B=4\cos 2\pi\left(hx-\frac{h}{4}\right)\cos 2\pi\left(ky+\frac{h}{4}\right)\sin 2\pi lz \quad =0$ if $l=0$

$h=2n$	$A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=4\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	
$h=2n+1$	$A=-4\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=-4\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$	
	$A=B=0$ if $k=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

$Pca2_1$ C_{2v}^{5}

No. 29

Origin on 2_1. | $x,y,z;\ \bar{x},\bar{y},\frac{1}{2}+z;\ \frac{1}{2}-x,y,\frac{1}{2}+z;\ \frac{1}{2}+x,\bar{y},z$ |

$A=4\cos 2\pi\left(hx-\frac{h+l}{4}\right)\cos 2\pi\left(ky+\frac{h}{4}\right)\cos 2\pi\left(lz+\frac{l}{4}\right)$ $\quad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$B=4\cos 2\pi\left(hx-\frac{h+l}{4}\right)\cos 2\pi\left(ky+\frac{h}{4}\right)\sin 2\pi\left(lz+\frac{l}{4}\right) \quad =0$ if $l=0$

$\begin{cases}h=2n\\ l=2n\end{cases}$	$A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=4\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	
$\begin{cases}h=2n\\ l=2n+1\end{cases}$	$A=-4\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$
	$B=4\sin 2\pi hx\cos 2\pi ky\cos 2\pi lz$	
	$A=B=0$ if $h=0$	
$\begin{cases}h=2n+1\\ l=2n\end{cases}$	$A=-4\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=-4\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$	
	$A=B=0$ if $k=0$	
$\begin{cases}h=2n+1\\ l=2n+1\end{cases}$	$A=-4\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$
	$B=4\cos 2\pi hx\sin 2\pi ky\cos 2\pi lz$	
	$A=B=0$ if $k=0$	

$$\rho(XYZ)=\frac{8}{V}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,l=2n+1}|F(hkl)|\sin 2\pi hX\cos 2\pi kY\sin[2\pi lZ-\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,l=2n}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,l=2n+1}|F(hkl)|\cos 2\pi hX\sin 2\pi kY\sin[2\pi lZ-\alpha(hkl)]\Big\}$$

No. 30 $Pnc2$ C_{2v}^{6}

Origin on 2. | $x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},\frac{1}{2}+y,\frac{1}{2}+z;\ x,\frac{1}{2}-y,\frac{1}{2}+z$ |

$A=4\cos 2\pi\left(hx-\frac{k+l}{4}\right)\cos 2\pi\left(ky+\frac{k+l}{4}\right)\cos 2\pi lz$ $\quad |F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(hk\bar{l})|=|F(hkl)|$

$B=4\cos 2\pi\left(hx-\frac{k+l}{4}\right)\cos 2\pi\left(ky+\frac{k+l}{4}\right)\sin 2\pi lz\ =0$ if $l=0$

$k+l=2n$	$A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(hk\bar{l})=-\alpha(hkl)$
	$B=4\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	
$k+l=2n+1$	$A=-4\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(hk\bar{l})=-\alpha(hkl)$
	$B=-4\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$	
	$A=B=0$ if $h=0$ or $k=0$	

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k+l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\Big\}$$

No. 31 $Pmn2_1$ C_{2v}^{7}

Origin on mn. | $x,y,z;\ \bar{x},y,z;\ \frac{1}{2}+x,\bar{y},\frac{1}{2}+z;\ \frac{1}{2}-x,\bar{y},\frac{1}{2}+z$ |

$A=4\cos 2\pi hx\cos 2\pi\left(ky-\frac{h+l}{4}\right)\cos 2\pi\left(lz+\frac{h+l}{4}\right)$ $\quad |F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(hk\bar{l})|=|F(hkl)|$

$B=4\cos 2\pi hx\cos 2\pi\left(ky-\frac{h+l}{4}\right)\sin 2\pi\left(lz+\frac{h+l}{4}\right)$

$h+l=2n$	$A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}l)=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=4\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz\ =0$ if $l=0$	
$h+l=2n+1$	$A=-4\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}l)=\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$
	$=0$ if $l=0$	
	$B=4\cos 2\pi hx\sin 2\pi ky\cos 2\pi lz$	
	$A=B=0$ if $k=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+l=2n+1}|F(hkl)|\cos 2\pi hX\sin 2\pi kY\sin[2\pi lZ-\alpha(hkl)]\right\}$$

$Pba2$ C_{2v}^{8}

No. 32

Origin on 2. | $x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}+y,z;\ \frac{1}{2}+x,\frac{1}{2}-y,z$ |

$$A=4\cos 2\pi\left(hx-\frac{h+k}{4}\right)\cos 2\pi\left(ky+\frac{h+k}{4}\right)\cos 2\pi lz$$

$$B=4\cos 2\pi\left(hx-\frac{h+k}{4}\right)\cos 2\pi\left(ky+\frac{h+k}{4}\right)\sin 2\pi lz\ =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}\bar{k}l)|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$h+k=2n$	$A=4\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}l)=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=4\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	
$h+k=2n+1$	$A=-4\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}l)=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$B=-4\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$	
	$A=B=0$ if $h=0$ or $k=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

$Pna2_1$ C_{2v}^{9}

No. 33

Origin on 2_1. | $x,y,z;\ \bar{x},\bar{y},\frac{1}{2}+z;\ \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}-y,z$ |

$$A=4\cos 2\pi\left(hx-\frac{h+k+l}{4}\right)\cos 2\pi\left(ky+\frac{h+k}{4}\right)\cos 2\pi\left(lz+\frac{l}{4}\right)$$

$$B=4\cos 2\pi\left(hx-\frac{h+k+l}{4}\right)\cos 2\pi\left(ky+\frac{h+k}{4}\right)\sin 2\pi\left(lz+\frac{l}{4}\right)\ =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}\bar{k}l)|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$\begin{cases} h+k=2n \\ l=2n \end{cases}$	$A=4\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz$ $B=4\cos 2\pi hx \cos 2\pi ky \sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$\begin{cases} h+k=2n \\ l=2n+1 \end{cases}$	$A=-4\sin 2\pi hx \cos 2\pi ky \sin 2\pi lz$ $B=4\sin 2\pi hx \cos 2\pi ky \cos 2\pi lz$ $A=B=0$ if $h=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$
$\begin{cases} h+k=2n+1 \\ l=2n \end{cases}$	$A=-4\sin 2\pi hx \sin 2\pi ky \cos 2\pi lz$ $B=-4\sin 2\pi hx \sin 2\pi ky \sin 2\pi lz$ $A=B=0$ if $h=0$ or $k=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$\begin{cases} h+k=2n+1 \\ l=2n+1 \end{cases}$	$A=-4\cos 2\pi hx \sin 2\pi ky \sin 2\pi lz$ $B=4\cos 2\pi hx \sin 2\pi ky \cos 2\pi lz$ $A=B=0$ if $k=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,l=2n+1}|F(hkl)|\sin 2\pi hX\cos 2\pi kY\sin[2\pi lZ-\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,l=2n}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,l=2n+1}|F(hkl)|\cos 2\pi hX\sin 2\pi kY\sin[2\pi lZ-\alpha(hkl)]\Big\}$$

No. 34 $Pnn2$ C_{2v}^{10}

Origin on 2. | $x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$ |

$$A=4\cos 2\pi\left(hx-\frac{h+k+l}{4}\right)\cos 2\pi\left(ky+\frac{h+k+l}{4}\right)\cos 2\pi lz$$
$$B=4\cos 2\pi\left(hx-\frac{h+k+l}{4}\right)\cos 2\pi\left(ky+\frac{h+k+l}{4}\right)\sin 2\pi lz \quad =0 \text{ if } l=0$$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$h+k+l=2n$	$A=4\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz$ $B=4\cos 2\pi hx \cos 2\pi ky \sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$h+k+l=2n+1$	$A=-4\sin 2\pi hx \sin 2\pi ky \cos 2\pi lz$ $B=-4\sin 2\pi hx \sin 2\pi ky \sin 2\pi lz$ $A=B=0$ if $h=0$ or $k=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\Big\}$$

$Cmm2$ C_{2v}^{11}

No. 35

Origin on $mm2$. $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) + \ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z\ |$

$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$

$B=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz \quad =0 \text{ if } l=0$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(hk\bar{l})|=|F(hk\bar{l})|$

$h+k=2n$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(hk\bar{l})=-\alpha(hk\bar{l})$
	$B=8\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	
$h+k=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]$$

$Cmc2_1$ C_{2v}^{12}

No. 36

Origin on $mc2_1$. $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) + \ |\ x,y,z;\ \bar{x},y,z;\ x,\bar{y},\frac{1}{2}+z;\ \bar{x},\bar{y},\frac{1}{2}+z\ |$

$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi\left(ky+\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{l}{4}\right)$

$B=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi\left(ky+\frac{l}{4}\right)\sin 2\pi\left(lz-\frac{l}{4}\right) \quad =0 \text{ if } l=0$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(hk\bar{l})|=|F(hk\bar{l})|$

$\begin{cases} h+k=2n \\ l=2n \end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(hk\bar{l})=-\alpha(hk\bar{l})$
	$B=8\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	
$\begin{cases} h+k=2n \\ l=2n+1 \end{cases}$	$A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\pi+\alpha(hk\bar{l})=\pi-\alpha(hk\bar{l})$
	$B=8\cos 2\pi hx\sin 2\pi ky\cos 2\pi lz$	
	$A=B=0$ if $k=0$	
$h+k=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^{l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^{l=2n+1}|F(hkl)|\cos 2\pi hX\sin 2\pi kY\sin[2\pi lZ-\alpha(hkl)]\right\}$$

No. 37 — $Ccc2$ — C_{2v}^{13}

Origin on $cc2$. $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) + \ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z\ |$

$$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)\cos 2\pi lz$$

$$B=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)\sin 2\pi lz \quad =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$\begin{cases} h+k=2n \\ l=2n \end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $B=8\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$\begin{cases} h+k=2n \\ l=2n+1 \end{cases}$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$ $B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $A=B=0$ if $h=0$ or $k=0$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$h+k=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

No. 38 — $Amm2$ — C_{2v}^{14}

Origin on $mm2$. $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2}) + \ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z\ |$

$$A=8\cos^2 2\pi\frac{k+l}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$$

$$B=8\cos^2 2\pi\frac{k+l}{4}\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz \quad =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$k+l=2n$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $B=8\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$k+l=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]$$

$Abm2$ C_{2v}^{15}

No. 39

Origin on 2. $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2})+\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},\frac{1}{2}+y,z;\ x,\frac{1}{2}-y,z\ |$

$$A=8\cos^2 2\pi\frac{k+l}{4}\cos 2\pi\left(hx+\frac{k}{4}\right)\cos 2\pi\left(ky-\frac{k}{4}\right)\cos 2\pi lz$$

$$B=8\cos^2 2\pi\frac{k+l}{4}\cos 2\pi\left(hx+\frac{k}{4}\right)\cos 2\pi\left(ky-\frac{k}{4}\right)\sin 2\pi lz\quad =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$\begin{cases} k+l=2n \\ k=2n \end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $B=8\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$\begin{cases} k+l=2n \\ k=2n+1 \end{cases}$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$ $B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$A=B=0$ if $h=0$	
$k+l=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

$Ama2$ C_{2v}^{16}

No. 40

Origin on 2. $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2})+\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,y,z;\ \frac{1}{2}+x,\bar{y},z\ |$

$$A=8\cos^2 2\pi\frac{k+l}{4}\cos 2\pi\left(hx-\frac{h}{4}\right)\cos 2\pi\left(ky+\frac{h}{4}\right)\cos 2\pi lz$$

$$B=8\cos^2 2\pi\frac{k+l}{4}\cos 2\pi\left(hx-\frac{h}{4}\right)\cos 2\pi\left(ky+\frac{h}{4}\right)\sin 2\pi lz\quad =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$\begin{cases} k+l=2n \\ h=2n \end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $B=8\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$\begin{cases} k+l=2n \\ h=2n+1 \end{cases}$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$ $B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$A=B=0$ if $k=0$	
$k+l=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

No. 41 $Aba2$ C_{2v}^{17}

Origin on 2. $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2}) + \ |\ x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}+y,z;\ \frac{1}{2}+x,\frac{1}{2}-y,z\ |$

$$A=8\cos^2 2\pi\frac{k+l}{4}\cos 2\pi\left(hx-\frac{h+k}{4}\right)\cos 2\pi\left(ky+\frac{h+k}{4}\right)\cos 2\pi lz$$

$$B=8\cos^2 2\pi\frac{k+l}{4}\cos 2\pi\left(hx-\frac{h+k}{4}\right)\cos 2\pi\left(ky+\frac{h+k}{4}\right)\sin 2\pi lz \quad =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}\bar{k}l)|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$\begin{cases} k+l=2n \\ h+k=2n \end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $B=8\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}l)=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$\begin{cases} k+l=2n \\ h+k=2n+1 \end{cases}$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$ $B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $A=B=0$ if $h=0$ or $k=0$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}l)=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$k+l=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

No. 42 $Fmm2$ C_{2v}^{18}

Origin on $mm2$. $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0) + \ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z\ |$

$$A=16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$$

$$B=16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz \quad =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}\bar{k}l)|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$\begin{cases} h+k=2n \\ k+l=2n \end{cases}$	$A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $B=16\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}l)=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$ (indices all even or all odd)
$h+k=2n+1$ or $k+l=2n+1$	$A=B=0$	(indices mixed even and odd)

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]$$

$Fdd2$
C_{2v}^{19}

No. 43

Origin on 2. $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0) + \ |\ x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{4}-x,\frac{1}{4}+y,\frac{1}{4}+z;\ \frac{1}{4}+x,\frac{1}{4}-y,\frac{1}{4}+z\ |$

$$A=8\cos 2\pi\frac{h+l}{4}\cos 2\pi\frac{k+l}{4}\left\{\cos 2\pi\frac{h-k}{4}\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(hx-ky)\cos 2\pi\left(lz-\frac{l}{4}\right)\right\}$$

$$B=8\cos 2\pi\frac{h+l}{4}\cos 2\pi\frac{k+l}{4}\left\{\cos 2\pi\frac{h-k}{4}\cos 2\pi(hx+ky)\sin 2\pi lz+\cos 2\pi(hx-ky)\sin 2\pi\left(lz-\frac{l}{4}\right)\right\}\ =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$\begin{cases} h+l=2n,\ k+l=2n \\ h+k+l=4n \end{cases}$ $A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$B=16\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$

$\begin{cases} h+l=2n,\ k+l=2n \\ h+k+l=4n+1 \\ (h,k,l \text{ all odd. Note. If } h+k+l=4n+1, \text{ then } -h-k-l=4n+3, \text{ etc.}) \end{cases}$

$A=8\,[\cos 2\pi(hx+ky)\cos 2\pi lz-\cos 2\pi(hx-ky)\sin 2\pi lz]$

$B=8\,[\cos 2\pi(hx+ky)\sin 2\pi lz+\cos 2\pi(hx-ky)\cos 2\pi lz]$

$\begin{cases} \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l}) \\ =\alpha(\bar{h}kl)+\pi/2 \\ =\alpha(h\bar{k}l)+\pi/2=-\alpha(hk\bar{l}) \end{cases}$

$\begin{cases} h+l=2n,\ k+l=2n \\ h+k+l=4n+2 \end{cases}$ $A=-16\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)$

$B=-16\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $\quad =\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$A=B=0$ if $h=0$ or $k=0$

$\begin{cases} h+l=2n,\ k+l=2n \\ h+k+l=4n+3 \\ (h,k,l \text{ all odd. Note. If } h+k+l=4n+3, \text{ then } -h-k-l=4n+1, \text{ etc.}) \end{cases}$

$A=8\,[\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(hx-ky)\sin 2\pi lz]$

$B=8\,[\cos 2\pi(hx+ky)\sin 2\pi lz-\cos 2\pi(hx-ky)\cos 2\pi lz]$

$\begin{cases} \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l}) \\ =\alpha(\bar{h}kl)-\pi/2 \\ =\alpha(h\bar{k}l)-\pi/2=-\alpha(hk\bar{l}) \end{cases}$

$h+l=2n+1$ or $k+l=2n+1$ (indices mixed even and odd) $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n+2}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}+$$
$$\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n+1}|F(hkl)|\{\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]-\cos 2\pi(hX-kY)\sin[2\pi lZ-\alpha(hkl)]\}+\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n+3}|F(hkl)|\{\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+\cos 2\pi(hX-kY)\sin[2\pi lZ-\alpha(hkl)]\}\right\}$$

$Imm2$
C_{2v}^{20}

No. 44

Origin on $mm2$. $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) + \ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z\ |$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$$B=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz\ =0 \text{ if } l=0$$

$h+k+l=2n$ $\quad A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$B=8\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$

$h+k+l=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]$$

No. 45 $Iba2$ C_{2v}^{21}

Origin on 2. $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) +\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z\ |$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)\cos 2\pi lz$$

$$B=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)\sin 2\pi lz \quad =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$\begin{cases} h+k+l=2n \\ l=2n \end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $B=8\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$\begin{cases} h+k+l=2n \\ l=2n+1 \end{cases}$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$ $B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$A=B=0$ if $h=0$ or $k=0$	
$h+k+l=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty\sum_{l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty\sum_{l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

No. 46 $Iam2$ C_{2v}^{22}

Origin on 2. $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) +\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,y,z;\ \frac{1}{2}+x,\bar{y},z\ |$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi\left(hx+\frac{h}{4}\right)\cos 2\pi\left(ky-\frac{h}{4}\right)\cos 2\pi lz$$

$$B=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi\left(hx+\frac{h}{4}\right)\cos 2\pi\left(ky-\frac{h}{4}\right)\sin 2\pi lz \quad =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$\begin{cases} h+k+l=2n \\ h=2n \end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $B=8\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$\begin{cases} h+k+l=2n \\ h=2n+1 \end{cases}$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$ $B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
	$A=B=0$ if $k=0$	
$h+k+l=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty\sum_{h=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty\sum_{h=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

$Pmmm$ D_{2h}^{1}

No. 47

Origin at centre (mmm). $\pm\ |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z\ |$

$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$B=0$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ$$

$Pnnn$ D_{2h}^{2}

No. 48

Origin at 222 (at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{1}$).

$|\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z;\ \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z\ |$

$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$B=-8\sin^2 2\pi\frac{h+k+l}{4}\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $h=0$ or $k=0$ or $l=0$

$h+k+l=2n$ $A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz;\quad B=0$

$\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\mathrm{m}\pi$

$h+k+l=2n+1$ $A=0;\quad B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $h=0$ or $k=0$ or $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{2}$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi\right\}$$

where $\mathrm{m}=0$ if A or B is positive, $\mathrm{m}=1$ if A or B is negative

$Pnnn$ D_{2h}^{2}

No. 48

Origin at $\bar{1}$. $\pm\ |\ x,y,z;\ \bar{x},\frac{1}{2}+y,\frac{1}{2}+z;\ \frac{1}{2}+x,\bar{y},\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}+y,\bar{z}\ |$

$A=8\cos 2\pi\left(hx-\frac{k-l}{4}\right)\cos 2\pi\left(ky-\frac{l-h}{4}\right)\cos 2\pi\left(lz-\frac{h-k}{4}\right);\quad B=0$

$\begin{cases} h+k=2n \\ k+l=2n \end{cases}$ $A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz;\quad B=0$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=2n \\ k+l=2n+1 \end{cases}$ $A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$ $=0$ if $h=0$ or $k=0$; $B=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=2n+1 \\ k+l=2n \end{cases}$ $A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $k=0$ or $l=0$; $B=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h+k=2n+1 \\ k+l=2n+1 \end{cases}$ $A=-8\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz$ $=0$ if $l=0$ or $h=0$; $B=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ k+l=2n}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ k+l=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\Big\}$$

No. 49

$Pccm$ D_{2h}^3

Origin at centre $(2/m)$. $\pm\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z\ |$

$A=8\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)\cos 2\pi lz;\quad B=0$

$l=2n$ $A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz;\quad B=0$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$l=2n+1$ $A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz;\quad A=B=0$ if $h=0$ or $k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\Big\}$$

No. 50

$Pban$ D_{2h}^4

Origin at 222 (at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$).

$|\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}-y,\bar{z};\ \frac{1}{2}-x,\frac{1}{2}+y,z;\ \frac{1}{2}+x,\frac{1}{2}-y,z;\ \frac{1}{2}+x,\frac{1}{2}+y,\bar{z}\ |$

$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$B=-8\sin^2 2\pi\frac{h+k}{4}\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $h=0$ or $k=0$ or $l=0$

$h+k=2n$ $A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz;\quad B=0$ $\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=m\pi$

$h+k=2n+1$ $A=0;\quad B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $h=0$ or $k=0$ or $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=m\pi+\frac{\pi}{2}$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos m\pi-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos m\pi\right\}$$

where m=0 if A or B is positive, m=1 if A or B is negative.

$Pban$ D_{2h}^4

No. 50

Origin at $\bar{1}$. $\pm\ |\ x,y,z;\ \frac{1}{2}-x,\frac{1}{2}-y,z;\ \frac{1}{2}-x,y,\bar{z};\ x,\frac{1}{2}-y,\bar{z}\ |$

$$A=8\cos 2\pi\left(hx-\frac{k}{4}\right)\cos 2\pi\left(ky-\frac{h}{4}\right)\cos 2\pi\left(lz+\frac{h+k}{4}\right);\quad B=0$$

$\begin{cases}h=2n\\k=2n\end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$
$\begin{cases}h=2n\\k=2n+1\end{cases}$	$A=-8\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz$ $=0$ if $h=0$ or $l=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$
$\begin{cases}h=2n+1\\k=2n\end{cases}$	$A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$ $=0$ if $k=0$ or $l=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$
$\begin{cases}h=2n+1\\k=2n+1\end{cases}$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\right\}$$

$Pmma$ D_{2h}^5

No. 51

Origin at centre (2/m). $\pm\ |\ x,y,z;\ x,\bar{y},z;\ \frac{1}{2}-x,y,z;\ \frac{1}{2}-x,\bar{y},z\ |$

$$A=8\cos 2\pi\left(hx+\frac{h}{4}\right)\cos 2\pi ky\cos 2\pi\left(lz-\frac{h}{4}\right);\quad B=0$$

$h=2n$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$
$h=2n+1$	$A=-8\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $l=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\right\}$$

No. 52 $Pnna$ D_{2h}^{6}

Origin at $\bar{1}$. $\pm\ |\ x,y,z;\ \frac{1}{2}-x,\bar{y},z;\ x,\frac{1}{2}-y,\frac{1}{2}-z;\ \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z\ |$

$A=8\cos 2\pi\left(hx+\frac{k+l}{4}\right)\cos 2\pi\left(ky-\frac{h+k+l}{4}\right)\cos 2\pi\left(lz+\frac{h}{4}\right);\quad B=0$

$\begin{cases} h=2n \\ k+l=2n \end{cases}$ $A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz;\quad B=0$ $\quad F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h=2n \\ k+l=2n+1 \end{cases}$ $A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz;\quad A=B=0$ if $h=0$ or $k=0$

$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h=2n+1 \\ k+l=2n \end{cases}$ $A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $k=0$ or $l=0$

$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h=2n+1 \\ k+l=2n+1 \end{cases}$ $A=-8\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $l=0$

$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k+l=2n}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k+l=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\Big\}$$

No. 53 $Pmna$ D_{2h}^{7}

Origin at centre $(2/m)$. $\pm\ |\ x,y,z;\ x,\bar{y},\bar{z};\ \frac{1}{2}-x,y,\frac{1}{2}-z;\ \frac{1}{2}-x,\bar{y},\frac{1}{2}+z\ |$

$A=8\cos 2\pi hx\cos 2\pi\left(ky+\frac{h+l}{4}\right)\cos 2\pi\left(lz-\frac{h+l}{4}\right);\quad B=0$

$h+l=2n$ $\quad A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $\quad F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$h+l=2n+1$ $\quad A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $k=0$ or $l=0$

$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+l=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\Big\}$$

No. 54 $Pcca$ D_{2h}^{8}

Origin at $\bar{1}$. $\pm\ |\ x,y,z;\ \frac{1}{2}-x,\bar{y},z;\ \frac{1}{2}+x,\bar{y},\frac{1}{2}-z;\ \bar{x},y,\frac{1}{2}-z\ |$

$A=8\cos 2\pi\left(hx-\frac{h+l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)\cos 2\pi\left(lz+\frac{h}{4}\right);\quad B=0$

$\begin{cases} h = 2n \\ l = 2n \end{cases}$ $A=8\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz$ $F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h = 2n \\ l = 2n+1 \end{cases}$ $A=-8\sin 2\pi hx \sin 2\pi ky \cos 2\pi lz$; $A=B=0$ if $h=0$ or $k=0$ $F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h = 2n+1 \\ l = 2n \end{cases}$ $A=-8\sin 2\pi hx \cos 2\pi ky \sin 2\pi lz$; $A=B=0$ if $l=0$ $F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h = 2n+1 \\ l = 2n+1 \end{cases}$ $A=-8\cos 2\pi hx \sin 2\pi ky \sin 2\pi lz$; $A=B=0$ if $k=0$ $F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,l=2n} F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,l=2n+1} F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,l=2n} F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,l=2n+1} F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\right\}$$

$Pbam$ D_{2h}^{9}

No. 55

Origin at centre $(2/m)$. $\pm\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}+x,\frac{1}{2}-y,\bar{z};\ \frac{1}{2}-x,\frac{1}{2}+y,\bar{z}\ |$

$A=8\cos 2\pi\left(hx+\frac{h+k}{4}\right)\cos 2\pi\left(ky-\frac{h+k}{4}\right)\cos 2\pi lz$; $B=0$

$h+k=2n$ $A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$h+k=2n+1$ $A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$; $A=B=0$ if $h=0$ or $k=0$ $F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n} F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1} F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\right\}$$

$Pccn$ D_{2h}^{10}

No. 56

Origin at $\bar{1}$. $\pm\ |\ x,y,z;\ \frac{1}{2}-x,\frac{1}{2}-y,z;\ \frac{1}{2}-x,y,\frac{1}{2}+z;\ x,\frac{1}{2}-y,\frac{1}{2}+z\ |$

$A=8\cos 2\pi\left(hx+\frac{l-h}{4}\right)\cos 2\pi\left(ky+\frac{k-l}{4}\right)\cos 2\pi\left(lz+\frac{h-k}{4}\right)$; $B=0$

$\begin{cases} h+k = 2n \\ h+l = 2n \end{cases}$ $A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k = 2n \\ h+l = 2n+1 \end{cases}$ $A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$; $A=B=0$ if $h=0$ or $k=0$ $F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k = 2n+1 \\ h+l = 2n \end{cases}$ $A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$; $A=B=0$ if $k=0$ or $l=0$ $F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h+k = 2n+1 \\ h+l = 2n+1 \end{cases}$ $A=-8\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz$; $A=B=0$ if $l=0$ or $h=0$ $F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ h+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ h+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ h+l=2n}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ h+l=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\Big\}$$

No. 57

$Pbcm$ D_{2h}^{11}

Origin at $\bar{1}$. $\pm\ |\ x,y,z;\ \bar{x},\bar{y},\frac{1}{2}+z;\ \bar{x},\frac{1}{2}+y,z;\ x,\frac{1}{2}-y,\frac{1}{2}+z\ |$

$A=8\cos 2\pi\left(hx+\frac{k}{4}\right)\cos 2\pi\left(ky-\frac{k+l}{4}\right)\cos 2\pi\left(lz+\frac{l}{4}\right);\quad B=0$

$\begin{cases}k=2n\\ l=2n\end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$
$\begin{cases}k=2n\\ l=2n+1\end{cases}$	$A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $k=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$
$\begin{cases}k=2n+1\\ l=2n\end{cases}$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz;\quad A=B=0$ if $h=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$
$\begin{cases}k=2n+1\\ l=2n+1\end{cases}$	$A=-8\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $h=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n,\ l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n,\ l=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n+1,\ l=2n}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n+1,\ l=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\Big\}$$

No. 58

$Pnnm$ D_{2h}^{12}

Origin at centre $(2/m)$. $\pm\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z;\ \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z\ |$

$A=8\cos 2\pi\left(hx+\frac{h+k+l}{4}\right)\cos 2\pi\left(ky-\frac{h+k+l}{4}\right)\cos 2\pi lz;\quad B=0$

$h+k+l=2n$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$
$h+k+l=2n+1$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz;\quad A=B=0$ if $h=0$ or $k=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\Big\}$$

$Pmmn$ D_{2h}^{13}

No. 59

Origin at mmn (at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$).

$| x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}-y,\bar{z};\ \frac{1}{2}+x,\frac{1}{2}+y,\bar{z};\ \frac{1}{2}-x,\frac{1}{2}+y,\bar{z};\ \frac{1}{2}+x,\frac{1}{2}-y,\bar{z} |$

$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $\qquad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$B=8\sin^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$ $=0$ if $l=0$ or $h+k=0$

$h+k=2n$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\mathrm{m}\pi$
	$B=0$	
$h+k=2n+1$	$A=0$	$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{2}$
	$B=8\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz$ $=0$ if $l=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi+\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi\right\}$$

where $\mathrm{m}=0$ if A or B is positive, $\mathrm{m}=1$ if A or B is negative.

$Pmmn$ D_{2h}^{13}

No. 59

Origin at $\bar{1}$. $\qquad \pm\ | x,y,z;\ \frac{1}{2}-x,y,z;\ x,\frac{1}{2}-y,z;\ \frac{1}{2}-x,\frac{1}{2}-y,z |$

$A=8\cos 2\pi\left(hx+\frac{h}{4}\right)\cos 2\pi\left(ky+\frac{k}{4}\right)\cos 2\pi\left(lz-\frac{h+k}{4}\right);\quad B=0$

$\begin{cases}h=2n\\k=2n\end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$
$\begin{cases}h=2n\\k=2n+1\end{cases}$	$A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $l=0$	$F(\bar{h}kl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}k\bar{l})=-F(h\bar{k}l)=-F(hk\bar{l})$
$\begin{cases}h=2n+1\\k=2n\end{cases}$	$A=-8\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $l=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$
$\begin{cases}h=2n+1\\k=2n+1\end{cases}$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\right\}$$

No. 60 $Pbcn$ D_{2h}^{14}

Origin at $\bar{1}$. $\pm\ |\ x,y,z;\ \frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}-y,\bar{z};\ \bar{x},y,\frac{1}{2}-z\ |$

$A=8\cos 2\pi\left(hx+\frac{h+k}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{h+k+l}{4}\right);\quad B=0$

$\begin{cases} h+k=2n \\ l=2n \end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$
$\begin{cases} h+k=2n \\ l=2n+1 \end{cases}$	$A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $k=0$	$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$
$\begin{cases} h+k=2n+1 \\ l=2n \end{cases}$	$A=-8\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $h=0$ or $l=0$	$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$
$\begin{cases} h+k=2n+1 \\ l=2n+1 \end{cases}$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz;\quad A=B=0$ if $h=0$ or $k=0$	$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ l=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ l=2n}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\Big\}$$

No. 61 $Pbca$ D_{2h}^{15}

Origin at $\bar{1}$. $\pm\ |\ x,y,z;\ \frac{1}{2}+x,\frac{1}{2}-y,\bar{z};\ \bar{x},\frac{1}{2}+y,\frac{1}{2}-z;\ \frac{1}{2}-x,\bar{y},\frac{1}{2}+z\ |$

$A=8\cos 2\pi\left(hx-\frac{h-k}{4}\right)\cos 2\pi\left(ky-\frac{k-l}{4}\right)\cos 2\pi\left(lz-\frac{l-h}{4}\right);\quad B=0$

$\begin{cases} h+k=2n \\ k+l=2n \end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$
$\begin{cases} h+k=2n \\ k+l=2n+1 \end{cases}$	$A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $k=0$ or $l=0$	$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$
$\begin{cases} h+k=2n+1 \\ k+l=2n \end{cases}$	$A=-8\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $h=0$ or $l=0$	$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$
$\begin{cases} h+k=2n+1 \\ k+l=2n+1 \end{cases}$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz;\quad A=B=0$ if $h=0$ or $k=0$	$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ k+l=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ k+l=2n}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\Big\}$$

$Pnma$ D_{2h}^{16}

No. 62

Origin at $\bar{1}$. $\pm\ |\ x,y,z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{1}{2}-z;\ \bar{x},\tfrac{1}{2}+y,\bar{z};\ \tfrac{1}{2}-x,\bar{y},\tfrac{1}{2}+z\ |$

$A=8\cos 2\pi\left(hx-\frac{h+k+l}{4}\right)\cos 2\pi\left(ky+\frac{k}{4}\right)\cos 2\pi\left(lz+\frac{h+l}{4}\right);\quad B=0$

$\begin{cases} h+l=2n \\ k=2n \end{cases}$	$A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$
$\begin{cases} h+l=2n \\ k=2n+1 \end{cases}$	$A=-8\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz;\quad A=B=0$ if $h=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$
$\begin{cases} h+l=2n+1 \\ k=2n \end{cases}$	$A=-8\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $h=0$ or $l=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$
$\begin{cases} h+l=2n+1 \\ k=2n+1 \end{cases}$	$A=-8\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $l=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+l=2n,\,k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+l=2n,\,k=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+l=2n+1,\,k=2n}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+l=2n+1,\,k=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\Big\}$$

$Cmcm$ D_{2h}^{17}

No. 63

Origin at centre $(2/m)$. $(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},0)\ \pm\ |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\tfrac{1}{2}-z;\ \bar{x},\bar{y},\tfrac{1}{2}+z\ |$

$A=16\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi\left(ky+\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{l}{4}\right);\quad B=0$

$\begin{cases} h+k=2n \\ l=2n \end{cases}$	$A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$
$\begin{cases} h+k=2n \\ l=2n+1 \end{cases}$	$A=-16\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $k=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$
$h+k=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\Big\}$$

No. 64 $Cmca$ D_{2h}^{18}

Origin at centre $(2/m)$. $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) \pm \ |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},\frac{1}{2}+y,\frac{1}{2}-z;\ \bar{x},\frac{1}{2}-y,\frac{1}{2}+z\ |$

$A=16\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi\left(ky+\frac{k+l}{4}\right)\cos 2\pi\left(lz-\frac{k+l}{4}\right);\quad B=0$

$\begin{cases} h+k=2n \\ k+l=2n \end{cases}$ $A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=2n \\ k+l=2n+1 \end{cases}$ $A=-16\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $k=0$ or $l=0$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$h+k=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k+l=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\right\}$$

No. 65 $Cmmm$ D_{2h}^{19}

Origin at centre (mmm). $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) \pm \ |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z\ |$

$A=16\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz;\quad B=0$

$h+k=2n$ $A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$h+k=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ$$

No. 66 $Cccm$ D_{2h}^{20}

Origin at centre $(2/m$ at $ccm)$. $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) \pm \ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}-z;\ x,\bar{y},\frac{1}{2}-z\ |$

$A=16\cos^2 2\pi\frac{h+k}{4}\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)\cos 2\pi lz;\quad B=0$

$\begin{cases} h+k=2n \\ l=2n \end{cases}$ $A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=2n \\ l=2n+1 \end{cases}$ $A=-16\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz;\quad A=B=0$ if $h=0$ or $k=0$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$h+k=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\right\}$$

$Cmma$ D_{2h}^{21}

No. 67

Origin at centre ($2/m$ at maa). $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) \pm \mid x,y,z;\ x,\bar{y},\bar{z};\ \frac{1}{2}-x,y,\bar{z};\ \frac{1}{2}-x,\bar{y},z \mid$

$$A=16\cos^2 2\pi\frac{h+k}{4}\cos 2\pi hx\cos 2\pi\left(ky+\frac{h}{4}\right)\cos 2\pi\left(lz-\frac{h}{4}\right);\quad B=0$$

$\begin{cases} h+k=2n \\ h=2n \end{cases}$ $A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ $F(hkl)=F(\bar{h}\bar{k}l)=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=2n \\ h=2n+1 \end{cases}$ $A=-16\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $l=0$

$F(hkl)=F(\bar{h}\bar{k}l)=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$h+k=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\right\}$$

$Ccca$ D_{2h}^{22}

No. 68

Origin at 222 (at $0,\frac{1}{4},\frac{1}{4}$ from $\bar{1}$ on nca).

$(0,0,0;\ \frac{1}{2},\frac{1}{2},0) + \mid x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ \bar{x},\frac{1}{2}-y,\frac{1}{2}-z;\ \bar{x},\frac{1}{2}+y,\frac{1}{2}+z;\ x,\frac{1}{2}-y,\frac{1}{2}+z;\ x,\frac{1}{2}+y,\frac{1}{2}-z \mid$

$$A=16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{h+l}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$$

$$B=-16\cos^2 2\pi\frac{h+k}{4}\sin^2 2\pi\frac{h+l}{4}\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz\quad =0 \text{ if } h=0 \text{ or } k=0 \text{ or } l=0 \text{ or } h+l=0$$

$|F(hkl)|=|F(\bar{h}\bar{k}l)|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$

$\begin{cases} h+k=2n \\ h+l=2n \end{cases}$ $A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz;\quad B=0$ $\alpha(hkl)=\alpha(\bar{h}\bar{k}l)=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\mathrm{m}\pi$

$\begin{cases} h+k=2n \\ h+l=2n+1 \end{cases}$ $A=0;\quad B=-16\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz\quad =0$ if $h=0$ or $k=0$ or $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}l)=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{2}$

$h+k=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi\right\}$$

where $\mathrm{m}=0$ if A or B is positive, $\mathrm{m}=1$ if A or B is negative.

No. 68 $Ccca$ D_{2h}^{22}

Origin at $\bar{1}$. $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) \pm \mid x,y,z;\ \frac{1}{2}-x,y,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z;\ \bar{x},\frac{1}{2}-y,z \mid$

$A=16\cos^2 2\pi\frac{h+k}{4}\cos 2\pi\left(hx-\frac{k+l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)\cos 2\pi\left(lz+\frac{k}{4}\right);\quad B=0$

$h+k=2n$:	$\begin{cases}k=2n\\ l=2n\end{cases}$	$A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$
	$\begin{cases}k=2n\\ l=2n+1\end{cases}$	$A=-16\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz;$	$A=B=0$ if $h=0$ or $k=0$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$
	$\begin{cases}k=2n+1\\ l=2n\end{cases}$	$A=-16\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz;$	$A=B=0$ if $l=0$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$
	$\begin{cases}k=2n+1\\ l=2n+1\end{cases}$	$A=-16\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$
$h+k=2n+1$		$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n,\,l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n,\,l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n+1,\,l=2n}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n+1,\,l=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\Big\}$$

No. 69 $Fmmm$ D_{2h}^{23}

Origin at centre (mmm). $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0) \pm \mid x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z \mid$

$A=32\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz;\quad B=0$

$\begin{cases}h+k=2n\\ \text{and}\\ k+l=2n\end{cases}$	$A=32\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$ (indices all even or all odd)	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$
$\begin{cases}h+k=2n+1\\ \text{or}\\ k+l=2n+1\end{cases}$	$A=B=0$ (indices mixed even and odd)	

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ$$

$Fddd$ D_{2h}^{24}

No. 70

Origin at 222 (at $\bar{\tfrac{1}{8}},\bar{\tfrac{1}{8}},\bar{\tfrac{1}{8}}$ from $\bar{1}$). $(0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0)+$

$|\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ \tfrac{1}{4}-x,\tfrac{1}{4}-y,\tfrac{1}{4}-z;\ \tfrac{1}{4}-x,\tfrac{1}{4}+y,\tfrac{1}{4}+z;\ \tfrac{1}{4}+x,\tfrac{1}{4}-y,\tfrac{1}{4}+z;\ \tfrac{1}{4}+x,\tfrac{1}{4}+y,\tfrac{1}{4}-z\ |$

$A=32\cos 2\pi\frac{h+k+l}{8}G;\quad B=32\sin 2\pi\frac{h+k+l}{8}G;$ where

$$G=\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\left[\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz\cos 2\pi\frac{h+k+l}{8}-\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz\sin 2\pi\frac{h+k+l}{8}\right]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|$$

$\begin{cases} h,k \text{ and } l \text{ even} \\ h+k+l=4n \end{cases}$ $A=32\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz;\quad B=0$

$\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\mathrm{m}\pi$

$\begin{cases} h,k \text{ and } l \text{ odd} \\ h+k+l=4n+1 \end{cases}$ $A=16(\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz-\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz);\quad B=A$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{4}$

$\begin{cases} h,k \text{ and } l \text{ even} \\ h+k+l=4n+2 \end{cases}$ $A=0;\quad B=-32\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz=0$ if $h=0$ or $k=0$ or $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{2}$

$\begin{cases} h,k \text{ and } l \text{ odd} \\ h+k+l=4n+3 \end{cases}$ $A=16(\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz);\quad B=-A$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi-\frac{\pi}{4}$

$h+k=2n+1$ or $k+l=2n+1$ (h,k,l mixed even and odd) $A=B=0$

Note: If $h+k+l=4n+1$, then $-h-k-l=4n+3$, $-h+k+l=4n+3$, etc.

$$\rho(XYZ)=\frac{8}{V_c}\Bigg\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi+$$
$$\frac{1}{\sqrt{2}}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n+1}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ]\cos \mathrm{m}\pi-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n+2}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi+$$
$$\frac{1}{\sqrt{2}}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n+3}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ+\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ]\cos \mathrm{m}\pi\Bigg\}$$

where $\mathrm{m}=0$ if A (or if $A=0$, B) is positive, $\mathrm{m}=1$ if A (or if $A=0$, B) is negative.

$Fddd$ D_{2h}^{24}

No. 70

Origin at $\bar{1}$ (at $\bar{\tfrac{1}{8}},\bar{\tfrac{1}{8}},\bar{\tfrac{1}{8}}$ from 222).

$(0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0)\pm\ |\ x,y,z;\ x,\tfrac{1}{4}-y,\tfrac{1}{4}-z;\ \tfrac{1}{4}-x,y,\tfrac{1}{4}-z;\ \tfrac{1}{4}-x,\tfrac{1}{4}-y,z\ |$

$$A=8\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\left\{\cos 2\pi(hx+ky+lz)+\cos 2\pi\left(hx+ky-lz-\frac{h+k}{4}\right)+\right.$$
$$\left.\cos 2\pi\left(hx-ky+lz-\frac{l+h}{4}\right)+\cos 2\pi\left(-hx+ky+lz-\frac{k+l}{4}\right)\right\};\quad B=0$$

$\begin{cases} h+k=4n; & l+h=4n \\ k+l=4n \end{cases}$ $A=32\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=4n; & l+h=4n+2 \\ k+l=4n+2 \end{cases}$ $A=-32\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz$; $A=B=0$ if $h=0$ or $k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=4n+2; & l+h=4n+2 \\ k+l=4n \end{cases}$ $A=-32\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz$; $A=B=0$ if $k=0$ or $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h+k=4n+2; & l+h=4n \\ k+l=4n+2 \end{cases}$ $A=-32\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz$; $A=B=0$ if $l=0$ or $h=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h+k=4n; & l+h=4n+2 \\ k+l=4n \end{cases}$ $A=16\{\cos 2\pi(hx+ky)\cos 2\pi lz+\sin 2\pi(hx-ky)\sin 2\pi lz\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$ [N.B. $-h+k=4n+2$, etc.]

$\begin{cases} h+k=4n; & l+h=4n \\ k+l=4n+2 \end{cases}$ $A=16\{\cos 2\pi(hx+ky)\cos 2\pi lz-\sin 2\pi(hx-ky)\sin 2\pi lz\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$ [N.B. $-h+k=4n+2$, etc.]

$\begin{cases} h+k=4n+2; & l+h=4n \\ k+l=4n \end{cases}$ $A=16\{\cos 2\pi(hx-ky)\cos 2\pi lz-\sin 2\pi(hx+ky)\sin 2\pi lz\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$ [N.B. $-h+k=4n$, etc.]

$\begin{cases} h+k=4n+2; & l+h=4n+2 \\ k+l=4n+2 \end{cases}$ $A=-16\{\cos 2\pi(hx-ky)\cos 2\pi lz+\sin 2\pi(hx+ky)\sin 2\pi lz\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$ [N.B. $-h+k=4n$, etc.]

$h+k=2n+1$ or $k+l=2n+1$ (indices mixed even and odd); $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=4n,\ k+l=4n,\ l+h=4n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=4n,\ k+l=4n+2,\ l+h=4n+2}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=4n+2,\ k+l=4n,\ l+h=4n+2}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=4n+2,\ k+l=4n+2,\ l+h=4n}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\Big\}+$$
$$\frac{4}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=4n,\ k+l=4n,\ l+h=4n+2}F(hkl)[\cos 2\pi(hX+kY)\cos 2\pi lZ+\sin 2\pi(hX-kY)\sin 2\pi lZ]+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=4n,\ k+l=4n+2,\ l+h=4n}F(hkl)[\cos 2\pi(hX+kY)\cos 2\pi lZ-\sin 2\pi(hX-kY)\sin 2\pi lZ]+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=4n+2,\ k+l=4n,\ l+h=4n}F(hkl)[\cos 2\pi(hX-kY)\cos 2\pi lZ-\sin 2\pi(hX+kY)\sin 2\pi lZ]-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=4n+2,\ k+l=4n+2,\ l+h=4n+2}F(hkl)[\cos 2\pi(hX-kY)\cos 2\pi lZ+\sin 2\pi(hX+kY)\sin 2\pi lZ]\Big\}$$

N.B. The last four terms can be expressed in a symmetrical form if desired.

$Immm$ D_{2h}^{25}

No. 71

Origin at centre (mmm). $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})\pm\ |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z\ |$

$A=16\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$; $B=0$

$h+k+l=2n$ $A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$; $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$h+k+l=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ$$

$Ibam$ D_{2h}^{26}

No. 72

Origin at centre (2/m). $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm \mid x,y,z;\ \bar{x},\bar{y},z;\ x,\bar{y},\frac{1}{2}-z;\ \bar{x},y,\frac{1}{2}-z \mid$

$A=16\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)\cos 2\pi lz;\quad B=0$

$h+k+l=2n;\quad l=2n \qquad A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz \qquad F(hkl)=F(\bar{h}\bar{k}l)=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$l=2n+1 \qquad A=-16\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz;\quad A=B=0$ if $h=0$ or $k=0$

$F(hkl)=F(\bar{h}\bar{k}l)=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$h+k+l=2n+1 \qquad A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\right\}$$

$Ibca$ D_{2h}^{27}

No. 73

Origin at $\bar{1}$ (at *cab*). $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm \mid x,y,z;\ x,\bar{y},\frac{1}{2}-z;\ \frac{1}{2}-x,y,\bar{z};\ \bar{x},\frac{1}{2}-y,z \mid$

$A=16\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{h}{4}\right)\cos 2\pi\left(lz+\frac{k}{4}\right);\quad B=0$

$h+k+l=2n \quad \begin{cases} h=2n \\ k=2n \end{cases} \qquad A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz \qquad F(hkl)=F(\bar{h}\bar{k}l)=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h=2n \\ k=2n+1 \end{cases} \qquad A=-16\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $h=0$

$F(hkl)=F(\bar{h}\bar{k}l)=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h=2n+1 \\ k=2n \end{cases} \qquad A=-16\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz;\quad A=B=0$ if $k=0$

$F(hkl)=F(\bar{h}\bar{k}l)=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h=2n+1 \\ k=2n+1 \end{cases} \qquad A=-16\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $l=0$

$F(hkl)=F(\bar{h}\bar{k}l)=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$h+k+l=2n+1 \qquad A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\right\}$$

No. 74 — $Imma$ D_{2h}^{28}

Origin at centre (mnb). $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm \ |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},\frac{1}{2}+y,\bar{z};\ \bar{x},\frac{1}{2}-y,z\ |$

$$A=16\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi hx\cos 2\pi\left(ky+\frac{k}{4}\right)\cos 2\pi\left(lz-\frac{k}{4}\right);\quad B=0$$

$h+k+l=2n;\quad k=2n \qquad A=16\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz \qquad F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$k=2n+1 \qquad A=-16\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz;\quad A=B=0$ if $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$h+k+l=2n+1 \qquad A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\right\}$$

No. 75 — $P4$ C_4^1

Origin on 4. $|\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{y},x,z;\ y,\bar{x},z\ |$

$A=4\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$B=4\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\sin 2\pi lz \quad =0$ if $l=0$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(khl)|$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(khl)$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\}$$

No. 76 — $P4_1$ C_4^2

Origin on 4_1. $|\ x,y,z;\ \bar{x},\bar{y},\frac{1}{2}+z;\ \bar{y},x,\frac{1}{4}+z;\ y,\bar{x},\frac{3}{4}+z\ |$

$$A=2\left[\cos 2\pi\left(hx+ky-\frac{l}{4}\right)\cos 2\pi\left(lz+\frac{l}{4}\right)+\cos 2\pi\left(hy-kx-\frac{l}{4}\right)\cos 2\pi lz\right]$$

$$B=2\left[\cos 2\pi\left(hx+ky-\frac{l}{4}\right)\sin 2\pi\left(lz+\frac{l}{4}\right)+\cos 2\pi\left(hy-kx-\frac{l}{4}\right)\sin 2\pi lz\right] \quad =0 \text{ if } l=0$$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(khl)|$

$l = 4n$ $\quad A=4\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$B=4\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\sin 2\pi lz \quad =0$ if $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(khl)$

$l = 4n+1$ $\quad A=-2[\sin 2\pi(hx+ky)\sin 2\pi lz-\sin 2\pi(hy-kx)\cos 2\pi lz]$

$B=2[\sin 2\pi(hx+ky)\cos 2\pi lz+\sin 2\pi(hy-kx)\sin 2\pi lz]$ $\quad \Big\}\, A=B=0$ if $h=k=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=\frac{3\pi}{2}+\alpha(khl)$

$l = 4n+2$ $\quad A=-4\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$B=-4\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz$ $\quad \Big\}\, A=B=0$ if $h=k=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\pi+\alpha(khl)$

$l = 4n+3$ $\quad A=-2[\sin 2\pi(hx+ky)\sin 2\pi lz+\sin 2\pi(hy-kx)\cos 2\pi lz]$

$B=2[\sin 2\pi(hx+ky)\cos 2\pi lz-\sin 2\pi(hy-kx)\sin 2\pi lz]$ $\quad \Big\}\, A=B=0$ if $h=k=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=\frac{\pi}{2}+\alpha(khl)$

$$\rho(XYZ)=\frac{4}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty\overset{l=2n}{\{}|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\}-\sum_0^\infty\sum_0^\infty\sum_0^\infty\overset{l=2n+1}{\{}|F(hkl)|\sin 2\pi(hX+kY)\sin[2\pi lZ-\alpha(hkl)]-|F(\bar{h}kl)|\sin 2\pi(hX-kY)\sin[2\pi lZ-\alpha(\bar{h}kl)]\}\Big\}$$

$P4_2$ C_4^3

No. 77

Origin on 4_2. $\quad |\, x,y,z;\ \bar{x},\bar{y},z;\ \bar{y},x,\frac{1}{2}+z;\ y,\bar{x},\frac{1}{2}+z\,|$

$A=4\cos\pi\left[(h-k)x+(h+k)y+\frac{l}{2}\right]\cos\pi\left[(h+k)x-(h-k)y-\frac{l}{2}\right]\cos 2\pi lz$

$B=4\cos\pi\left[(h-k)x+(h+k)y+\frac{l}{2}\right]\cos\pi\left[(h+k)x-(h-k)y-\frac{l}{2}\right]\sin 2\pi lz \quad =0$ if $l=0$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|; \quad |F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(khl)|$

$l = 2n$ $\quad A=4\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$B=4\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\sin 2\pi lz \quad =0$ if $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(khl)$

$l = 2n+1$ $\quad A=-4\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$B=-4\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz$ $\quad \Big\}\, A=B=0$ if $h=k=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\}$$

No. 78

$P4_3$
C_4^4

Origin on 4_3. $\quad | \; x,y,z;\; \bar{x},\bar{y},\tfrac{1}{2}+z;\; \bar{y},x,\tfrac{3}{4}+z;\; y,\bar{x},\tfrac{1}{4}+z \; |$

$$A=2\left[\cos 2\pi\left(hx+ky-\frac{l}{4}\right)\cos 2\pi\left(lz+\frac{l}{4}\right)+\cos 2\pi\left(hy-kx+\frac{l}{4}\right)\cos 2\pi lz\right]$$

$$B=2\left[\cos 2\pi\left(hx+ky-\frac{l}{4}\right)\sin 2\pi\left(lz+\frac{l}{4}\right)+\cos 2\pi\left(hy-kx+\frac{l}{4}\right)\sin 2\pi lz\right] \quad =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|; \quad |F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(khl)|$$

$l=4n$

$$A=4\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$$

$$B=4\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\sin 2\pi lz \quad =0 \text{ if } l=0$$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(khl)$$

$l=4n+1$

$$\left.\begin{aligned}A&=-2[\sin 2\pi(hx+ky)\sin 2\pi lz+\sin 2\pi(hy-kx)\cos 2\pi lz]\\ B&=2[\sin 2\pi(hx+ky)\cos 2\pi lz-\sin 2\pi(hy-kx)\sin 2\pi lz]\end{aligned}\right\} A=B=0 \text{ if } h=k=0$$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=\frac{\pi}{2}+\alpha(khl)$$

$l=4n+2$

$$\left.\begin{aligned}A&=-4\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\cos 2\pi lz\\ B&=-4\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz\end{aligned}\right\} A=B=0 \text{ if } h=k=0$$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\pi+\alpha(khl)$$

$l=4n+3$

$$\left.\begin{aligned}A&=-2[\sin 2\pi(hx+ky)\sin 2\pi lz-\sin 2\pi(hy-kx)\cos 2\pi lz]\\ B&=2[\sin 2\pi(hx+ky)\cos 2\pi lz+\sin 2\pi(hy-kx)\sin 2\pi lz]\end{aligned}\right\} A=B=0 \text{ if } h=k=0$$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=\frac{3\pi}{2}+\alpha(khl)$$

$$\rho(XYZ)=\frac{4}{V_c}\Bigg\{\sum_0^\infty\sum_0^\infty\sum_0^\infty\Big\{|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+ |F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\Big\}- \sum_0^\infty\sum_0^\infty\sum_0^\infty\Big\{|F(hkl)|\sin 2\pi(hX+kY)\sin[2\pi lZ-\alpha(hkl)]-|F(\bar{h}kl)|\sin 2\pi(hX-kY)\sin[2\pi lZ-\alpha(\bar{h}kl)]\Big\}\Bigg\}$$

No. 79

$I4$
C_4^5

Origin on 4. $\quad (0,0,0;\; \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) + \; | \; x,y,z;\; \bar{x},\bar{y},z;\; \bar{y},x,z;\; y,\bar{x},z \; |$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$$

$$B=8\cos^2 2\pi\frac{h+k+l}{4}\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\sin 2\pi lz \quad =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|; \quad |F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(khl)|$$

$h+k+l=2n$ $\quad A=8\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$B=8\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\sin 2\pi lz \quad =0$ if $l=0$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(khl)$

$h+k+l=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\}$$

$I4_1$ C_4^6

No. 80

Origin on 2. $\quad (0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{y},\tfrac{1}{2}+x,\tfrac{1}{4}+z;\ y,\tfrac{1}{2}-x,\tfrac{1}{4}+z\ |$

$$A=4\cos^2 2\pi\frac{h+k+l}{4}\left[\cos 2\pi(hx+ky)\cos 2\pi lz+\cos\pi h\cos 2\pi(hy-kx)\cos 2\pi\left(lz-\frac{l}{4}\right)\right]$$

$$B=4\cos^2 2\pi\frac{h+k+l}{4}\left[\cos 2\pi(hx+ky)\sin 2\pi lz+\cos\pi h\cos 2\pi(hy-kx)\sin 2\pi\left(lz-\frac{l}{4}\right)\right] \quad =0 \text{ if } l=0$$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|; \quad |F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(khl)|$

$\begin{cases} h+k+l=2n \\ 2h+l=4n \end{cases}$ $\quad A=8\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$B=8\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\sin 2\pi lz \quad =0$ if $l=0$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(khl)$

$\begin{cases} h+k+l=2n \\ 2h+l=4n+1 \end{cases}$ $\quad A=4[\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(hy-kx)\sin 2\pi lz]$

$B=4[\cos 2\pi(hx+ky)\sin 2\pi lz-\cos 2\pi(hy-kx)\cos 2\pi lz]$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\frac{\pi}{2}+\alpha(khl)$

$\begin{cases} h+k+l=2n \\ 2h+l=4n+2 \end{cases}$ $\quad \left.\begin{array}{l} A=-8\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\cos 2\pi lz \\ B=-8\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz \end{array}\right\} A=B=0 \text{ if } h=k=0$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\pi+\alpha(khl)$

$\begin{cases} h+k+l=2n \\ 2h+l=4n+3 \end{cases}$ $\quad A=4[\cos 2\pi(hx+ky)\cos 2\pi lz-\cos 2\pi(hy-kx)\sin 2\pi lz]$

$B=4[\cos 2\pi(hx+ky)\sin 2\pi lz+\cos 2\pi(hy-kx)\cos 2\pi lz]$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\frac{3\pi}{2}+\alpha(khl)$

$h+k+l=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]-|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\}$$

No. 81 $P\bar{4}$ S_4^1

Origin at $\bar{4}$. $\quad | \; x,y,z;\; \bar{x},\bar{y},z;\; y,\bar{x},\bar{z};\; \bar{y},x,\bar{z} \; |$

$A=4\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$B=-4\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz \quad =0$ if $h=k=0$ or $l=0$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|; \quad |F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(khl)|$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(khl)$

$h=k \quad A=4\cos 2\pi hx\cos 2\pi hy\cos 2\pi lz; \quad B=-4\sin 2\pi hx\sin 2\pi hy\sin 2\pi lz \qquad |F(hhl)|=|F(\bar{h}hl)|$

$h=-k \quad A=4\cos 2\pi hx\cos 2\pi hy\cos 2\pi lz; \quad B=4\sin 2\pi hx\sin 2\pi hy\sin 2\pi lz \qquad \alpha(hhl)=-\alpha(\bar{h}hl)$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\}$$

No. 82 $I\bar{4}$ S_4^2

Origin at $\bar{4}$. $\quad (0,0,0;\; \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) + \; | \; x,y,z;\; \bar{x},\bar{y},z;\; y,\bar{x},\bar{z};\; \bar{y},x,\bar{z} \; |$

$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$B=-8\cos^2 2\pi\frac{h+k+l}{4}\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|; \quad |F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(khl)|; \quad |F(hhl)|=|F(\bar{h}hl)|$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(hk\bar{l})\neq\pm\alpha(\bar{h}kl); \quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(khl); \quad \alpha(hhl)=-\alpha(\bar{h}hl)$

$h+k+l=2n \quad A=8\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$B=-8\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz \quad =0$ if $h=k=0$ or $l=0$

$h+k+l=2n+1 \quad A=B=0$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\}$$

No. 83 $P4/m$ C_{4h}^1

Origin at centre $(4/m)$. $\quad \pm \; | \; x,y,z;\; \bar{x},\bar{y},z;\; \bar{y},x,z;\; y,\bar{x},z \; |$

$A=8\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz; \quad B=0$

$F(hkl)=F(\bar{h}k\bar{l})=F(hk\bar{l})\neq F(\bar{h}kl); \quad F(\bar{h}kl)=F(h\bar{k}l)=F(khl); \quad F(hhl)=F(\bar{h}hl)$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(hX-kY)\}\cos 2\pi lZ$$

$P4_2/m$ C_{4h}^2

No. 84

Origin at centre $(2/m)$ on 4_2. $\pm\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{y},x,\frac{1}{2}+z;\ y,\bar{x},\frac{1}{2}+z\ |$

$$A=8\cos\pi\left[(h-k)x+(h+k)y-\frac{l}{2}\right]\cos\pi\left[(h+k)x-(h-k)y+\frac{l}{2}\right]\cos 2\pi lz;\quad B=0$$

$$F(hkl)=F(\bar{h}k\bar{l})=F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(h\bar{k}l)$$

$l=2n$ $\quad A=8\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz;\quad B=0;$

$$F(\bar{h}kl)=F(khl);\quad F(hhl)=F(\bar{h}hl)$$

$l=2n+1$ $\quad A=-8\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\cos 2\pi lz;\quad A=B=0$ if $h=k=0$;

$$F(\bar{h}kl)=-F(khl);\quad F(hhl)=-F(\bar{h}hl)$$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(hX-kY)\}\cos 2\pi lZ$$

$P4/n$ C_{4h}^3

No. 85

Origin at $\bar{4}$ (at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$).

$|\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ \frac{1}{2}-x,\frac{1}{2}-y,\bar{z};\ \frac{1}{2}+x,\frac{1}{2}+y,\bar{z};\ \frac{1}{2}+y,\frac{1}{2}-x,z;\ \frac{1}{2}-y,\frac{1}{2}+x,z\ |$

$$A=8\cos^2 2\pi\frac{h+k}{4}\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$$

$$B=-8\sin^2 2\pi\frac{h+k}{4}\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz\quad =0 \text{ if } l=0$$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(khl)|$$

$h+k=2n$ $\quad A=8\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz;\quad B=0;\quad |F(hhl)|=|F(\bar{h}hl)|$

$$\alpha(hkl)=\alpha(\bar{h}k\bar{l})=\alpha(hk\bar{l})=\mathrm{m}\pi;\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(khl)=\mathrm{m}'\pi;\quad \alpha(hhl)=\alpha(\bar{h}hl)=\mathrm{m}\pi$$

$h+k=2n+1$ $\quad A=0;\quad B=-8\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{2};\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(khl)=\mathrm{m}'\pi+\frac{\pi}{2}$$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}[|F(hkl)|\cos 2\pi(hX+kY)\cos\mathrm{m}\pi+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos\mathrm{m}'\pi]\cos 2\pi lZ+\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}[|F(hkl)|\cos 2\pi(hX+kY)\cos\mathrm{m}\pi+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos\mathrm{m}'\pi]\sin 2\pi lZ\right\}$$

where m, m′ may be 0 or 1 according to the sign of A or B under the given conditions of h, k, l.

(See, for example, space group 48.)

No. 85 $P4/n$ C_{4h}^{3}

Origin at $\bar{1}$ (at $\frac{1}{4},\bar{\frac{1}{4}},0$ from $\bar{4}$). $\pm\ |\ x,y,z;\ \frac{1}{2}-x,\frac{1}{2}-y,z;\ \frac{1}{2}+y,\bar{x},\bar{z};\ \bar{y},\frac{1}{2}+x,\bar{z}\ |$

$$A=8\cos\pi\left[(h-k)x+(h+k)y-\frac{h}{2}\right]\cos\pi\left[(h+k)x-(h-k)y-\frac{k}{2}\right]\cos 2\pi\left(lz+\frac{h+k}{4}\right);\quad B=0$$

$\begin{cases} h=2n \\ k=2n \end{cases}$ $A=8\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz;$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(h\bar{k}l)=F(khl);\quad F(hhl)=F(\bar{h}hl)$

$\begin{cases} h=2n \\ k=2n+1 \end{cases}$ $A=-8\cos\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz;\quad A=B=0$ if $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=-F(h\bar{k}l)=F(khl)$

$\begin{cases} h=2n+1 \\ k=2n \end{cases}$ $A=-8\sin\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\sin 2\pi lz;\quad A=B=0$ if $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=-F(h\bar{k}l)=-F(khl)$

$\begin{cases} h=2n+1 \\ k=2n+1 \end{cases}$ $A=-8\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(h\bar{k}l)=-F(khl);\quad F(hhl)=-F(\bar{h}hl)$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}[F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(hX-kY)]\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}[F(hkl)\sin 2\pi(hX+kY)-F(\bar{h}kl)\sin 2\pi(hX-kY)]\sin 2\pi lZ\right\}$$

No. 86 $P4_2/n$ C_{4h}^{4}

Origin at $\bar{4}$ (at $\bar{\frac{1}{4}},\bar{\frac{1}{4}},\bar{\frac{1}{4}}$ from $\bar{1}$).

$|\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ \frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z;\ \frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z;\ \frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z;\ \frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z\ |$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$$

$$B=-8\sin^2 2\pi\frac{h+k+l}{4}\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz\quad =0 \text{ if } l=0$$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(khl)|$

$h+k+l=2n$ $A=8\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz;\quad B=0$

$|F(hhl)|=|F(\bar{h}hl)|;\quad \alpha(hhl)=\alpha(\bar{h}hl)=\mathrm{m}\pi$

$\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(hk\bar{l})=\mathrm{m}\pi;\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(khl)=\mathrm{m}'\pi$

$h+k+l=2n+1$ $A=0;\quad B=-8\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz$

$A=B=0$ if $h=k=0$ or if $l=0$; $|F(hhl)|=|F(\bar{h}hl)|;\quad \alpha(hhl)=-\alpha(\bar{h}hl)=\mathrm{m}\pi+\frac{\pi}{2}$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{2};\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(khl)=\mathrm{m}'\pi+\frac{\pi}{2}$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}[|F(hkl)|\cos 2\pi(hX+kY)\cos\mathrm{m}\pi+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos\mathrm{m}'\pi]\cos 2\pi lZ+\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}[|F(hkl)|\cos 2\pi(hX+kY)\cos\mathrm{m}\pi+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos\mathrm{m}'\pi]\sin 2\pi lZ\right\}$$

where m, m′=0 or 1 according as A (or if $A=0$, then B) is positive or negative.

$P4_2/n$ C_{4h}^4

No. 86

Origin at $\bar{1}$ (at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{4}$). $\pm\ |\ x,y,z;\ \frac{1}{2}-x,\frac{1}{2}-y,z;\ \bar{y},\frac{1}{2}+x,\frac{1}{2}+z;\ \frac{1}{2}+y,\bar{x},\frac{1}{2}+z\ |$

$$A=8\cos\pi\left[(h-k)x+(h+k)y-\frac{k+l}{2}\right]\cos\pi\left[(h+k)x-(h-k)y-\frac{h-l}{2}\right]\cos 2\pi\left(lz+\frac{h+k}{4}\right);\quad B=0$$

$\begin{cases} h+k=2n \\ k+l=2n \end{cases}$ $A=8\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(h\bar{k}l)=F(khl);\quad F(hhl)=F(\bar{h}\bar{h}l)$

$\begin{cases} h+k=2n \\ k+l=2n+1 \end{cases}$ $A=-8\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\cos 2\pi lz;\quad A=B=0$ if $h=k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(h\bar{k}l)=-F(khl);\quad F(hhl)=-F(\bar{h}\bar{h}l)$

$\begin{cases} h+k=2n+1 \\ k+l=2n \end{cases}$ $A=-8\cos\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz;\quad A=B=0$ if $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=-F(h\bar{k}l)=F(khl)$

$\begin{cases} h+k=2n+1 \\ k+l=2n+1 \end{cases}$ $A=-8\sin\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\sin 2\pi lz;\quad A=B=0$ if $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=-F(h\bar{k}l)=-F(khl)$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}[F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(hX-kY)]\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}[F(hkl)\sin 2\pi(hX+kY)-F(\bar{h}kl)\sin 2\pi(hX-kY)]\sin 2\pi lZ\right\}$$

$I4/m$ C_{4h}^5

No. 87

Origin at centre $(4/m)$. $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})\ \pm\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{y},x,z;\ y,\bar{x},z\ |$

$$A=16\cos^2 2\pi\frac{h+k+l}{4}\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz;\quad B=0$$

$h+k+l=2n$ $A=16\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(h\bar{k}l)=F(khl);\quad F(hhl)=F(\bar{h}\bar{h}l)$

$h+k+l=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(hX-kY)\}\cos 2\pi lZ$$

Origin at $\bar{4}$ (at $0,\frac{1}{4},\frac{1}{8}$ from $\bar{1}$).

$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) + \ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ \bar{x},\frac{1}{2}-y,\frac{1}{4}-z;\ x,\frac{1}{2}+y,\frac{1}{4}-z;\ y,\frac{1}{2}-x,\frac{1}{4}+z;\ \bar{y},\frac{1}{2}+x,\frac{1}{4}+z\ |$

$A=G\cos 2\pi\,\frac{2k+l}{8};\quad B=G\sin 2\pi\,\frac{2k+l}{8},$ where

$$G=8\cos^2 2\pi\frac{h+k+l}{4}\left[\cos 2\pi(hx+ky)\cos 2\pi\left(lz-\frac{2k+l}{8}\right)+\cos 2\pi(hy-kx)\cos 2\pi\left(lz+\frac{2k+l}{8}\right)\right]$$

$$=16\cos^2 2\pi\frac{h+k+l}{4}\left\{\cos 2\pi\frac{2k+l}{8}\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz-\right.$$
$$\left.\sin 2\pi\frac{2k+l}{8}\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz\right\}$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(khl)|;\quad \alpha(\bar{h}kl)=-\alpha(khl)$$

$\begin{cases} h+k+l=2n \\ 2k+l=4n \end{cases}$ $\quad A=16\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz;\quad B=0$

$|F(hhl)|=|F(\bar{h}hl)|;\quad \alpha(hhl)=\alpha(\bar{h}hl)=\mathrm{m}\pi$

$\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(hk\bar{l})=\mathrm{m}\pi;\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\mathrm{m}'\pi$

$\begin{cases} h+k+l=2n \\ 2k+l=4n+1 \end{cases}$ $\quad A=8\{\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz-$

$\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz\};\quad B=A$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{4};\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\mathrm{m}'\pi+\frac{\pi}{4}$

$\begin{cases} h+k+l=2n \\ 2k+l=4n+2 \end{cases}$ $\quad A=0;\quad B=-16\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz$

$A=B=0$ if $h=k=0$ or $l=0$; $\quad |F(hhl)|=|F(\bar{h}hl)|;\quad \alpha(hhl)=-\alpha(\bar{h}hl)=\mathrm{m}\pi+\frac{\pi}{2}$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{2};\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\mathrm{m}'\pi+\frac{\pi}{2}$

$\begin{cases} h+k+l=2n \\ 2k+l=4n+3 \end{cases}$ $\quad A=8\{\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz+$

$\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz\};\quad B=-A$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\mathrm{m}\pi-\frac{\pi}{4};\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\mathrm{m}'\pi-\frac{\pi}{4}$

$h+k+l=2n+1\quad A=B=0$

N.B. If $h+k+l=2n$ and $2k+l=4n+1$, then $-2k-l=4n+3$, $2k-l=4n+3$, $-2k+l=4n+1$, etc.

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2k+l=4n}[|F(hkl)|\cos 2\pi(hX+kY)\cos\mathrm{m}\pi+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos\mathrm{m}'\pi]\cos 2\pi lZ+\right.$$
$$\frac{1}{\sqrt{2}}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2k+l=4n+1}[|F(hkl)|\cos 2\pi(hX+kY)\cos\mathrm{m}\pi+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos\mathrm{m}'\pi](\cos 2\pi lZ+\sin 2\pi lZ)+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2k+l=4n+2}[|F(hkl)|\cos 2\pi(hX+kY)\cos\mathrm{m}\pi+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos\mathrm{m}'\pi]\sin 2\pi lZ+$$
$$\left.\frac{1}{\sqrt{2}}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2k+l=4n+3}[|F(hkl)|\cos 2\pi(hX+kY)\cos\mathrm{m}\pi+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos\mathrm{m}'\pi](\cos 2\pi lZ-\sin 2\pi lZ)\right\}$$

where m, m′=0 or 1 according as A (or if $A=0$, then B) is positive or negative.

$I4_1/a$ C_{4h}^6

No. 88

Origin at $\bar{1}$ (at $0,\frac{1}{4},\frac{1}{8}$ from $\bar{4}$). $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm \ |\ x,y,z;\ \bar{x},\frac{1}{2}-y,z;\ \frac{3}{4}-y,\frac{1}{4}+x,\frac{1}{4}+z;\ \frac{1}{4}+y,\frac{1}{4}-x,\frac{1}{4}+z\ |$

$$A=8\cos 2\pi\frac{h+k+l}{4}\left\{\cos 2\pi\frac{h+k+l}{4}\cos 2\pi\left(hx+ky-\frac{k}{4}\right)\cos 2\pi\left(lz+\frac{k}{4}\right)+\cos 2\pi\left(hy-kx-\frac{h}{4}\right)\cos 2\pi\left(lz+\frac{h}{4}\right)\right\}$$

$B=0$

$h+k+l=4n$; $h=2n$; $k=2n$	$A=8[\cos 2\pi(hx+ky)+\cos 2\pi(hy-kx)]\cos 2\pi lz$; $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})\neq F(\bar{h}kl)$; $F(\bar{h}kl)=F(h\bar{k}l)=F(khl)$; $F(hhl)=F(\bar{h}hl)$
$h+k+l=4n$; $h=2n$; $k=2n+1$	$A=-8[\sin 2\pi(hx+ky)\sin 2\pi lz-\cos 2\pi(hy-kx)\cos 2\pi lz]$; $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(hk\bar{l})\neq F(\bar{h}kl)$; $F(\bar{h}kl)=-F(h\bar{k}l)=F(khl)$
$h+k+l=4n$; $h=2n+1$; $k=2n$	$A=8[\cos 2\pi(hx+ky)\cos 2\pi lz-\sin 2\pi(hy-kx)\sin 2\pi lz]$; $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})\neq F(\bar{h}kl)$; $F(\bar{h}kl)=F(h\bar{k}l)=F(khl)$
$h+k+l=4n$; $h=2n+1$; $k=2n+1$	$A=-8[\sin 2\pi(hx+ky)+\sin 2\pi(hy-kx)]\sin 2\pi lz$; $A=B=0$ if $l=0$; $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(hk\bar{l})\neq F(\bar{h}kl)$; $F(\bar{h}kl)=-F(h\bar{k}l)=F(khl)$; $F(hhl)=F(\bar{h}hl)$
$h+k+l=4n+2$; $h=2n$; $k=2n$	$A=8[\cos 2\pi(hx+ky)-\cos 2\pi(hy-kx)]\cos 2\pi lz$; $A=B=0$ if $h=k=0$; $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})\neq F(\bar{h}kl)$; $F(\bar{h}kl)=F(h\bar{k}l)=-F(khl)$; $F(hhl)=-F(\bar{h}hl)$
$h+k+l=4n+2$; $h=2n$; $k=2n+1$	$A=-8[\sin 2\pi(hx+ky)\sin 2\pi lz+\cos 2\pi(hy-kx)\cos 2\pi lz]$; $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(hk\bar{l})\neq F(\bar{h}kl)$; $F(\bar{h}kl)=-F(h\bar{k}l)=-F(khl)$
$h+k+l=4n+2$; $h=2n+1$; $k=2n$	$A=8[\cos 2\pi(hx+ky)\cos 2\pi lz+\sin 2\pi(hy-kx)\sin 2\pi lz]$; $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})\neq F(\bar{h}kl)$; $F(\bar{h}kl)=F(h\bar{k}l)=-F(khl)$
$h+k+l=4n+2$; $h=2n+1$; $k=2n+1$	$A=-8[\sin 2\pi(hx+ky)-\sin 2\pi(hy-kx)]\sin 2\pi lz$; $A=B=0$ if $l=0$; $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(hk\bar{l})\neq F(\bar{h}kl)$; $F(\bar{h}kl)=-F(h\bar{k}l)=-F(khl)$;
$h+k+l=2n+1$	$A=B=0$; $F(hhl)=-F(\bar{h}hl)$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n}[F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(hX-kY)]\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n+1}[F(hkl)\sin 2\pi(hX+kY)-F(\bar{h}kl)\sin 2\pi(hX-kY)]\sin 2\pi lZ\right\}$$

$P422$ D_4^1

No. 89

Origin at 422. $|\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\bar{z};\ x,\bar{y},\bar{z};\ \bar{y},\bar{x},\bar{z};\ y,x,\bar{z};\ y,\bar{x},z;\ \bar{y},x,z\ |$

$A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=-4\sin 2\pi lz\,[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$ or $l=0$ or $h=\pm k$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$\alpha(h\bar{k}l)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(hk\bar{l})=-\alpha(hkl)=-\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\{\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)\}$$

No. 90

$P4_12$
D_4^2

Origin at 222. | x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}+x,z$; $\frac{1}{2}+y,\frac{1}{2}-x,z$ |

$$A=4\cos 2\pi lz\left[\cos 2\pi\left(hx-\frac{h+k}{4}\right)\cos 2\pi\left(ky+\frac{h+k}{4}\right)+\cos 2\pi\left(kx-\frac{h+k}{4}\right)\cos 2\pi\left(hy+\frac{h+k}{4}\right)\right]$$

$$B=-4\sin 2\pi lz\left[\sin 2\pi\left(hx-\frac{h+k}{4}\right)\sin 2\pi\left(ky+\frac{h+k}{4}\right)-\sin 2\pi\left(kx-\frac{h+k}{4}\right)\sin 2\pi\left(hy+\frac{h+k}{4}\right)\right]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}l)|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k=2n$

$$A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$$

$$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]\quad =0 \text{ if } h=0 \text{ or } k=0 \text{ or } l=0 \text{ or } h=\pm k$$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}l)=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$$

$h+k=2n+1$

$$A=-4\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]\quad =0 \text{ if } h=0 \text{ or } k=0$$

$$B=4\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]\quad =0 \text{ if } l=0$$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}l)=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]+\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)]\right\}$$

No. 91

$P4_122$
D_4^3

Enantiomorphous to $P4_322$. Origin at 4_121.

| x,y,z; $\bar{x},y,\bar{z}$; $\bar{x},\bar{y},\frac{1}{2}+z$; $x,\bar{y},\frac{1}{2}-z$; $\bar{y},\bar{x},\frac{1}{4}-z$; $\bar{y},x,\frac{1}{4}+z$; $y,\bar{x},\frac{3}{4}+z$; $y,x,\frac{3}{4}-z$ |

$$A=4\left[\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi ky\cos 2\pi\left(lz+\frac{l}{4}\right)+\cos 2\pi kx\cos 2\pi\left(hy-\frac{l}{4}\right)\cos 2\pi lz\right]$$

$$B=-4\left[\sin 2\pi\left(hx-\frac{l}{4}\right)\sin 2\pi ky\sin 2\pi\left(lz+\frac{l}{4}\right)-\sin 2\pi kx\sin 2\pi\left(hy-\frac{l}{4}\right)\sin 2\pi lz\right]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}l)|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$l = 4n$ $\quad A=4\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky+\cos 2\pi kx \cos 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx \sin 2\pi ky-\sin 2\pi kx \sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$ or $l=0$ or $h=\pm k$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$$

$l = 4n+1$ $\quad A=4[-\sin 2\pi hx \cos 2\pi ky \sin 2\pi lz+\cos 2\pi kx \sin 2\pi hy \cos 2\pi lz]$ $=0$ if $h=0$

$B=4[\cos 2\pi hx \sin 2\pi ky \cos 2\pi lz-\sin 2\pi kx \cos 2\pi hy \sin 2\pi lz]$ $=0$ if $k=0$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})=\frac{\pi}{2}-\alpha(khl);\quad A=B \text{ if } h=k;\quad A=-B \text{ if } h=-k$$

$l = 4n+2$ $\quad A=4\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky-\cos 2\pi kx \cos 2\pi hy]$ $=0$ if $h=\pm k$

$B=-4\sin 2\pi lz[\sin 2\pi hx \sin 2\pi ky+\sin 2\pi kx \sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\frac{\pi}{2}-\alpha(khl)$$

$l = 4n+3$ $\quad A=-4[\sin 2\pi hx \cos 2\pi ky \sin 2\pi lz+\cos 2\pi kx \sin 2\pi hy \cos 2\pi lz]$ $=0$ if $h=0$

$B=4[\cos 2\pi hx \sin 2\pi ky \cos 2\pi lz+\sin 2\pi kx \cos 2\pi hy \sin 2\pi lz]$ $=0$ if $k=0$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})=\frac{3\pi}{2}-\alpha(khl);\quad A=-B \text{ if } h=k;\ A=B \text{ if } h=-k$$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty\sum_{l=2n}|F(hkl)|\,[\cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ \cos\alpha(hkl)-\sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ \sin\alpha(hkl)]+$$
$$\tfrac{1}{2}\sum_0^\infty\sum_0^\infty\sum_0^\infty\sum_{l=2n+1}|F(hkl)|\{-\sin 2\pi(hX+kY)\quad[2\pi lZ-\alpha(hkl)]-\sin 2\pi(hX-kY)\sin[2\pi lZ+\alpha(hkl)]\}\Big\}$$

$P4_12_12$ D_4^4

No. 92

Enantiomorphous to $P4_32_12$; Origin at 2_12 (2_1 along z axis).

$|\ x,y,z;\ \bar{x},\bar{y},\tfrac{1}{2}+z;\ y,x,\bar{z};\ \bar{y},\bar{x},\tfrac{1}{2}-z;\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{4}-z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{3}{4}-z;\ \tfrac{1}{2}-y,\tfrac{1}{2}+x,\tfrac{1}{4}+z;\ \tfrac{1}{2}+y,\tfrac{1}{2}-x,\tfrac{3}{4}+z\ |$

$$A=4\Big\{\cos\pi(h+k)(x+y)\cos\pi\Big[(h-k)(x-y)-\frac{l}{2}\Big]\cos 2\pi\Big(lz+\frac{l}{4}\Big)+$$
$$\cos\pi(h+k)\cos\pi\Big[(h-k)(x+y)-\frac{l}{2}\Big]\cos\pi(h+k)(x-y)\cos 2\pi lz\Big\}$$
$$B=-4\Big\{\sin\pi(h+k)(x+y)\sin\pi\Big[(h-k)(x-y)-\frac{l}{2}\Big]\sin 2\pi\Big(lz+\frac{l}{4}\Big)-$$
$$\cos\pi(h+k)\sin\pi\Big[(h-k)(x+y)-\frac{l}{2}\Big]\sin\pi(h+k)(x-y)\sin 2\pi lz\Big\}$$
$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$2h+2k+l=4n$

$A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$

$B=0$ if $h=0$ or $k=0$ or $l=0$ or $h=\pm k$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$$

$2h+2k+l=4n+1$

$A=4\{-\cos\pi(h+k)(x+y)\sin\pi(h-k)(x-y)\sin 2\pi lz+$
$\sin\pi(h-k)(x+y)\cos\pi(h+k)(x-y)\cos 2\pi lz\}$

$B=4\{\sin\pi(h+k)(x+y)\cos\pi(h-k)(x-y)\cos 2\pi lz-$
$\cos\pi(h-k)(x+y)\sin\pi(h+k)(x-y)\sin 2\pi lz\}$

$A=0$ if $h=k$; $B=0$ if $h=-k$; $A=B$ if $k=0$; $A=-B$ if $h=0$.

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\frac{3\pi}{2}-\alpha(\bar{h}kl)=\frac{\pi}{2}-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})=\pi-\alpha(khl)$$

$2h+2k+l=4n+2$

$A=-4\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$

$B=4\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $h=\pm k$ or $l=0$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$$

$2h+2k+l=4n+3$

$A=-4\{\cos\pi(h+k)(x+y)\sin\pi(h-k)(x-y)\sin 2\pi lz+$
$\sin\pi(h-k)(x+y)\cos\pi(h+k)(x-y)\cos 2\pi lz\}$

$B=4\{\sin\pi(h+k)(x+y)\cos\pi(h-k))(x-y)\cos 2\pi lz+$
$\cos\pi(h-k)(x+y)\sin\pi(h+k)(x-y)\sin 2\pi lz\}$

$A=0$ if $h=k$; $B=0$ if $h=-k$; $A=B$ if $h=0$; $A=-B$ if $k=0$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\frac{\pi}{2}-\alpha(\bar{h}kl)=\frac{3\pi}{2}-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})=\pi-\alpha(khl)$$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+2k+l=4n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]+$$
$$\tfrac{1}{2}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+2k+l=4n+1}|F(hkl)|\{-\sin 2\pi(hX+kY)\sin[2\pi lZ-\alpha(hkl)]+\sin 2\pi(hX-kY)\cos[2\pi lZ+\alpha(hkl)]\}+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+2k+l=4n+2}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)]+$$
$$\tfrac{1}{2}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+2k+l=4n+3}|F(hkl)|\{-\sin 2\pi(hX+kY)\sin[2\pi lZ-\alpha(hkl)]-\sin 2\pi(hX-kY)\cos[2\pi lZ+\alpha(hkl)]\}\Big\}$$

No. 93

$P4_22$
D_4^5

Origin at 4_221. | x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\bar{z}$; $x,\bar{y},\bar{z}$; $y,x,\frac{1}{2}-z$; $\bar{y},\bar{x},\frac{1}{2}-z$; $\bar{y},x,\frac{1}{2}+z$; $y,\bar{x},\frac{1}{2}+z$ |

$A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos\pi l\cos 2\pi kx\cos 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\cos\pi l\sin 2\pi kx\sin 2\pi hy]$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$l = 2n$ $\quad A=4\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky + \cos 2\pi kx \cos 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx \sin 2\pi ky - \sin 2\pi kx \sin 2\pi hy] \quad =0$ if $h=0$ or $k=0$ or $l=0$ or $h=\pm k$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$

$l = 2n+1$ $\quad A=4\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky - \cos 2\pi kx \cos 2\pi hy] \quad =0$ if $h=\pm k$

$B=-4\sin 2\pi lz[\sin 2\pi hx \sin 2\pi ky + \sin 2\pi kx \sin 2\pi hy] \quad =0$ if $h=0$ or $k=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi-\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|[\cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ \cos\alpha(hkl) - \sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ \sin\alpha(hkl)]$$

$P4_22_12$ D_4^6

No. 94

Origin at 222.

$|\ x,y,z;\ \bar{x},\bar{y},z;\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{2}-z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{1}{2}-z;\ y,x,\bar{z};\ \bar{y},\bar{x},\bar{z};\ \tfrac{1}{2}+y,\tfrac{1}{2}-x,\tfrac{1}{2}+z;\ \tfrac{1}{2}-y,\tfrac{1}{2}+x,\tfrac{1}{2}+z\ |$

$$A=4\cos 2\pi lz\left\{\cos 2\pi\left(hx-\frac{h+k+l}{4}\right)\cos 2\pi\left(ky+\frac{h+k+l}{4}\right)+\cos 2\pi\left(kx-\frac{h+k+l}{4}\right)\cos 2\pi\left(hy+\frac{h+k+l}{4}\right)\right\}$$

$$B=-4\sin 2\pi lz\left\{\sin 2\pi\left(hx-\frac{h+k+l}{4}\right)\sin 2\pi\left(ky+\frac{h+k+l}{4}\right)-\sin 2\pi\left(kx-\frac{h+k+l}{4}\right)\sin 2\pi\left(hy+\frac{h+k+l}{4}\right)\right\}$$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$h+k+l=2n$ $\quad A=4\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky + \cos 2\pi kx \cos 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx \sin 2\pi ky - \sin 2\pi kx \sin 2\pi hy] \quad =-\alpha(khl)$

$B=0$ if $h=0$ or $k=0$ or $l=0$ or $h=\pm k$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$h+k+l=2n+1$ $\quad A=-4\cos 2\pi lz[\sin 2\pi hx \sin 2\pi ky + \sin 2\pi kx \sin 2\pi hy] \quad =0$ if $h=0$ or $k=0$

$B=4\sin 2\pi lz[\cos 2\pi hx \cos 2\pi ky - \cos 2\pi kx \cos 2\pi hy] \quad =0$ if $h=\pm k$ or $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|[\cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ \cos\alpha(hkl) - \sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ \sin\alpha(hkl)]+\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|[\cos 2\pi hX \cos 2\pi kY \sin 2\pi lZ \sin\alpha(hkl) - \sin 2\pi hX \sin 2\pi kY \cos 2\pi lZ \cos\alpha(hkl)]\right\}$$

$P4_322$ D_4^7

No. 95

Enantiomorphous to $P4_122$; Origin at 4_321.

$|\ x,y,z;\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},\tfrac{1}{2}+z;\ x,\bar{y},\tfrac{1}{2}-z;\ y,x,\tfrac{1}{4}-z;\ y,\bar{x},\tfrac{1}{4}+z;\ \bar{y},x,\tfrac{3}{4}+z;\ \bar{y},\bar{x},\tfrac{3}{4}-z\ |$

$$A=4\left[\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi ky \cos 2\pi\left(lz+\frac{l}{4}\right)+\cos 2\pi kx \cos 2\pi\left(hy+\frac{l}{4}\right)\cos 2\pi lz\right]$$

$$B=-4\left[\sin 2\pi\left(hx-\frac{l}{4}\right)\sin 2\pi ky \sin 2\pi\left(lz+\frac{l}{4}\right)-\sin 2\pi kx \sin 2\pi\left(hy+\frac{l}{4}\right)\sin 2\pi lz\right]$$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$l = 4n$ $\quad A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$ or $l=0$ or $h=\pm k$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$$

$l = 4n+1$ $\quad A=-4[\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz+\cos 2\pi kx\sin 2\pi hy\cos 2\pi lz]$ $=0$ if $h=0$

$B=4[\cos 2\pi hx\sin 2\pi ky\cos 2\pi lz+\sin 2\pi kx\cos 2\pi hy\sin 2\pi lz]$ $=0$ if $k=0$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})=\frac{3\pi}{2}-\alpha(khl);\quad A=-B \text{ if } h=k;\quad A=B \text{ if } h=-k$$

$l = 4n+2$ $\quad A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $h=\pm k$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi-\alpha(khl)$$

$l = 4n+3$ $\quad A=4[-\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz+\cos 2\pi kx\sin 2\pi hy\cos 2\pi lz]$ $=0$ if $h=0$

$B=4[\cos 2\pi hx\sin 2\pi ky\cos 2\pi lz-\sin 2\pi kx\cos 2\pi hy\sin 2\pi lz]$ $=0$ if $k=0$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})=\frac{\pi}{2}-\alpha(khl);\quad A=B \text{ if } h=k;\quad A=-B \text{ if } h=-k$$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]+$$
$$\tfrac{1}{2}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}|F(hkl)|\{-\sin 2\pi(hX+kY)\sin[2\pi lZ-\alpha(hkl)]-\sin 2\pi(hX-kY)\sin[2\pi lZ+\alpha(hkl)]\}\Big\}$$

No. 96

$P4_32_12$
D_4^8

Enantiomorphous to $P4_12_12$; Origin at 2_12 (2_1 along z axis).

| x,y,z; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,x,\bar{z}$; $\bar{y},\bar{x},\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{4}-z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{3}{4}-z$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{4}+z$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{3}{4}+z$ |

$$A=4\Big\{\cos\pi(h+k)(x+y)\cos\pi\Big[(h-k)(x-y)-\frac{l}{2}\Big]\cos 2\pi\Big(lz+\frac{l}{4}\Big)+$$
$$\cos\pi(h+k)\cos\pi\Big[(h-k)(x+y)+\frac{l}{2}\Big]\cos\pi(h+k)(x-y)\cos 2\pi lz\Big\}$$
$$B=-4\Big\{\sin\pi(h+k)(x+y)\sin\pi\Big[(h-k)(x-y)-\frac{l}{2}\Big]\sin 2\pi\Big(lz+\frac{l}{4}\Big)-$$
$$\cos\pi(h+k)\sin\pi\Big[(h-k)(x+y)+\frac{l}{2}\Big]\sin\pi(h+k)(x-y)\sin 2\pi lz\Big\}$$
$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$2h+2k+l=4n$ $\quad A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$

$B=0$ if $h=0$ or $k=0$ or $l=0$ or $h=\pm k$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$$

$2h+2k+l=4n+1$ $\quad A=-4\{\cos\pi(h+k)(x+y)\sin\pi(h-k)(x-y)\sin 2\pi lz+$

$\sin\pi(h-k)(x+y)\cos\pi(h+k)(x-y)\cos 2\pi lz\}$

$B=4\{\sin\pi(h+k)(x+y)\cos\pi(h-k)(x-y)\cos 2\pi lz+$

$\cos\pi(h-k)(x+y)\sin\pi(h+k)(x-y)\sin 2\pi lz\}$

$A=0$ if $h=k$; $B=0$ if $h=-k$; $A=B$ if $h=0$; $A=-B$ if $k=0$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\frac{\pi}{2}-\alpha(\bar{h}kl)=\frac{3\pi}{2}-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})=\pi-\alpha(khl)$

$2h+2k+l=4n+2$ $\quad A=-4\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$

$B=4\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $h=\pm k$ or $l=0$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$

$2h+2k+l=4n+3$ $\quad A=4\{-\cos\pi(h+k)(x+y)\sin\pi(h-k)(x-y)\sin 2\pi lz+$

$\sin\pi(h-k)(x+y)\cos\pi(h+k)(x-y)\cos 2\pi lz\}$

$B=4\{\sin\pi(h+k)(x+y)\cos\pi(h-k)(x-y)\cos 2\pi lz-$

$\cos\pi(h-k)(x+y)\sin\pi(h+k)(x-y)\sin 2\pi lz\}$

$A=0$ if $h=k$; $B=0$ if $h=-k$; $A=B$ if $k=0$; $A=-B$ if $h=0$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\frac{3\pi}{2}-\alpha(\bar{h}kl)=\frac{\pi}{2}-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})=\pi-\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+2k+l=4n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]+$$
$$\tfrac{1}{2}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+2k+l=4n+1}|F(hkl)|\{-\sin 2\pi(hX+kY)\sin[2\pi lZ-\alpha(hkl)]-\sin 2\pi(hX-kY)\cos[2\pi lZ+\alpha(hkl)]\}+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+2k+l=4n+2}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)]+$$
$$\tfrac{1}{2}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+2k+l=4n+3}|F(hkl)|\{-\sin 2\pi(hX+kY)\sin[2\pi lZ-\alpha(hkl)]+\sin 2\pi(hX-kY)\cos[2\pi lZ+\alpha(hkl)]\}\Big\}$$

$I422$
D_4^9

No. 97

Origin at 422. $\quad (0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})\ +\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\bar{z};\ x,\bar{y},\bar{z};\ \bar{y},\bar{x},\bar{z};\ y,x,\bar{z};\ y,\bar{x},z;\ \bar{y},x,z\ |$

$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=-8\cos^2 2\pi\frac{h+k+l}{4}\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$h+k+l=2n$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=-8\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$

$B=0$ if $h=0$ or $k=0$ or $l=0$ or $h=\pm k$; $\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$h+k+l=2n+1$ $\quad A=B=0$ $\quad =-\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]$$

$I4_122$ D_4^{10}

Origin at 222.

$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) +\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},\tfrac{1}{2}+y,\tfrac{1}{4}-z;\ x,\tfrac{1}{2}-y,\tfrac{1}{4}-z;\ \bar{y},\bar{x},\bar{z};\ y,x,\bar{z};\ \bar{y},\tfrac{1}{2}+x,\tfrac{1}{4}+z;\ y,\tfrac{1}{2}-x,\tfrac{1}{4}+z\ |$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\Big\{\cos\pi(h+k)(x+y)\cos\pi(h-k)(x-y)\cos 2\pi lz+$$
$$\cos\pi k\cos\pi\Big[(h-k)(x+y)+\frac{l}{2}\Big]\cos\pi\Big[(h+k)(x-y)+\frac{l}{2}\Big]\cos 2\pi\Big(lz+\frac{l}{4}\Big)\Big\}$$

$$B=-8\cos^2 2\pi\frac{h+k+l}{4}\Big\{\sin\pi(h+k)(x+y)\sin\pi(h-k)(x-y)\sin 2\pi lz-$$
$$\cos\pi k\sin\pi\Big[(h-k)(x+y)+\frac{l}{2}\Big]\sin\pi\Big[(h+k)(x-y)+\frac{l}{2}\Big]\sin 2\pi\Big(lz+\frac{l}{4}\Big)\Big\}$$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$\begin{cases} h+k+l=2n \\ 2k+l=4n \end{cases}$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=-8\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$

$B=0$ if $h=0$ or $k=0$ or $l=0$ or $h=\pm k$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$\begin{cases} h+k+l=2n \\ 2k+l=4n+1 \end{cases}$ $\quad A=8\{\cos\pi(h+k)(x+y)\cos\pi(h-k)(x-y)\cos 2\pi lz-$ $\quad =-\alpha(khl)$

$\sin\pi(h-k)(x+y)\sin\pi(h+k)(x-y)\sin 2\pi lz\}$

$B=8\{-\sin\pi(h+k)(x+y)\sin\pi(h-k)(x-y)\sin 2\pi lz+$

$\cos\pi(h-k)(x+y)\cos\pi(h+k)(x-y)\cos 2\pi lz\}$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\frac{\pi}{2}-\alpha(\bar{h}kl)=\frac{\pi}{2}-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$

$\begin{cases} h+k+l=2n \\ 2k+l=4n+2 \end{cases}$ $\quad A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$

$B=8\sin 2\pi lz\,[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $h=\pm k$ or $l=0$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$

$\begin{cases} h+k+l=2n \\ 2k+l=4n+3 \end{cases}$ $\quad A=8\{\cos\pi(h+k)(x+y)\cos\pi(h-k)(x-y)\cos 2\pi lz+$

$\sin\pi(h-k)(x+y)\sin\pi(h+k)(x-y)\sin 2\pi lz\}$

$B=-8\{\sin\pi(h+k)(x+y)\sin\pi(h-k)(x-y)\sin 2\pi lz+$

$\cos\pi(h-k)(x+y)\cos\pi(h+k)(x-y)\cos 2\pi lz\}$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\frac{3\pi}{2}-\alpha(\bar{h}kl)=\frac{3\pi}{2}-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$

$h+k+l=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2k+l=4n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]+$$
$$\tfrac{1}{2}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2k+l=4n+1}|F(hkl)|\{\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+\cos 2\pi(hX-kY)\sin[2\pi lZ+\alpha(hkl)]\}+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2k+l=4n+2}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)]+$$
$$\tfrac{1}{2}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2k+l=4n+3}|F(hkl)|\{\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]-\cos 2\pi(hX-kY)\sin[2\pi lZ+\alpha(hkl)]\}\Big\}$$

$P4mm$ C_{4v}^{1}

No. 99

Origin on $4mm$. | x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,z$; $x,\bar{y},z$; y,x,z; $\bar{y},\bar{x},z$; $\bar{y},x,z$; $y,\bar{x},z$ |

$A=4\cos 2\pi lz.G$; $B=4\sin 2\pi lz.G$, where $G=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy$

$B=0$ if $l=0$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]$$

$P4bm$ C_{4v}^{2}

No. 100

Origin on 4. | x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $\frac{1}{2}+x,\frac{1}{2}-y,z$; $\bar{y},x,z$; $y,\bar{x},z$; $\frac{1}{2}+y,\frac{1}{2}+x,z$; $\frac{1}{2}-y,\frac{1}{2}-x,z$ |

$A=4\cos 2\pi lz.G$; $B=4\sin 2\pi lz.G$, where

$$G=\cos 2\pi\left(hx-\frac{h+k}{4}\right)\cos 2\pi\left(ky+\frac{h+k}{4}\right)+\cos 2\pi\left(kx+\frac{h+k}{4}\right)\cos 2\pi\left(hy+\frac{h+k}{4}\right)$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k=2n$ $A=4\cos 2\pi lz.G'$; $B=4\sin 2\pi lz.G'$, where $G'=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy$

$B=0$ if $l=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$h+k=2n+1$ $A=4\cos 2\pi lz.G''$; $B=4\sin 2\pi lz.G''$, where $G''=-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy$

$A=B=0$ if $h=0$ or $k=0$; $B=0$ if $l=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

$P4_2cm$ C_{4v}^{3}

No. 101

Origin on 4_2. | x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\frac{1}{2}+z$; $x,\bar{y},\frac{1}{2}+z$; y,x,z; $\bar{y},\bar{x},z$; $\bar{y},x,\frac{1}{2}+z$; $y,\bar{x},\frac{1}{2}+z$ |

$A=4\cos 2\pi lz.G$; $B=4\sin 2\pi lz.G$, where

$$G=\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)+\cos 2\pi\left(kx-\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$l=2n$ $A=4\cos 2\pi lz.G'$; $B=4\sin 2\pi lz.G'$, where $G'=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy$

$B=0$ if $l=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$l=2n+1$ $A=4\cos 2\pi lz.G''$; $B=4\sin 2\pi lz.G''$, where $G''=-[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$A=B=0$ if $h=0$ or $k=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

No. 102 $P4_2nm$ C_{4v}^4

Origin on *mm*.

| x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$; y,x,z; $\bar{y},\bar{x},z$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$ |

$A=4\cos 2\pi lz.G$; $B=4\sin 2\pi lz.G$, where

$$G=\cos 2\pi\left(hx-\frac{h+k+l}{4}\right)\cos 2\pi\left(ky+\frac{h+k+l}{4}\right)+\cos 2\pi\left(kx-\frac{h+k+l}{4}\right)\cos 2\pi\left(hy+\frac{h+k+l}{4}\right)$$

$B=0$ if $l=0$ $\quad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$h+k+l=2n$ $\quad A=4\cos 2\pi lz.G'$; $B=4\sin 2\pi lz.G'$, where $G'=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy$

$B=0$ if $l=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$h+k+l=2n+1$ $\quad A=4\cos 2\pi lz.G''$; $B=4\sin 2\pi lz.G''$, where $G''=-[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$A=B=0$ if $h=0$ or $k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

No. 103 $P4cc$ C_{4v}^5

Origin on 4. | x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\frac{1}{2}+z$; $x,\bar{y},\frac{1}{2}+z$; $y,\bar{x},z$; $\bar{y},x,z$; $y,x,\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}+z$ |

$A=4\cos 2\pi lz.G$; $B=4\sin 2\pi lz.G$, where

$$G=\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)+\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)$$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$l=2n$ $\quad A=4\cos 2\pi lz.G'$; $B=4\sin 2\pi lz.G'$, where $G'=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy$

$B=0$ if $l=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$l=2n+1$ $\quad A=4\cos 2\pi lz.G''$; $B=4\sin 2\pi lz.G''$, where $G''=-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy$

$A=B=0$ if $h=0$ or $k=0$ or $h=\pm k$; $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

$P4nc$ C_{4v}^{6} No. 104

Origin on 4.

$|\ x,y,z;\ \bar{x},\bar{y},z;\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{2}+z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{1}{2}+z;\ \bar{y},x,z;\ y,\bar{x},z;\ \tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}+z;\ \tfrac{1}{2}-y,\tfrac{1}{2}-x,\tfrac{1}{2}+z\ |$

$A=4\cos 2\pi lz.G$; $B=4\sin 2\pi lz.G$, where

$$G=\cos 2\pi\left(hx-\frac{h+k+l}{4}\right)\cos 2\pi\left(ky+\frac{h+k+l}{4}\right)+\cos 2\pi\left(kx+\frac{h+k+l}{4}\right)\cos 2\pi\left(hy+\frac{h+k+l}{4}\right)$$

$B=0$ if $l=0$ $\qquad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$h+k+l=2n$ $\quad A=4\cos 2\pi lz.G'$; $B=4\sin 2\pi lz.G'$, where $G'=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy$

$B=0$ if $l=0$ $\qquad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$h+k+l=2n+1$ $\quad A=4\cos 2\pi lz.G''$; $B=4\sin 2\pi lz.G''$, where $G''=-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy$

$A=B=0$ if $h=0$ or $k=0$ or $h=\pm k$ $\qquad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

$P4_2mc$ C_{4v}^{7} No. 105

Origin on 4_2. $\qquad |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z;\ y,x,\tfrac{1}{2}+z;\ \bar{y},\bar{x},\tfrac{1}{2}+z;\ \bar{y},x,\tfrac{1}{2}+z;\ y,\bar{x},\tfrac{1}{2}+z\ |$

$A=4\cos 2\pi lz.G$; $B=4\sin 2\pi lz.G$, where $G=\cos 2\pi hx\cos 2\pi ky+\cos\pi l\cos 2\pi kx\cos 2\pi hy$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$l=2n$ $\quad A=4\cos 2\pi lz.G'$; $B=4\sin 2\pi lz.G'$, where $G'=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy$

$B=0$ if $l=0$ $\qquad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$l=2n+1$ $\quad A=4\cos 2\pi lz.G''$; $B=4\sin 2\pi lz.G''$, where $G''=\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy$

$A=B=0$ if $h=\pm k$ $\qquad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]$$

No. 106

$P4_2bc$ C_{4v}^8

Origin on 4_2.

$|\ x,y,z;\ \bar{x},\bar{y},z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,z;\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,z;\ \bar{y},x,\tfrac{1}{2}+z;\ y,\bar{x},\tfrac{1}{2}+z;\ \tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}+z;\ \tfrac{1}{2}-y,\tfrac{1}{2}-x,\tfrac{1}{2}+z\ |$

$A=4\cos 2\pi lz.G$; $B=4\sin 2\pi lz.G$, where

$$G=\cos 2\pi\left(hx-\frac{h+k}{4}\right)\cos 2\pi\left(ky+\frac{h+k}{4}\right)+\cos\pi l\cos 2\pi\left(kx+\frac{h+k}{4}\right)\cos 2\pi\left(hy+\frac{h+k}{4}\right)$$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$\begin{cases} h+k=2n \\ l=2n \end{cases}$ $A=4\cos 2\pi lz.G'$; $B=4\sin 2\pi lz.G'$, where $G'=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy$

$B=0$ if $l=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$\begin{cases} h+k=2n \\ l=2n+1 \end{cases}$ $A=4\cos 2\pi lz.G''$; $B=4\sin 2\pi lz.G''$, where $G''=\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy$

$A=B=0$ if $h=\pm k$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl)$

$\begin{cases} h+k=2n+1 \\ l=2n \end{cases}$ $A=4\cos 2\pi lz.G'''$; $B=4\sin 2\pi lz.G'''$, where $G'''=-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy$

$A=B=0$ if $h=0$ or $k=0$; $B=0$ if $l=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$\begin{cases} h+k=2n+1 \\ l=2n+1 \end{cases}$ $A=4\cos 2\pi lz.G''''$; $B=4\sin 2\pi lz.G''''$, where $=\pi+\alpha(khl)$

$G''''=-[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$A=B=0$ if $h=0$ or $k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

No. 107

$I4mm$ C_{4v}^9

Origin on $4mm$. $\quad (0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z;\ y,x,z;\ \bar{y},\bar{x},z;\ \bar{y},x,z;\ y,\bar{x},z\ |$

$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi lz.G$; $B=8\cos^2 2\pi\frac{h+k+l}{4}\sin 2\pi lz.G$, where

$G=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy$ $\quad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$h+k+l=2n$ $\quad A=8\cos 2\pi lz.G'$; $B=8\sin 2\pi lz.G'$, where $G'=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy$

$B=0$ if $l=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$h+k+l=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]$$

$I4cm$ C_{4v}^{10}

No. 108

Origin on 4.

$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) +\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}+y,z;\ \frac{1}{2}+x,\frac{1}{2}-y,z;\ \bar{y},x,z;\ y,\bar{x},z;\ \frac{1}{2}+y,\frac{1}{2}+x,z;\ \frac{1}{2}-y,\frac{1}{2}-x,z\ |$

$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi lz.G;\quad B=8\cos^2 2\pi\frac{h+k+l}{4}\sin 2\pi lz.G$, where

$G=\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)+\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$\begin{cases} h+k+l=2n \\ l=2n \end{cases}$ $A=8\cos 2\pi lz.G';\quad B=8\sin 2\pi lz.G'$, where $G'=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy$; $B=0$ if $l=0$; $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$\begin{cases} h+k+l=2n \\ l=2n+1 \end{cases}$ $A=8\cos 2\pi lz.G'';\quad B=8\sin 2\pi lz.G''$, where $G''=-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy$; $A=B=0$ if $h=0$ or $k=0$; $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl)$

$h+k+l=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

$I4_1md$ C_{4v}^{11}

No. 109

Origin on mm.

$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) +\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z;\ y,\frac{1}{2}+x,\frac{1}{4}+z;\ \bar{y},\frac{1}{2}-x,\frac{1}{4}+z;\ \bar{y},\frac{1}{2}+x,\frac{1}{4}+z;\ y,\frac{1}{2}-x,\frac{1}{4}+z\ |$

$A=8\cos^2 2\pi\frac{h+k+l}{4}\left[\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos\pi k\cos 2\pi kx\cos 2\pi hy\cos 2\pi\left(lz+\frac{l}{4}\right)\right]$

$B=8\cos^2 2\pi\frac{h+k+l}{4}\left[\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz+\cos\pi k\cos 2\pi kx\cos 2\pi hy\sin 2\pi\left(lz+\frac{l}{4}\right)\right]\quad =0$ if $l=0$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$\begin{cases} h+k+l=2n \\ 2k+l=4n \end{cases}$ $A=8\cos 2\pi lz.G;\quad B=8\sin 2\pi lz.G$, where $G=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy$; $B=0$ if $l=0$; $\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$\begin{cases} h+k+l=2n \\ 2k+l=4n+1 \end{cases}$ $A=8[\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz-\cos 2\pi kx\cos 2\pi hy\sin 2\pi lz]$; $B=8[\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz+\cos 2\pi kx\cos 2\pi hy\cos 2\pi lz]$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\frac{\pi}{2}+\alpha(khl)$

$\begin{cases} h+k+l=2n & A=8\cos 2\pi lz.G'; \quad B=8\sin 2\pi lz.G', \text{ where } G'=\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy \\ 2k+l=4n+2 & A=B=0 \text{ if } h=\pm k; \quad B=0 \text{ if } l=0 \quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl) \end{cases}$

$\begin{cases} h+k+l=2n & A=8[\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi hy\sin 2\pi lz] \\ 2k+l=4n+3 & B=8[\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz-\cos 2\pi kx\cos 2\pi hy\cos 2\pi lz] \end{cases}$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\frac{3\pi}{2}+\alpha(khl)$

Note. If $h+k+l=2n$, $2k+l=4n+1$, then $-2k-l=4n+3$, etc.

$h+k+l=2n+1 \quad A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]$$

No. 110

$I4_1cd$ C_{4v}^{12}

Origin on 2.

$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})+\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z;\ y,\frac{1}{2}-x,\frac{1}{4}+z;\ \bar{y},\frac{1}{2}+x,\frac{1}{4}+z;\ y,\frac{1}{2}+x,\frac{3}{4}+z;\ \bar{y},\frac{1}{2}-x,\frac{3}{4}+z\ |$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\left\{\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)\cos 2\pi lz+\cos\pi k\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\cos 2\pi\left(lz+\frac{l}{4}\right)\right\}$$

$$B=8\cos^2 2\pi\frac{h+k+l}{4}\left\{\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)\sin 2\pi lz+\cos\pi k\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\sin 2\pi\left(lz+\frac{l}{4}\right)\right\}$$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$\begin{cases} h+k+l=2n & A=8\cos 2\pi lz.G; \quad B=8\sin 2\pi lz.G, \text{ where } G=\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy \\ 2k+l=4n & B=0 \text{ if } l=0 \quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl) \end{cases}$

$\begin{cases} h+k+l=2n & A=-8[\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz+\sin 2\pi kx\sin 2\pi hy\sin 2\pi lz] \\ 2k+l=4n+1 & B=-8[\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz-\sin 2\pi kx\sin 2\pi hy\cos 2\pi lz] \end{cases}\Bigg\}A=B=0 \text{ if } h=0 \text{ or } k=0$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\frac{3\pi}{2}+\alpha(khl)$

$\begin{cases} h+k+l=2n & A=8\cos 2\pi lz.G'; \quad B=8\sin lz.G', \text{ where } G'=\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy \\ 2k+l=4n+2 & A=B=0 \text{ if } h=\pm k; \quad B=0 \text{ if } l=0 \quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl) \end{cases}$

$\begin{cases} h+k+l=2n & A=-8[\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz-\sin 2\pi kx\sin 2\pi hy\sin 2\pi lz] \\ 2k+l=4n+3 & B=-8[\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi hy\cos 2\pi lz] \end{cases}\Bigg\}A=B=0 \text{ if } h=0 \text{ or } k=0$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\frac{\pi}{2}+\alpha(khl)$

$h+k+l=2n+1 \quad A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^{2k+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^{2k+l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

$P\bar{4}2m$ D_{2d}^{1}

No. 111

Origin at $\bar{4}2m$. | x,y,z; $x,\bar{y},\bar{z}$; $\bar{x},y,\bar{z}$; $\bar{x},\bar{y},z$; y,x,z; $y,\bar{x},\bar{z}$; $\bar{y},x,\bar{z}$; $\bar{y},\bar{x},z$ |

$A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$ or $l=0$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$h=k$ $A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$

$B=-8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$

$h=-k$ $A=8\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz$

$B=8\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\{\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)\}$$

$P\bar{4}2c$ D_{2d}^{2}

No. 112

Origin at $\bar{4}$. | x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\frac{1}{2}-z$; $x,\bar{y},\frac{1}{2}-z$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; $y,x,\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}+z$ |

$$A=4\cos 2\pi lz\left[\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)+\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\right]$$

$$B=-4\sin 2\pi lz\left[\sin 2\pi\left(hx+\frac{l}{4}\right)\sin 2\pi\left(ky-\frac{l}{4}\right)+\sin 2\pi\left(kx+\frac{l}{4}\right)\sin 2\pi\left(hy+\frac{l}{4}\right)\right]$$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$l=2n$ $A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$ or $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$l=2n+1$ $A=4\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$

$B=-4\sin 2\pi lz[-\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$A=B=0$ if $h=\pm k$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^{l=2n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]+\sum_0^\infty\sum_0^\infty\sum_0^{l=2n+1}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)]\right\}$$

No. 113 $P\bar{4}2_1m$ D_{2d}^3

Origin at $\bar{4}$. | x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $y,\bar{x},\bar{z}$; $\bar{y},x,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,z$; $\frac{1}{2}-y,\frac{1}{2}-x,z$ |

$$A=4\cos 2\pi lz\left[\cos 2\pi\left(hx+\frac{h+k}{4}\right)\cos 2\pi\left(ky-\frac{h+k}{4}\right)+\cos 2\pi\left(kx+\frac{h+k}{4}\right)\cos 2\pi\left(hy+\frac{h+k}{4}\right)\right]$$

$$B=-4\sin 2\pi lz\left[\sin 2\pi\left(hx+\frac{h+k}{4}\right)\sin 2\pi\left(ky-\frac{h+k}{4}\right)+\sin 2\pi\left(kx+\frac{h+k}{4}\right)\sin 2\pi\left(hy+\frac{h+k}{4}\right)\right]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k=2n$

$A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$ or $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$h+k=2n+1$

$A=4\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$

$B=-4\sin 2\pi lz[-\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]+\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)]\right\}$$

No. 114 $P\bar{4}2_1c$ D_{2d}^4

Origin at $\bar{4}$.

| x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$ |

$$A=4\cos 2\pi lz\left[\cos 2\pi\left(hx+\frac{h+k+l}{4}\right)\cos 2\pi\left(ky-\frac{h+k+l}{4}\right)+\cos 2\pi\left(kx+\frac{h+k+l}{4}\right)\cos 2\pi\left(hy+\frac{h+k+l}{4}\right)\right]$$

$$B=-4\sin 2\pi lz\left[\sin 2\pi\left(hx+\frac{h+k+l}{4}\right)\sin 2\pi\left(ky-\frac{h+k+l}{4}\right)+\sin 2\pi\left(kx+\frac{h+k+l}{4}\right)\sin 2\pi\left(hy+\frac{h+k+l}{4}\right)\right]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k+l=2n$

$A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$ or $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$h+k+l=2n+1$

$A=4\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$

$B=-4\sin 2\pi lz[-\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $l=0$

$A=B=0$ if $h=\pm k$ $\quad\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]+\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)]\right\}$$

$P\bar{4}m2$ D_{2d}^{5}

No. 115

Origin at $\bar{4}m2$. | x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,z$; $x,\bar{y},z$; $y,x,\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$ |

$A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=4\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $l=0$ or $h=\pm k$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]$$

$P\bar{4}c2$ D_{2d}^{6}

No. 116

Origin at $\bar{4}$. | x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\frac{1}{2}+z$; $x,\bar{y},\frac{1}{2}+z$; $y,\bar{x},\bar{z}$; $\bar{y},x,\bar{z}$; $y,x,\frac{1}{2}-z$; $\bar{y},\bar{x},\frac{1}{2}-z$ |

$$A=4\cos 2\pi lz\left[\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)+\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\right]$$

$$B=4\sin 2\pi lz\left[\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)-\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\right]$$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$l=2n$ $\quad A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=4\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $l=0$ or $h=\pm k$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$

$l=2n+1$ $\quad A=4\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=\pm k$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$A=B=0$ if $h=0$ or $k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi-\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

No. 117 $P\bar{4}b2$ D_{2d}^{7}

Origin at $\bar{4}$. | x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $\frac{1}{2}+x,\frac{1}{2}-y,z$; $y,\bar{x},\bar{z}$; $\bar{y},x,\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}-x,\bar{z}$ |

$$A=4\cos 2\pi lz\left[\cos 2\pi\left(hx+\frac{h+k}{4}\right)\cos 2\pi\left(ky-\frac{h+k}{4}\right)+\cos 2\pi\left(kx+\frac{h+k}{4}\right)\cos 2\pi\left(hy+\frac{h+k}{4}\right)\right]$$

$$B=4\sin 2\pi lz\left[\cos 2\pi\left(hx+\frac{h+k}{4}\right)\cos 2\pi\left(ky-\frac{h+k}{4}\right)-\cos 2\pi\left(kx+\frac{h+k}{4}\right)\cos 2\pi\left(hy+\frac{h+k}{4}\right)\right]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k=2n$

$A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=4\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $l=0$ or $h=\pm k$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$$

$h+k=2n+1$

$A=4\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $l=0$

$A=B=0$ if $h=0$ or $k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi-\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

No. 118 $P\bar{4}n2$ D_{2d}^{8}

Origin at $\bar{4}$.

| x,y,z; $\bar{x},\bar{y},z$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$; $\bar{y},x,\bar{z}$; $y,\bar{x},\bar{z}$; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}-z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$ |

$$A=4\cos 2\pi lz\left[\cos 2\pi\left(hx+\frac{h+k+l}{4}\right)\cos 2\pi\left(ky-\frac{h+k+l}{4}\right)+\cos 2\pi\left(kx+\frac{h+k+l}{4}\right)\cos 2\pi\left(hy+\frac{h+k+l}{4}\right)\right]$$

$$B=4\sin 2\pi lz\left[\cos 2\pi\left(hx+\frac{h+k+l}{4}\right)\cos 2\pi\left(ky-\frac{h+k+l}{4}\right)-\cos 2\pi\left(kx+\frac{h+k+l}{4}\right)\cos 2\pi\left(hy+\frac{h+k+l}{4}\right)\right]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k+l=2n$

$A=4\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=4\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $l=0$ or $h=\pm k$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$$

$h+k+l=2n+1$

$A=4\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=\pm k$

$B=-4\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $l=0$

$A=B=0$ if $h=0$ or $k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi-\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

$I\bar{4}m2$ D_{2d}^{9}

No. 119

Origin at $\bar{4}m2$. $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) +$ | $x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z;\ y,x,\bar{z};\ \bar{y},\bar{x},\bar{z};\ \bar{y},x,\bar{z};\ y,\bar{x},\bar{z}$ |

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$$

$$B=8\cos^2 2\pi\frac{h+k+l}{4}\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k+l=2n$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=8\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $l=0$ or $h=\pm k$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$$

$h+k+l=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]$$

$I\bar{4}c2$ D_{2d}^{10}

No. 120

Origin at $\bar{4}$.

$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) +$ | $x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z;\ y,\bar{x},\bar{z};\ \bar{y},x,\bar{z};\ y,x,\frac{1}{2}-z;\ \bar{y},\bar{x},\frac{1}{2}-z$ |

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi lz\left[\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)+\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\right]$$

$$B=8\cos^2 2\pi\frac{h+k+l}{4}\sin 2\pi lz\left[\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)-\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\right]$$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$\begin{cases} h+k+l=2n \\ l=2n \end{cases}$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=8\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $l=0$ or $h=\pm k$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$$

$\begin{cases} h+k+l=2n \\ l=2n+1 \end{cases}$ $\quad \left.\begin{array}{l} A=8\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy] \\ B=-8\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy] \end{array}\right\} A=B=0$ if $h=0$ or $k=0$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi-\alpha(khl)$$

$h+k+l=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^{l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos[2\pi lZ-\alpha(hkl)]-\sum_0^\infty\sum_0^\infty\sum_0^{l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos[2\pi lZ-\alpha(hkl)]\right\}$$

No. 121 $I\bar{4}2m$ D_{2d}^{11}

Origin at $\bar{4}2m$. $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) +\ |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ y,x,z;\ y,\bar{x},\bar{z};\ \bar{y},x,\bar{z};\ \bar{y},\bar{x},z\ |$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$$

$$B=-8\cos^2 2\pi\frac{h+k+l}{4}\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k+l=2n$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$B=-8\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$ or $l=0$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$$

$h+k+l=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\{\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)\}$$

No. 122 $I\bar{4}2d$ D_{2d}^{12}

Origin at $\bar{4}$.

$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) +\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},\frac{1}{2}+y,\frac{1}{4}-z;\ x,\frac{1}{2}-y,\frac{1}{4}-z;\ y,\bar{x},\bar{z};\ \bar{y},x,\bar{z};\ y,\frac{1}{2}+x,\frac{1}{4}+z;\ \bar{y},\frac{1}{2}-x,\frac{1}{4}+z\ |$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\Big\{\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz+$$
$$\cos\pi h\cos\pi\left[(h+k)x+(h-k)y-\frac{l}{2}\right]\cos\pi\left[(h-k)x-(h+k)y+\frac{l}{2}\right]\cos 2\pi\left(lz+\frac{l}{4}\right)\Big\}$$

$$B=-8\cos^2 2\pi\frac{h+k+l}{4}\Big\{\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz-$$
$$\cos\pi h\sin\pi\left[(h+k)x+(h-k)y-\frac{l}{2}\right]\sin\pi\left[(h-k)x-(h+k)y+\frac{l}{2}\right]\sin 2\pi\left(lz+\frac{l}{4}\right)\Big\}$$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$\begin{cases} h+k+l=2n \\ 2h+l=4n \end{cases}$ $\quad A=8\cos 2\pi lz\{\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]+$
$\cos\pi[(h+k)x+(h-k)y]\cos\pi[(h-k)x-(h+k)y]\}$

$B=-8\sin 2\pi lz\{\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]-$
$\sin\pi[(h+k)x+(h-k)y]\sin\pi[(h-k)x-(h+k)y]\}$

$B=0$ if $h=0$ or $k=0$ or $l=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

$\begin{cases} h+k+l=2n \\ 2h+l=4n+1 \end{cases}$ $\quad A=8\{\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz+$
$\sin\pi[(h+k)x+(h-k)y]\sin\pi[(h-k)x-(h+k)y]\sin 2\pi lz\}$

$B=-8\{\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz+$
$\cos\pi[(h+k)x+(h-k)y]\cos\pi[(h-k)x-(h+k)y]\cos 2\pi lz\}$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\frac{3\pi}{2}-\alpha(\bar{h}kl)=\frac{3\pi}{2}-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\frac{\pi}{2}+\alpha(khl)$$

$\begin{cases} h+k+l=2n \\ 2h+l=4n+2 \end{cases}$ $A=8\cos 2\pi lz\{\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]-$
$\cos\pi[(h+k)x+(h-k)y]\cos\pi[(h-k)x-(h+k)y]\}$

$B=-8\sin 2\pi lz\{\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]+$
$\sin\pi[(h+k)x+(h-k)y]\sin\pi[(h-k)x-(h+k)y]\}$

$A=B=0$ if $h=\pm k$; $B=0$ if $l=0$ $\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$\begin{cases} h+k+l=2n \\ 2h+l=4n+3 \end{cases}$ $A=8\{\cos\pi[(h-k)x+(h+k)y]\cos\pi[(h+k)x-(h-k)y]\cos 2\pi lz-$ $=\pi+\alpha(khl)$
$\sin\pi[(h+k)x+(h-k)y]\sin\pi[(h-k)x-(h+k)y]\sin 2\pi lz\}$

$B=-8\{\sin\pi[(h-k)x+(h+k)y]\sin\pi[(h+k)x-(h-k)y]\sin 2\pi lz-$
$\cos\pi[(h+k)x+(h-k)y]\cos\pi[(h-k)x-(h+k)y]\cos 2\pi lz\}$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\frac{\pi}{2}-\alpha(\bar{h}kl)=\frac{\pi}{2}-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\frac{3\pi}{2}+\alpha(khl)$

Note. If $2h+l=4n+1$, $-2h-l=4n+3$, $-2h+l=4n+1$, etc. (since $h+k+l=2n$)

$h+k+l=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+l=4n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]+$$
$$\tfrac{1}{2}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+l=4n+1}|F(hkl)|\{\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]-\cos 2\pi(hX-kY)\sin[2\pi lZ+\alpha(hkl)]\}+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+l=4n+2}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)]+$$
$$\tfrac{1}{2}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+l=4n+3}|F(hkl)|\{\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+\cos 2\pi(hX-kY)\sin[2\pi lZ+\alpha(hkl)]\}\Big\}$$

$P4/mmm$ D_{4h}^1

No. 123

Origin at centre $(4/mmm)$. $\pm\ |\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ y,x,z;\ y,\bar{x},\bar{z};\ \bar{y},x,\bar{z};\ \bar{y},\bar{x},z\ |$

$A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$; $B=0$ $F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ$$

$P4/mcc$ D_{4h}^2

No. 124

Origin at centre $(4/m)$. $\pm\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z;\ \bar{y},x,z;\ y,\bar{x},z;\ y,x,\frac{1}{2}+z;\ \bar{y},\bar{x},\frac{1}{2}+z\ |$

$$A=8\cos 2\pi lz\left[\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)+\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\right];\quad B=0$$

$l=2n$ $A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$ $F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$l=2n+1$ $A=8\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$ $=0$ if $h=0$ or $k=0$ or $h=\pm k$ $=F(khl)$

$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\Big\}$$

No. 125

$P4/nbm$ D_{4h}^3

Origin at 422 (at $\bar{\frac{1}{4}},\bar{\frac{1}{4}},0$ from centre, $2/m$).

$$\left|\begin{array}{llllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & \frac{1}{2}-x,\frac{1}{2}-y,\bar{z}; & \frac{1}{2}-x,\frac{1}{2}+y,z; & \frac{1}{2}+x,\frac{1}{2}-y,z; & \frac{1}{2}+x,\frac{1}{2}+y,\bar{z}; \\ \bar{y},\bar{x},\bar{z}; & \bar{y},x,z; & y,\bar{x},z; & y,x,\bar{z}; & \frac{1}{2}+y,\frac{1}{2}+x,z; & \frac{1}{2}+y,\frac{1}{2}-x,\bar{z}; & \frac{1}{2}-y,\frac{1}{2}+x,\bar{z}; & \frac{1}{2}-y,\frac{1}{2}-x,z \end{array}\right|$$

$$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$$

$$B=-8\sin^2 2\pi\frac{h+k}{4}\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k=2n$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy];\quad B=0$

$$\alpha(hkl)=\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\alpha(khl)=\mathrm{m}\pi$$

$h+k=2n+1$ $\quad A=0;\quad B=-8\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$

$A=B=0$ if $h=0$ or $k=0$ or $l=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)=\mathrm{m}\pi+\frac{\pi}{2}$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi\right\}$$

where m=0 if A or B is positive, m=1 if A or B is negative.

No. 125

$P4/nbm$ D_{4h}^3

Origin at centre ($2/m$) (at $\frac{1}{4},\frac{1}{4},0$ from 422).

$$\pm\ \left|\ x,y,z;\ \bar{x},\tfrac{1}{2}+y,z;\ \tfrac{1}{2}+x,\bar{y},z;\ \tfrac{1}{2}-x,\tfrac{1}{2}-y,z;\ y,x,\bar{z};\ \bar{y},\tfrac{1}{2}+x,\bar{z};\ \tfrac{1}{2}+y,\bar{x},\bar{z};\ \tfrac{1}{2}-y,\tfrac{1}{2}-x,\bar{z}\ \right|$$

$$A=8\cos 2\pi\left(lz+\frac{h+k}{4}\right)\left\{\cos 2\pi\left(hx-\frac{k}{4}\right)\cos 2\pi\left(ky-\frac{h}{4}\right)+\cos 2\pi\left(kx+\frac{h}{4}\right)\cos 2\pi\left(hy+\frac{k}{4}\right)\right\};\quad B=0$$

$\begin{cases}h=2n\\k=2n\end{cases}$ $\quad A=8\cos 2\pi lz\{\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy\}$

$$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$$

$\begin{cases}h=2n\\k=2n+1\end{cases}$ $\quad A=-8\sin 2\pi lz\{\sin 2\pi hx\cos 2\pi ky-\cos 2\pi kx\sin 2\pi hy\};\quad A=B=0$ it $h=0$ or $l=0$

$$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$$

$\begin{cases}h=2n+1\\k=2n\end{cases}$ $\quad A=-8\sin 2\pi lz\{\cos 2\pi hx\sin 2\pi ky-\sin 2\pi kx\cos 2\pi hy\};\quad A=B=0$ if $k=0$ or $l=0$

$$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$$

$\begin{cases}h=2n+1\\k=2n+1\end{cases}$ $\quad A=-8\cos 2\pi lz\{\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy\}$

$$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\right\}$$

$P4/nnc$ D_{4h}^{4} No. 126

Origin at 422 (at $\bar{\tfrac{1}{4}},\bar{\tfrac{1}{4}},\bar{\tfrac{1}{4}}$ from $\bar{1}$).

x,y,z;	$x,\bar{y},\bar{z}$;	$\bar{x},y,\bar{z}$;	$\bar{x},\bar{y},z$;	$\tfrac{1}{2}+x,\tfrac{1}{2}+y,\tfrac{1}{2}-z$;	$\tfrac{1}{2}-x,\tfrac{1}{2}-y,\tfrac{1}{2}-z$;	$\tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{1}{2}+z$;	$\tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{2}+z$
$\bar{y},\bar{x},\bar{z}$;	$\bar{y},x,z$;	$y,\bar{x},z$;	$y,x,\bar{z}$;	$\tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}+z$;	$\tfrac{1}{2}-y,\tfrac{1}{2}-x,\tfrac{1}{2}+z$;	$\tfrac{1}{2}-y,\tfrac{1}{2}+x,\tfrac{1}{2}-z$;	$\tfrac{1}{2}+y,\tfrac{1}{2}-x,\tfrac{1}{2}-z$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$$

$$B=-8\sin^2 2\pi\frac{h+k+l}{4}\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k+l=2n$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$; $\quad B=0$

$$\alpha(hkl)=\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\alpha(khl)=\mathrm{m}\pi$$

$h+k+l=2n+1$ $\quad A=0$; $\quad B=-8\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$

$A=B=0$ if $h=0$ or $k=0$ or $l=0$ or $h=\pm k$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)=\mathrm{m}\pi+\frac{\pi}{2}$$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\mathrm{m}\pi-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos\mathrm{m}\pi\right\}$$

where $\mathrm{m}=0$ if A or B is positive, $\mathrm{m}=1$ if A or B is negative.

$P4/nnc$ D_{4h}^{4} No. 126

Origin at $\bar{1}$ (at $\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$ from 422).

$\pm$ | x,y,z; $\bar{x},\tfrac{1}{2}+y,\tfrac{1}{2}+z$; $\tfrac{1}{2}+x,\bar{y},\tfrac{1}{2}+z$; $\tfrac{1}{2}+x,\tfrac{1}{2}+y,\bar{z}$; $\tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}+z$; $\tfrac{1}{2}-y,x,z$; $y,\tfrac{1}{2}-x,z$; $y,x,\tfrac{1}{2}-z$ |

$$A=8\cos 2\pi\left(lz+\frac{h+k}{4}\right)\left\{\cos\pi l\cos 2\pi\left(hx-\frac{k+l}{4}\right)\cos 2\pi\left(ky-\frac{h+l}{4}\right)+\cos 2\pi\left(kx+\frac{h+l}{4}\right)\cos 2\pi\left(hy+\frac{k+l}{4}\right)\right\};\ B=0$$

$\begin{cases}h+k=2n;\ l=2n\\ k+l=2n\end{cases}$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$ (Note. h, k, l all even)

$\begin{cases}h+k=2n;\ l=2n\\ k+l=2n+1\end{cases}$ $\quad A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$ (Note. h, k odd; l even)

$\begin{cases}h+k=2n+1;\ l=2n\\ k+l=2n\end{cases}$ $\quad A=-8\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky-\sin 2\pi kx\cos 2\pi hy]$; $A=B=0$ if $k=0$ or $l=0$

$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$ (Note. h odd; k, l even, etc.)

$\begin{cases}h+k=2n+1;\ l=2n\\ k+l=2n+1\end{cases}$ $\quad A=-8\sin 2\pi lz[\sin 2\pi hx\cos 2\pi ky-\cos 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $h=0$ or $l=0$

$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$

$\begin{cases}h+k=2n;\ l=2n+1\\ k+l=2n\end{cases}$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$; $A=B=0$ if $h=\pm k$

$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

$\begin{cases} h+k=2n;\ l=2n+1 \\ k+l=2n+1 \end{cases}$ $A=-8\cos 2\pi lz[\sin 2\pi hx \sin 2\pi ky - \sin 2\pi kx \sin 2\pi hy]$

$A=B=0$ if $h=\pm k$ or $h=0$ or $k=0$; $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=2n+1;\ l=2n+1 \\ k+l=2n \end{cases}$ $A=-8\sin 2\pi lz[\cos 2\pi hx \sin 2\pi ky + \sin 2\pi kx \cos 2\pi hy]$ $=-F(khl)$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$

$\begin{cases} h+k=2n+1;\ l=2n+1 \\ k+l=2n+1 \end{cases}$ $A=-8\sin 2\pi lz[\sin 2\pi hx \cos 2\pi ky + \cos 2\pi kx \sin 2\pi hy]$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\Big\}$$

No. 127 $P4/mbm$ D_{4h}^5

Origin at centre $(4/m)$.

$\pm\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,z;\ \bar{y},x,z;\ y,\bar{x},z;\ \tfrac{1}{2}+y,\tfrac{1}{2}+x,z;\ \tfrac{1}{2}-y,\tfrac{1}{2}-x,z\ |$

$$A=8\cos 2\pi lz\left[\cos 2\pi\left(hx-\frac{h+k}{4}\right)\cos 2\pi\left(ky+\frac{h+k}{4}\right)+\cos 2\pi\left(kx+\frac{h+k}{4}\right)\cos 2\pi\left(hy+\frac{h+k}{4}\right)\right];\quad B=0$$

$h+k=2n$ $A=8\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky + \cos 2\pi kx \cos 2\pi hy]$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$h+k=2n+1$ $A=8\cos 2\pi lz[-\sin 2\pi hx \sin 2\pi ky + \sin 2\pi kx \sin 2\pi hy]$; $A=B=0$ if $h=0$ or $k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\Big\}$$

No. 128 $P4/mnc$ D_{4h}^6

Origin at centre $(4/m)$.

$\pm\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{2}+z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{1}{2}+z;\ \bar{y},x,z;\ y,\bar{x},z;\ \tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}+z;\ \tfrac{1}{2}-y,\tfrac{1}{2}-x,\tfrac{1}{2}+z\ |$

$$A=8\cos 2\pi lz\left[\cos 2\pi\left(hx-\frac{h+k+l}{4}\right)\cos 2\pi\left(ky+\frac{h+k+l}{4}\right)+\cos 2\pi\left(kx+\frac{h+k+l}{4}\right)\cos 2\pi\left(hy+\frac{h+k+l}{4}\right)\right]$$
$B=0$

$h+k+l=2n$ $A=8\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky + \cos 2\pi kx \cos 2\pi hy]$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$h+k+l=2n+1$ $A=8\cos 2\pi lz[-\sin 2\pi hx \sin 2\pi ky + \sin 2\pi kx \sin 2\pi hy]$;

$A=B=0$ if $h=0$ or $k=0$ or $h=\pm k$; $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\Big\}$$

$P4/nmm$ D_{4h}^{7} No. 129

Origin at $\bar{4}m2$ (at $\frac{1}{4},\frac{1}{4},0$ from centre, $2/m$).

$$\left|\begin{array}{lllllll} x,y,z; & \bar{x},\bar{y},z; & \bar{x},y,z; & x,\bar{y},z; & \frac{1}{2}+x,\frac{1}{2}+y,\bar{z}; & \frac{1}{2}-x,\frac{1}{2}-y,\bar{z}; & \frac{1}{2}+x,\frac{1}{2}-y,\bar{z}; \\ \bar{y},\bar{x},\bar{z}; & y,x,\bar{z}; & \bar{y},x,\bar{z}; & y,\bar{x},\bar{z}; & \frac{1}{2}+y,\frac{1}{2}+x,z; & \frac{1}{2}-y,\frac{1}{2}-x,z; & \frac{1}{2}-y,\frac{1}{2}+x,z; \end{array}\right. \quad \left.\begin{array}{l} \frac{1}{2}-x,\frac{1}{2}+y,\bar{z}; \\ \frac{1}{2}+y,\frac{1}{2}-x,z \end{array}\right|$$

$$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$$

$$B=8\sin^2 2\pi\frac{h+k}{4}\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k=2n$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$; $\quad B=0$

$$\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\alpha(khl)=\mathrm{m}\pi$$

$h+k=2n+1$ $\quad A=0$; $\quad B=8\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$; $\quad A=B=0$ if $l=0$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)=\mathrm{m}\pi+\frac{\pi}{2}$$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi+\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi\right\}$$

where $m=0$ if A or B is positive, $\mathrm{m}=1$ if A or B is negative.

$P4/nmm$ D_{4h}^{7} No. 129

Origin at centre $(2/m)$ (at $\frac{1}{4},\frac{\bar{1}}{4},0$ from $\bar{4}m2$).

$$\pm\ \left|\ x,y,z;\ \tfrac{1}{2}-x,y,z;\ x,\tfrac{1}{2}-y,z;\ \tfrac{1}{2}-x,\tfrac{1}{2}-y,z;\ y,x,z;\ \tfrac{1}{2}-y,x,z;\ y,\tfrac{1}{2}-x,z;\ \tfrac{1}{2}-y,\tfrac{1}{2}-x,z\ \right|$$

$$A=8\cos 2\pi\left(lz+\frac{h+k}{4}\right)\left\{\cos 2\pi\left(hx-\frac{h}{4}\right)\cos 2\pi\left(ky-\frac{k}{4}\right)+\cos 2\pi\left(kx-\frac{k}{4}\right)\cos 2\pi\left(hy-\frac{h}{4}\right)\right\};\quad B=0$$

$\begin{cases} h=2n \\ k=2n \end{cases}$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$$

$\begin{cases} h=2n \\ k=2n+1 \end{cases}$ $\quad A=-8\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky+\sin 2\pi kx\cos 2\pi hy]$; $\quad A=B=0$ if $l=0$

$$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$$

$\begin{cases} h=2n+1 \\ k=2n \end{cases}$ $\quad A=-8\sin 2\pi lz[\sin 2\pi hx\cos 2\pi ky+\cos 2\pi kx\sin 2\pi hy]$; $\quad A=B=0$ if $l=0$

$$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$$

$\begin{cases} h=2n+1 \\ k=2n+1 \end{cases}$ $\quad A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)-F(hk\bar{l})=F(khl)$$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\right\}$$

Origin at $\bar{4}$ (at $\frac{1}{4},\frac{1}{4}$ 0 from $\bar{1}$).

$$\left|\begin{array}{lllllll} x,y,z; & \bar{x},\bar{y},z; & \bar{x},y,\frac{1}{2}+z; & x,\bar{y},\frac{1}{2}+z; & \frac{1}{2}+x,\frac{1}{2}+y,\bar{z}; & \frac{1}{2}-x,\frac{1}{2}-y,\bar{z}; & \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z; \\ y,\bar{x},\bar{z}; & \bar{y},x,\bar{z}; & y,x,\frac{1}{2}-z; & \bar{y},\bar{x},\frac{1}{2}-z; & \frac{1}{2}-y,\frac{1}{2}+x,z; & \frac{1}{2}+y,\frac{1}{2}-x,z; & \frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z; \end{array}\right.$$

$$\left.\begin{array}{l} \frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z \\ \frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}-z \end{array}\right|$$

$$A=8\cos^2 2\pi\frac{h+k}{4}\cos 2\pi lz\left[\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)+\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\right]$$

$$B=8\sin^2 2\pi\frac{h+k}{4}\sin 2\pi lz\left[\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)-\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\right]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$\begin{cases} h+k=2n \\ l=2n \end{cases}$ $A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$; $B=0$

$\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=-\alpha(khl)=\mathrm{m}\pi$

$\begin{cases} h+k=2n \\ l=2n+1 \end{cases}$ $A=8\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$; $B=0$

$A=B=0$ if $h=0$ or $k=0$ or $h=\pm k$ $\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\pi-\alpha(khl)=\mathrm{m}\pi$

$\begin{cases} h+k=2n+1 \\ l=2n \end{cases}$ $A=0$; $B=8\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$

$A=B=0$ if $l=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)=\mathrm{m}\pi+\frac{\pi}{2}$

$\begin{cases} h+k=2n+1 \\ l=2n+1 \end{cases}$ $A=0$; $B=-8\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$A=B=0$ if $h=0$ or $k=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi-\alpha(khl)=\mathrm{m}\pi+\frac{\pi}{2}$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi\Big\}$$

where m=0 if A or B is positive, m=1 if A or B is negative.

Origin at $\bar{1}$ (at $\frac{1}{4},\frac{\bar{1}}{4},0$ from $\bar{4}$).

$$\pm\left|\begin{array}{lllllll} x,y,z; & \frac{1}{2}-x,\frac{1}{2}-y,z; & \frac{1}{2}-x,y,\frac{1}{2}+z; & x,\frac{1}{2}-y,\frac{1}{2}+z; & y,x,\frac{1}{2}+z; & \frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z; & \frac{1}{2}-y,x,z; \\ y,\frac{1}{2}-x,z & & & & & & \end{array}\right|$$

$$A=8\cos 2\pi\left(lz+\frac{h+k}{4}\right)\left\{\cos 2\pi\left(hx-\frac{h+l}{4}\right)\cos 2\pi\left(ky-\frac{k+l}{4}\right)\cos \pi l+\cos 2\pi\left(kx-\frac{k+l}{4}\right)\cos 2\pi\left(hy-\frac{h+l}{4}\right)\right\}$$

$B=0$

$\begin{cases} h+k=2n; & l=2n \\ k+l=2n \end{cases}$ $A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$F(hkl=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$ (Note. h, k, l all even)

$\begin{cases} h+k=2n; & l=2n \\ k+l=2n+1 \end{cases}$ $A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$ (Note. h, k odd; l even)

$\begin{cases} h+k=2n+1; & l=2n \\ k+l=2n \end{cases}$ $A=-8\sin 2\pi lz[\sin 2\pi hx\cos 2\pi ky+\cos 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$ (Note. h odd; k, l even, etc.)

$\begin{cases} h+k=2n+1; & l=2n \\ k+l=2n+1 \end{cases}$ $A=-8\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky+\sin 2\pi kx\cos 2\pi hy]$; $A=B=0$ if $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$

$\begin{cases} h+k=2n; & l=2n+1 \\ k+l=2n \end{cases}$ $A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$; $A=B=0$ if $h=\pm k$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

$\begin{cases} h+k=2n; & l=2n+1 \\ k+l=2n+1 \end{cases}$ $A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$

$A=B=0$ if $h=0$ or $k=0$ or $h=\pm k$; $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

$\begin{cases} h+k=2n+1; & l=2n+1 \\ k+l=2n \end{cases}$ $A=-8\sin 2\pi lz[\sin 2\pi hx\cos 2\pi ky-\cos 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $h=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$

$\begin{cases} h+k=2n+1; & l=2n+1 \\ k+l=2n+1 \end{cases}$ $A=-8\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky-\sin 2\pi kx\cos 2\pi hy]$; $A=B=0$ if $k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\Big\}$$

$P4_2/mmc$ D_{4h}^9

No. 131

Origin at centre (mmm) on 4_2.

$\pm$ | x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\bar{z}$; $x,\bar{y},\bar{z}$; $y,x,\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}+z$; $\bar{y},x,\frac{1}{2}-z$; $y,\bar{x},\frac{1}{2}-z$ |

$A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos \pi l\cos 2\pi kx\cos 2\pi hy]$; $B=0$

$l=2n$ $A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$l=2n+1$ $A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$; $A=B=0$ if $h=\pm k$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ$$

No. 132 $P4_2/mcm$ D_{4h}^{10}

Origin at centre (mmm) on 4_2.

$\pm$ | x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\frac{1}{2}+z$; $x,\bar{y},\frac{1}{2}+z$; y,x,z; $\bar{y},\bar{x},z$; $\bar{y},x,\frac{1}{2}+z$; $y,\bar{x},\frac{1}{2}+z$ |

$$A=8\cos 2\pi lz\left\{\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)+\cos 2\pi\left(kx-\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\right\};\quad B=0$$

$l=2n$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$l=2n+1$ $\quad A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$; $\quad A=B=0$ if $h=0$ or $k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^{l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^{l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\right\}$$

No. 133 $P4_2/nbc$ D_{4h}^{11}

Origin at $\bar{4}$ (at $\bar{\frac{1}{4}},\frac{1}{4},\frac{1}{4}$ from $\bar{1}$).

x,y,z; $\bar{x},\bar{y},z$; $\bar{x},y,\frac{1}{2}-z$; $x,\bar{y},\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z$; $\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $\frac{1}{2}+x,\frac{1}{2}-y,z$;
$y,\bar{x},\bar{z}$; $\bar{y},x,\bar{z}$; $y,x,\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}+y,\frac{1}{2}+x,\bar{z}$; $\frac{1}{2}-y,\frac{1}{2}-x,\bar{z}$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi lz\left\{\cos 2\pi\left(hx-\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)+\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\right\}$$

$$B=-8\sin^2 2\pi\frac{h+k+l}{4}\sin 2\pi lz\left\{\sin 2\pi\left(hx-\frac{l}{4}\right)\sin 2\pi\left(ky+\frac{l}{4}\right)+\sin 2\pi\left(kx+\frac{l}{4}\right)\sin 2\pi\left(hy+\frac{l}{4}\right)\right\}$$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$\begin{cases} h+k+l=2n \\ l=2n \end{cases}$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$; $\quad B=0$

$\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\alpha(khl)=m\pi$

$\begin{cases} h+k+l=2n \\ l=2n+1 \end{cases}$ $\quad A=8\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$; $\quad B=0$

$A=B=0$ if $h=0$ or $k=0$ $\quad \alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\pi+\alpha(khl)=m\pi$

$\begin{cases} h+k+l=2n+1 \\ l=2n \end{cases}$ $\quad A=0$; $\quad B=-8\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$A=B=0$ if $h=0$ or $k=0$ or $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)=m\pi+\frac{\pi}{2}$

$\begin{cases} h+k+l=2n+1 \\ l=2n+1 \end{cases}$ $\quad A=0$; $\quad B=8\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$

$A=B=0$ if $h=\pm k$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl)=m\pi+\frac{\pi}{2}$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n,\ l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos m\pi-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n,\ l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos m\pi-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1,\ l=2n}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos m\pi+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1,\ l=2n+1}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\cos m\pi\Big\}$$

where m=0 if A or B is positive, m=1 if A or B is negative.

$P4_2/nbc$
D_{4h}^{11}

No. 133

Origin at $\bar{1}$ (at $\frac{1}{4},\bar{\frac{1}{4}},\frac{1}{4}$ from $\bar{4}$).

$\pm\ |\ x,y,z;\ \bar{x},\frac{1}{2}+y,z;\ \frac{1}{2}+x,\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}-y,z;\ \frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z;\ \frac{1}{2}-y,x,\frac{1}{2}+z;\ y,\frac{1}{2}-x,\frac{1}{2}+z;\ \bar{y},\bar{x},\frac{1}{2}+z\ |$

$$A=8\cos 2\pi\left(lz+\frac{h+k}{4}\right)\left\{\cos 2\pi\left(hx-\frac{k}{4}\right)\cos 2\pi\left(ky-\frac{h}{4}\right)+\cos\pi l\cos 2\pi\left(hy+\frac{k}{4}\right)\cos 2\pi\left(kx+\frac{h}{4}\right)\right\};\quad B=0$$

$\begin{cases}h=2n; & l=2n\\ k=2n\end{cases}$ $A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$\begin{cases}h=2n; & l=2n\\ k=2n+1\end{cases}$ $A=-8\sin 2\pi lz[\sin 2\pi hx\cos 2\pi ky-\cos 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $h=0$ or $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$

$\begin{cases}h=2n+1; & l=2n\\ k=2n\end{cases}$ $A=-8\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky-\sin 2\pi kx\cos 2\pi hy]$; $A=B=0$ if $k=0$ or $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$

$\begin{cases}h=2n+1; & l=2n\\ k=2n+1\end{cases}$ $A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$\begin{cases}h=2n; & l=2n+1\\ k=2n\end{cases}$ $A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$; $A=B=0$ if $h=\pm k$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

$\begin{cases}h=2n; & l=2n+1\\ k=2n+1\end{cases}$ $A=-8\sin 2\pi lz[\sin 2\pi hx\cos 2\pi ky+\cos 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $h=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$

$\begin{cases}h=2n+1; & l=2n+1\\ k=2n\end{cases}$ $A=-8\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky+\sin 2\pi kx\cos 2\pi hy]$; $A=B=0$ if $k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$

$\begin{cases}h=2n+1; & l=2n+1\\ k=2n+1\end{cases}$ $A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $h=\pm k$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\ k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\ k=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\ k=2n}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\ k=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\Big\}$$

No. 134 $P4_2/nnm$ D_{4h}^{12}

Origin at $\bar{4}2m$ (at $\bar{\frac{1}{4}},\frac{1}{4},\bar{\frac{1}{4}}$ from centre, $2/m$).

$$\left|\begin{array}{l} x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ \tfrac{1}{2}-x,\tfrac{1}{2}-y,\tfrac{1}{2}-z;\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{2}+z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{1}{2}+z;\ \tfrac{1}{2}+x,\tfrac{1}{2}+y,\tfrac{1}{2}-z; \\ y,x,z;\ y,\bar{x},\bar{z};\ \bar{y},x,\bar{z};\ \bar{y},\bar{x},z;\ \tfrac{1}{2}-y,\tfrac{1}{2}-x,\tfrac{1}{2}-z;\ \tfrac{1}{2}-y,\tfrac{1}{2}+x,\tfrac{1}{2}+z;\ \tfrac{1}{2}+y,\tfrac{1}{2}-x,\tfrac{1}{2}+z;\ \tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}-z \end{array}\right|$$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$$

$$B=-8\sin^2 2\pi\frac{h+k+l}{4}\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k+l=2n$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy];\quad B=0$

$$\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\alpha(khl)=\mathrm{m}\pi$$

$h+k+l=2n+1$ $\quad A=0;\quad B=-8\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$A=B=0$ if $h=0$ or $k=0$ or $l=0$ or $h=\pm k$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)=\mathrm{m}\pi+\frac{\pi}{2}$$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi\right\}$$

where $\mathrm{m}=0$ if A or B is positive, $\mathrm{m}=1$ if A or B is negative.

No. 134 $P4_2/nnm$ D_{4h}^{12}

Origin at centre $(2/m)$ (at $\frac{1}{4},\bar{\frac{1}{4}},\frac{1}{4}$ from $\bar{4}2m$).

$$\pm\ \left|\ x,y,z;\ \bar{x},\tfrac{1}{2}+y,\tfrac{1}{2}+z;\ \tfrac{1}{2}+x,\bar{y},\tfrac{1}{2}+z;\ \tfrac{1}{2}-x,\tfrac{1}{2}-y,z;\ \tfrac{1}{2}+y,\tfrac{1}{2}+x,z;\ \tfrac{1}{2}-y,x,\tfrac{1}{2}+z;\ y,\tfrac{1}{2}-x,\tfrac{1}{2}+z;\ \bar{y},\bar{x},z\ \right|$$

$$A=8\cos 2\pi\left(lz+\frac{h+k}{4}\right)\left\{\cos 2\pi\left(hx-\frac{k+l}{4}\right)\cos 2\pi\left(ky-\frac{h-l}{4}\right)+\cos 2\pi\left(kx+\frac{h-l}{4}\right)\cos 2\pi\left(hy+\frac{k+l}{4}\right)\right\};\quad B=0$$

$\begin{cases} h+k=2n \\ k+l=2n \end{cases}$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$ $\quad$ (Note. $(h+k)-(k+l)=h-l=2n$)

$\begin{cases} h+k=2n \\ k+l=2n+1 \end{cases}$ $\quad A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy];\quad A=B=0$ if $h=0$ or $k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$\begin{cases} h+k=2n+1 \\ k+l=2n \end{cases}$ $\quad A=-8\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky-\sin 2\pi kx\cos 2\pi hy];\quad A=B=0$ if $k=0$ or $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$

$\begin{cases} h+k=2n+1 \\ k+l=2n+1 \end{cases}$ $\quad A=-8\sin 2\pi lz[\sin 2\pi hx\cos 2\pi ky-\cos 2\pi kx\sin 2\pi hy];\quad A=B=0$ if $h=0$ or $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\right\}$$

$P4_2/mbc$ D_{4h}^{13}

No. 135

Origin at centre $(2/m)$ on 4_2.

$\pm\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,z;\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,z;\ \bar{y},x,\tfrac{1}{2}+z;\ y,\bar{x},\tfrac{1}{2}+z;\ \tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}+z;\ \tfrac{1}{2}-y,\tfrac{1}{2}-x,\tfrac{1}{2}+z\ |$

$$A=8\cos 2\pi lz\left[\cos 2\pi\left(hx+\frac{h+k}{4}\right)\cos 2\pi\left(ky-\frac{h+k}{4}\right)+\cos \pi l\cos 2\pi\left(kx+\frac{h+k}{4}\right)\cos 2\pi\left(hy+\frac{h+k}{4}\right)\right]$$

$B=0$

$\begin{cases} h+k=2n \\ l=2n \end{cases}$ $A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$\begin{cases} h+k=2n \\ l=2n+1 \end{cases}$ $A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$; $A=B=0$ if $h=\pm k$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

$\begin{cases} h+k=2n+1 \\ l=2n \end{cases}$ $A=8\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $h=0$ or $k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

$\begin{cases} h+k=2n+1 \\ l=2n+1 \end{cases}$ $A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $h=0$ or $k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\right\}$$

$P4_2/mnm$ D_{4h}^{14}

No. 136

Origin at centre (mmm).

$\pm\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{2}+z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{1}{2}+z;\ y,x,z;\ \bar{y},\bar{x},z;\ \tfrac{1}{2}-y,\tfrac{1}{2}+x,\tfrac{1}{2}+z;\ \tfrac{1}{2}+y,\tfrac{1}{2}-x,\tfrac{1}{2}+z\ |$

$$A=8\cos 2\pi lz\left[\cos 2\pi\left(hx-\frac{h+k+l}{4}\right)\cos 2\pi\left(ky+\frac{h+k+l}{4}\right)+\cos 2\pi\left(kx-\frac{h+k+l}{4}\right)\cos 2\pi\left(hy+\frac{h+k+l}{4}\right)\right]$$

$B=0$

$h+k+l=2n$ $A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$h+k+l=2n+1$ $A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $h=0$ or $k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\right\}$$

No. 137 $P4_2/nmc$ D_{4h}^{15}

Origin at $\bar{4}m2$ (at $\frac{\bar{1}}{4},\frac{1}{4},\frac{\bar{1}}{4}$ from $\bar{1}$).

x,y,z;	$\bar{x},\bar{y},z$;	$\bar{x},y,z$;	$x,\bar{y},z$;	$\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z$;	$\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z$;	$\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$;	$\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z$;
$y,x,\bar{z}$;	$\bar{y},\bar{x},\bar{z}$;	$\bar{y},x,\bar{z}$;	$y,\bar{x},\bar{z}$;	$\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$;	$\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$;	$\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$;	$\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$$

$$B=8\sin^2 2\pi\frac{h+k+l}{4}\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$h+k+l=2n$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$; $\quad B=0$

$$\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=-\alpha(khl)=\mathrm{m}\pi$$

$h+k+l=2n+1$ $\quad A=0$; $\quad B=8\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$

$A=B=0$ if $h=\pm k$ or $l=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)=\mathrm{m}\pi+\frac{\pi}{2}$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi+\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi\right\}$$

where m=0 if A or B is positive, m=1 if A or B is negative.

No. 137 $P4_2/nmc$ D_{4h}^{15}

Origin at $\bar{1}$ (at $\frac{1}{4},\frac{\bar{1}}{4},\frac{1}{4}$ from $\bar{4}m2$).

$\pm$ | x,y,z; $\frac{1}{2}-x,\frac{1}{2}-y,z$; $\frac{1}{2}-x,y,z$; $x,\frac{1}{2}-y,z$; $y,x,\frac{1}{2}+z$; $\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z$; $\frac{1}{2}-y,x,\frac{1}{2}+z$; $y,\frac{1}{2}-x,\frac{1}{2}+z$ |

$$A=8\cos 2\pi\left(lz+\frac{h+k}{4}\right)\left[\cos 2\pi\left(hx-\frac{h}{4}\right)\cos 2\pi\left(ky-\frac{k}{4}\right)+\cos \pi l\cos 2\pi\left(kx-\frac{k}{4}\right)\cos 2\pi\left(hy-\frac{h}{4}\right)\right];\quad B=0$$

$\begin{cases}h=2n; & l=2n\\ k=2n\end{cases}$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$$

$\begin{cases}h=2n; & l=2n\\ k=2n+1\end{cases}$ $\quad A=-8\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky+\sin 2\pi kx\cos 2\pi hy]$; $\quad A=B=0$ if $l=0$

$$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$$

$\begin{cases}h=2n+1; & l=2n\\ k=2n\end{cases}$ $\quad A=-8\sin 2\pi lz[\sin 2\pi hx\cos 2\pi ky+\cos 2\pi kx\sin 2\pi hy]$; $\quad A=B=0$ if $l=0$

$$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$$

$\begin{cases}h=2n+1; & l=2n\\ k=2n+1\end{cases}$ $\quad A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$

$$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$$

$\begin{cases}h=2n; & l=2n+1\\ k=2n\end{cases}$ $\quad A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$; $\quad A=B=0$ if $h=\pm k$

$$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$$

$\begin{cases}h=2n; & l=2n+1\\ k=2n+1\end{cases}$ $\quad A=-8\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky-\sin 2\pi kx\cos 2\pi hy]$

$$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$$

$\begin{cases} h = 2n+1; \quad l = 2n+1 \\ k = 2n \end{cases}$ $A = -8 \sin 2\pi lz[\sin 2\pi hx \cos 2\pi ky - \cos 2\pi kx \sin 2\pi hy]$

$F(hkl) = F(\bar{h}\bar{k}\bar{l}) = -F(\bar{h}kl) = F(h\bar{k}l) = -F(hk\bar{l}) = -F(khl)$

$\begin{cases} h = 2n+1; \quad l = 2n+1 \\ k = 2n+1 \end{cases}$ $A = -8 \cos 2\pi lz[\sin 2\pi hx \sin 2\pi ky - \sin 2\pi kx \sin 2\pi hy]$; $A = B = 0$ if $h = \pm k$

$F(hkl) = F(\bar{h}\bar{k}\bar{l}) = -F(\bar{h}kl) = -F(h\bar{k}l) = F(hk\bar{l}) = -F(khl)$

$$\rho(XYZ) = \frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n} F(hkl) \cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ - \sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n+1} F(hkl) \cos 2\pi hX \sin 2\pi kY \sin 2\pi lZ -$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n} F(hkl) \sin 2\pi hX \cos 2\pi kY \sin 2\pi lZ - \sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n+1} F(hkl) \sin 2\pi hX \sin 2\pi kY \cos 2\pi lZ\Big\}$$

$P4_2/ncm$ D_{4h}^{16}

No. 138

Origin at $\bar{4}$ (at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from centre, $2/m$).

x,y,z;	$\bar{x},\bar{y},z$;	$\bar{x},y,\frac{1}{2}+z$;	$x,\bar{y},\frac{1}{2}+z$;	$\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$;	$\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$;	$\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z$;	$\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z$;
$\bar{y},x,\bar{z}$;	$y,\bar{x},\bar{z}$;	$y,x,\frac{1}{2}-z$;	$\bar{y},\bar{x},\frac{1}{2}-z$;	$\frac{1}{2}+y,\frac{1}{2}+x,z$;	$\frac{1}{2}-y,\frac{1}{2}-x,z$;	$\frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}+z$;	$\frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}+z$

$$A = 8 \cos^2 2\pi\frac{h+k+l}{4} \cos 2\pi lz\left[\cos 2\pi\left(hx-\frac{l}{4}\right) \cos 2\pi\left(ky+\frac{l}{4}\right) + \cos 2\pi\left(kx+\frac{l}{4}\right) \cos 2\pi\left(hy+\frac{l}{4}\right)\right]$$

$$B = 8 \sin^2 2\pi\frac{h+k+l}{4} \sin 2\pi lz\left[\cos 2\pi\left(hx-\frac{l}{4}\right) \cos 2\pi\left(ky+\frac{l}{4}\right) - \cos 2\pi\left(kx+\frac{l}{4}\right) \cos 2\pi\left(hy+\frac{l}{4}\right)\right]$$

$|F(hkl)| = |F(\bar{h}\bar{k}\bar{l})| = |F(\bar{h}kl)| = |F(h\bar{k}l)| = |F(hk\bar{l})| = |F(khl)|$

$\begin{cases} h+k+l = 2n \\ l = 2n \end{cases}$ $A = 8 \cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky + \cos 2\pi kx \cos 2\pi hy]$; $B = 0$

$\alpha(hkl) = \alpha(\bar{h}\bar{k}\bar{l}) = \alpha(\bar{h}kl) = \alpha(h\bar{k}l) = \alpha(hk\bar{l}) = -\alpha(khl) = \mathrm{m}\pi$

$\begin{cases} h+k+l = 2n \\ l = 2n+1 \end{cases}$ $A = 8 \cos 2\pi lz[-\sin 2\pi hx \sin 2\pi ky + \sin 2\pi kx \sin 2\pi hy]$; $B = 0$

$A = B = 0$ if $h = 0$ or $k = 0$ $\quad \alpha(hkl) = \alpha(\bar{h}\bar{k}\bar{l}) = -\alpha(\bar{h}kl) = -\alpha(h\bar{k}l) = \alpha(hk\bar{l}) = \pi - \alpha(khl) = \mathrm{m}\pi$

$\begin{cases} h+k+l = 2n+1 \\ l = 2n \end{cases}$ $A = 0$; $B = 8 \sin 2\pi lz[\cos 2\pi hx \cos 2\pi ky - \cos 2\pi kx \cos 2\pi hy]$

$A = B = 0$ if $l = 0$ $\quad \alpha(hkl) = -\alpha(\bar{h}\bar{k}\bar{l}) = \alpha(\bar{h}kl) = \alpha(h\bar{k}l) = -\alpha(hk\bar{l}) = -\alpha(khl) = \mathrm{m}\pi + \frac{\pi}{2}$

$\begin{cases} h+k+l = 2n+1 \\ l = 2n+1 \end{cases}$ $A = 0$; $B = -8 \sin 2\pi lz[\sin 2\pi hx \sin 2\pi ky + \sin 2\pi kx \sin 2\pi hy]$

$A = B = 0$ if $h = 0$ or $k = 0$ $\quad \alpha(hkl) = -\alpha(\bar{h}\bar{k}\bar{l}) = -\alpha(\bar{h}kl) = -\alpha(h\bar{k}l) = -\alpha(hk\bar{l}) = \pi - \alpha(khl) = \mathrm{m}\pi + \frac{\pi}{2}$

$$\rho(XYZ) = \frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n,\,l=2n} |F(hkl)| \cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ \cos \mathrm{m}\pi -$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n,\,l=2n+1} |F(hkl)| \sin 2\pi hX \sin 2\pi kY \cos 2\pi lZ \cos \mathrm{m}\pi +$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1,\,l=2n} |F(hkl)| \cos 2\pi hX \cos 2\pi kY \sin 2\pi lZ \cos \mathrm{m}\pi -$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1,\,l=2n+1} |F(hkl)| \sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ \cos \mathrm{m}\pi\Big\}$$

where $\mathrm{m} = 0$ if A or B is positive, $\mathrm{m} = 1$ if A or B is negative.

No. 138 $P4_2/ncm$ D_{4h}^{16}

Origin at centre $(2/m)$ (at $\frac{1}{4},\bar{\frac{1}{4}},\frac{1}{4}$ from $\bar{4}$).

$\pm\ |\ x,y,z;\ \frac{1}{2}+x,\frac{1}{2}+y,\bar{z};\ \frac{1}{2}-x,y,\frac{1}{2}+z;\ \bar{x},\frac{1}{2}+y,\frac{1}{2}-z;\ y,x,z;\ \frac{1}{2}+y,\frac{1}{2}+x,\bar{z};\ \frac{1}{2}-y,x,\frac{1}{2}+z;\ \bar{y},\frac{1}{2}+x,\frac{1}{2}-z\ |$

$$A=8\cos 2\pi\left(lz+\frac{h+k}{4}\right)\left\{\cos 2\pi\left(hx-\frac{h-l}{4}\right)\cos 2\pi\left(ky-\frac{k+l}{4}\right)+\cos 2\pi\left(kx-\frac{k+l}{4}\right)\cos 2\pi\left(hy-\frac{h-l}{4}\right)\right\}$$

$B=0$

$\begin{cases} h+k=2n \\ k+l=2n \end{cases}$ $A=8\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$\begin{cases} h+k=2n \\ k+l=2n+1 \end{cases}$ $A=-8\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $h=0$ or $k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$\begin{cases} h+k=2n+1 \\ k+l=2n \end{cases}$ $A=-8\sin 2\pi lz[\sin 2\pi hx\cos 2\pi ky+\cos 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $h=0$ or $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$

$\begin{cases} h+k=2n+1 \\ k+l=2n+1 \end{cases}$ $A=-8\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky+\sin 2\pi kx\cos 2\pi hy]$; $A=B=0$ if $k=0$ or $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ k+l=2n}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ k+l=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\right\}$$

No. 139 $I4/mmm$ D_{4h}^{17}

Origin at centre $(4/mmm)$.

$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})\ \pm\ |\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\bar{z};\ x,\bar{y},\bar{z};\ y,x,z;\ \bar{y},\bar{x},z;\ \bar{y},x,\bar{z};\ y,\bar{x},\bar{z}\ |$

$$A=16\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$$

$B=0$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$h+k+l=2n$ $A=16\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$h+k+l=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ$$

$I4/mcm$ D_{4h}^{18}

No. 140

Origin at centre $(4/m)$.

$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm \left|\ x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\frac{1}{2}+z;\ x,\bar{y},\frac{1}{2}+z;\ \bar{y},x,z;\ y,\bar{x},z;\ y,x,\frac{1}{2}+z;\ \bar{y},\bar{x},\frac{1}{2}+z\ \right|$

$$A=16\cos^2 2\pi\frac{h+k+l}{4}\cos 2\pi lz\left[\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)+\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\right];\quad B=0$$

$\begin{cases} h+k+l=2n \\ l=2n \end{cases}$ $A=16\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$\begin{cases} h+k+l=2n \\ l=2n+1 \end{cases}$ $A=16\cos 2\pi lz[-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $h=0$ or $k=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

$h+k+l=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\right\}$$

$I4_1/amd$ D_{4h}^{19}

No. 141

Origin at $\bar{4}m2$ (at $0,\frac{1}{4},\frac{\bar{1}}{8}$ from centre, $2/m$).

$$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) + \left|\begin{array}{l} x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z;\ x,\frac{1}{2}+y,\frac{1}{4}-z;\ \bar{x},\frac{1}{2}-y,\frac{1}{4}-z;\ \bar{x},\frac{1}{2}+y,\frac{1}{4}-z;\ x,\frac{1}{2}-y,\frac{1}{4}-z; \\ y,x,\bar{z};\ \bar{y},\bar{x},\bar{z};\ \bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ y,\frac{1}{2}+x,\frac{1}{4}+z;\ \bar{y},\frac{1}{2}-x,\frac{1}{4}+z;\ \bar{y},\frac{1}{2}+x,\frac{1}{4}+z;\ y,\frac{1}{2}-x,\frac{1}{4}+z \end{array}\right|$$

$A=G\cos 2\pi\frac{2h+l}{8}$; $B=-G\sin 2\pi\frac{2h+l}{8}$, where

$$G=16\cos^2 2\pi\frac{h+k+l}{4}\left[\cos 2\pi hx\cos 2\pi ky\cos 2\pi\left(lz+\frac{2h+l}{8}\right)+\cos 2\pi kx\cos 2\pi hy\cos 2\pi\left(lz-\frac{2h+l}{8}\right)\right]$$

$\alpha(hkl)=-\alpha(khl)$ $|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$\begin{cases} h+k+l=2n \\ 2h+l=4n \end{cases}$ $A=16\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$; $B=0$

$\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\mathrm{m}\pi$

$\begin{cases} h+k+l=2n \\ 2h+l=4n+1 \end{cases}$ $A=-B=8[\cos 2\pi lz(\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy)-$
$\sin 2\pi lz(\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy)]$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi-\frac{\pi}{4}$

$\begin{cases} h+k+l=2n \\ 2h+l=4n+2 \end{cases}$ $A=0$; $B=16\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $l=0$ or $h=\pm k$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{2}$

$\begin{cases} h+k+l=2n \\ 2h+l=4n+3 \end{cases}$ $A=B=8[\cos 2\pi lz(\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy)+$
$\sin 2\pi lz(\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy)]$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{4}$

$h+k+l=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+l=4n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos m\pi+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+l=4n+1}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi(lZ+\tfrac{1}{8})\cos m\pi+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+l=4n+2}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\cos m\pi+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+l=4n+3}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi(lZ-\tfrac{1}{8})\cos m\pi\Big\}$$

where m=0 or 1 according as A (or if $A=0$, then B) is positive or negative.

$I4_1/amd$ D_{4h}^{19}

No. 141

Origin at centre $(2/m)$ (at $0,\bar{\tfrac{1}{4}},\tfrac{1}{8}$ from $\bar{4}m2$).

$$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})\pm\left|\begin{matrix} x,y,z; & \bar{x},y,z; & x,\tfrac{1}{2}-y,z; & \bar{x},\tfrac{1}{2}-y,z; & \tfrac{1}{4}+y,\tfrac{1}{4}+x,\tfrac{3}{4}+z; \\ \tfrac{1}{4}+y,\tfrac{1}{4}-x,\tfrac{3}{4}+z; & \tfrac{3}{4}-y,\tfrac{1}{4}+x,\tfrac{3}{4}+z; & \tfrac{3}{4}-y,\tfrac{1}{4}-x,\tfrac{3}{4}+z \end{matrix}\right|$$

$$A=16\cos 2\pi\frac{h+k+l}{4}\Big\{\cos 2\pi\frac{h+k+l}{4}\cos 2\pi hx\cos 2\pi\Big(ky+\frac{k}{4}\Big)\cos 2\pi\Big(lz-\frac{k}{4}\Big)+$$
$$\cos\pi k\cos 2\pi kx\cos 2\pi\Big(hy+\frac{h}{4}\Big)\cos 2\pi\Big(lz+\frac{h}{4}\Big)\Big\}$$

$B=0$

$h+k+l=4n$; $h=2n$; $k=2n$	$A=16\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$
$h+k+l=4n$; $h=2n$; $k=2n+1$	$A=-16[\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz+\cos 2\pi kx\cos 2\pi hy\cos 2\pi lz]$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$
$h+k+l=4n$; $h=2n+1$; $k=2n$	$A=16[\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\sin 2\pi hy\sin 2\pi lz]$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$
$h+k+l=4n$; $h=2n+1$; $k=2n+1$	$A=-16\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky+\cos 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $l=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$
$h+k+l=4n+2$; $h=2n$; $k=2n$	$A=16\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$; $A=B=0$ if $h=\pm k$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$
$h+k+l=4n+2$; $h=2n$; $k=2n+1$	$A=-16[\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz-\cos 2\pi kx\cos 2\pi hy\cos 2\pi lz]$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$
$h+k+l=4n+2$; $h=2n+1$; $k=2n$	$A=16[\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz-\cos 2\pi kx\sin 2\pi hy\sin 2\pi lz]$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$
$h+k+l=4n+2$; $h=2n+1$; $k=2n+1$	$A=-16\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky-\cos 2\pi kx\sin 2\pi hy]$; $A=B=0$ if $l=0$	$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$
$h+k+l=2n+1$	$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{k=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\Big\}$$

$I4_1/acd$ D_{4h}^{20}

No. 142

Origin at $\bar{4}$ (at $0,\frac{1}{4},\frac{\bar{1}}{8}$ from $\bar{1}$).

$$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) + \left|\begin{array}{l} x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,\tfrac{1}{2}+z;\ x,\bar{y},\tfrac{1}{2}+z;\ x,\tfrac{1}{2}+y,\tfrac{1}{4}-z;\ \bar{x},\tfrac{1}{2}-y,\tfrac{1}{4}-z;\ x,\tfrac{1}{2}-y,\tfrac{3}{4}-z;\ \bar{x},\tfrac{1}{2}+y,\tfrac{3}{4}-z; \\ \bar{y},x,\bar{z};\ y,\bar{x},\bar{z};\ y,x,\tfrac{1}{2}-z;\ \bar{y},\bar{x},\tfrac{1}{2}-z;\ \bar{y},\tfrac{1}{2}+x,\tfrac{1}{4}+z;\ y,\tfrac{1}{2}-x,\tfrac{1}{4}+z;\ y,\tfrac{1}{2}+x,\tfrac{3}{4}+z;\ \bar{y},\tfrac{1}{2}-x,\tfrac{3}{4}+z \end{array}\right|$$

$A=G\cos 2\pi\frac{2h+l}{8}$; $B=-G\sin 2\pi\frac{2h+l}{8}$, where

$$G=16\cos^2 2\pi\frac{h+k+l}{4}\left[\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{l}{4}\right)\cos 2\pi\left(lz+\frac{2h+l}{8}\right)+\right.$$
$$\left.\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{2h+l}{8}\right]\right)$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$\begin{cases} h+k+l=2n \\ 2h+l=4n \end{cases}$ $A=16\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$; $B=0$

$\alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=-\alpha(khl)=\mathrm{m}\pi$

$\begin{cases} h+k+l=2n \\ 2h+l=4n+1 \end{cases}$ $A=-B=8[\cos 2\pi lz(-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy)+$
$\sin 2\pi lz(\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy)]$

$A=B=0$ if $h=0$ or $k=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi-\alpha(khl)$
$=\mathrm{m}\pi-\frac{\pi}{4}$

$\begin{cases} h+k+l=2n \\ 2h+l=4n+2 \end{cases}$ $A=0$; $B=16\sin 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $=0$ if $l=0$ or $h=\pm k$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)=\mathrm{m}\pi-\frac{\pi}{2}$

$\begin{cases} h+k+l=2n \\ 2h+l=4n+3 \end{cases}$ $A=B=8[\cos 2\pi lz(-\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy)-$
$\sin 2\pi lz(\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy)]$

$A=B=0$ if $h=0$ or $k=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi-\alpha(khl)$
$=\mathrm{m}\pi+\frac{\pi}{4}$

$h+k+l=2n+1$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+l=4n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi-\right.$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+l=4n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos 2\pi(lZ+\tfrac{1}{8})\cos \mathrm{m}\pi+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+l=4n+2}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi-$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{2h+l=4n+3}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\cos 2\pi(lZ-\tfrac{1}{8})\cos \mathrm{m}\pi\right\}$$

where $\mathrm{m}=0$ or 1 according as A (or if $A=0$, then B) is positive or negative.

No. 142

$I4_1/acd$ D_{4h}^{20}

Origin at $\bar{1}$ (at $0,\frac{1}{4},\frac{1}{8}$ from $\bar{4}$).

$$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) \pm \left|\begin{matrix} x,y,z; & \bar{x},y,\frac{1}{2}+z; & \frac{1}{4}+y,\frac{1}{4}+x,\frac{1}{4}+z; & \frac{3}{4}-y,\frac{1}{4}+x,\frac{3}{4}+z; \\ x,\frac{1}{2}-y,\frac{1}{2}+z; & \bar{x},\frac{1}{2}-y,z; & \frac{1}{4}+y,\frac{1}{4}-x,\frac{3}{4}+z; & \frac{3}{4}-y,\frac{1}{4}-x,\frac{1}{4}+z \end{matrix}\right|$$

$$A=16\cos 2\pi\frac{h+k+l}{4}\left\{\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{h}{4}\right)\cos 2\pi\left(lz+\frac{k}{4}\right)+\right.$$

$$B=0 \qquad \left.\cos 2\pi\frac{h+k+l}{4}\cos 2\pi\left(hy-\frac{k}{4}\right)\cos 2\pi\left(kx-\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{h}{4}\right)\right\}$$

$h+k+l=4n$; $h=2n$; $k=2n$	$A=16\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$
$h+k+l=4n$; $h=2n$; $k=2n+1$	$A=-16[\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi hy\cos 2\pi lz]$ $A=B=0$ if $h=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$
$h+k+l=4n$; $h=2n+1$; $k=2n$	$A=-16[\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz+\sin 2\pi kx\cos 2\pi hy\sin 2\pi lz]$ $A=B=0$ if $k=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$
$h+k+l=4n$; $h=2n+1$; $k=2n+1$	$A=-16\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky+\cos 2\pi kx\sin 2\pi hy]$ $A=B=0$ if $l=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$
$h+k+l=4n+2$; $h=2n$; $k=2n$	$A=16\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]$ $A=B=0$ if $h=\pm k$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$
$h+k+l=4n+2$; $h=2n$; $k=2n+1$	$A=-16[\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz-\sin 2\pi kx\sin 2\pi hy\cos 2\pi lz]$ $A=B=0$ if $h=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$
$h+k+l=4n+2$; $h=2n+1$; $k=2n$	$A=-16[\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz-\sin 2\pi kx\cos 2\pi hy\sin 2\pi lz]$ $A=B=0$ if $k=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$
$h+k+l=4n+2$; $h=2n+1$; $k=2n+1$	$A=-16\sin 2\pi lz[\cos 2\pi hx\sin 2\pi ky-\cos 2\pi kx\sin 2\pi hy]$ $A=B=0$ if $l=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$
$h+k+l=2n+1$	$A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\right\}$$

$P3$ C_3^1 No. 143

Origin on 3. | $x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z$ |

$A=\cos 2\pi(hx+ky+lz)+\cos 2\pi(kx+iy+lz)+\cos 2\pi(ix+hy+lz)$

$B=\sin 2\pi(hx+ky+lz)+\sin 2\pi(kx+iy+lz)+\sin 2\pi(ix+hy+lz)$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(kil)|\neq|F(\bar{h}kl)|\neq|F(h\bar{k}l)|\neq|F(hk\bar{l})|\neq|F(khl)|$$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})\neq\alpha(khl)$$

$$\rho(XYZ)=\frac{2}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos[2\pi(hX+kY+lZ)-\alpha(hkl)]+|F(\bar{h}kl)|\cos[2\pi(-hX+kY+lZ)-\alpha(\bar{h}kl)]+$$
$$|F(h\bar{k}l)|\cos[2\pi(hX-kY+lZ)-\alpha(h\bar{k}l)]+|F(hk\bar{l})|\cos[2\pi(hX+kY-lZ)-\alpha(hk\bar{l})]\}$$

$P3_1$ C_3^2 No. 144

Enantiomorphous to $P3_2$; Origin on 3_1. | $x,y,z;\ \bar{y},x-y,\frac{1}{3}+z;\ y-x,\bar{x},\frac{2}{3}+z$ |

$$\left.\begin{aligned}A&=\cos 2\pi(hx+ky+lz)+\cos 2\pi\left(kx+iy+lz+\frac{l}{3}\right)+\cos 2\pi\left(ix+hy+lz-\frac{l}{3}\right)\\ B&=\sin 2\pi(hx+ky+lz)+\sin 2\pi\left(kx+iy+lz+\frac{l}{3}\right)+\sin 2\pi\left(ix+hy+lz-\frac{l}{3}\right)\end{aligned}\right\}A=B=0 \text{ if } h=k=0 \text{ and } l=3n\pm1$$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})\neq\alpha(khl)$$

$l=3n$	$\alpha(hkl)=\alpha(kil)$
$l=3n+1$	$\alpha(hkl)=\alpha(kil)+\frac{2}{3}\pi$
$l=3n+2$	$\alpha(hkl)=\alpha(kil)-\frac{2}{3}\pi$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 143 (above).

$P3_2$ C_3^3 No. 145

Enantiomorphous to $P3_1$; Origin on 3_2. | $x,y,z;\ \bar{y},x-y,\frac{2}{3}+z;\ y-x,\bar{x},\frac{1}{3}+z$ |

$$\left.\begin{aligned}A&=\cos 2\pi(hx+ky+lz)+\cos 2\pi\left(kx+iy+lz-\frac{l}{3}\right)+\cos 2\pi\left(ix+hy+lz+\frac{l}{3}\right)\\ B&=\sin 2\pi(hx+ky+lz)+\sin 2\pi\left(kx+iy+lz-\frac{l}{3}\right)+\sin 2\pi\left(ix+hy+lz+\frac{l}{3}\right)\end{aligned}\right\}A=B=0 \text{ if } h=k=0 \text{ and } l=3n\pm1$$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})\neq\alpha(khl)$$

$l=3n$	$\alpha(hkl)=\alpha(kil)$
$l=3n+1$	$\alpha(hkl)=\alpha(kil)-\frac{2}{3}\pi$
$l=3n+2$	$\alpha(hkl)=\alpha(kil)+\frac{2}{3}\pi$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 143 (above).

No. 146 $R3$ C_3^4

Origin on 3. Rhombohedral co-ordinates: | x,y,z; y,z,x; z,x,y |

$A = \cos 2\pi(\mathrm{hx+ky+lz}) + \cos 2\pi(\mathrm{kx+ly+hz}) + \cos 2\pi(\mathrm{lx+hy+kz})$

$B = \sin 2\pi(\mathrm{hx+ky+lz}) + \sin 2\pi(\mathrm{kx+ly+hz}) + \sin 2\pi(\mathrm{lx+hy+kz})$

$|F(hkl)| = |F(\bar{h}\bar{k}\bar{l})| = |F(klh)| \neq |F(\bar{h}kl)| \neq |F(h\bar{k}l)| \neq |F(hk\bar{l})|$; $\alpha(hkl) = -\alpha(\bar{h}\bar{k}\bar{l}) = \alpha(klh) \neq \alpha(\bar{h}kl) \neq \alpha(h\bar{k}l) \neq \alpha(hk\bar{l})$

Hexagonal co-ordinates: $(0,0,0;\ \frac{1}{3},\frac{2}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3},\frac{1}{3}) + |\ x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z\ |$

$$A = \left(1 + 2\cos 2\pi\frac{-h+k+l}{3}\right)[\cos 2\pi(hx+ky+lz) + \cos 2\pi(kx+iy+lz) + \cos 2\pi(ix+hy+lz)]$$

$$B = \left(1 + 2\cos 2\pi\frac{-h+k+l}{3}\right)[\sin 2\pi(hx+ky+lz) + \sin 2\pi(kx+iy+lz) + \sin 2\pi(ix+hy+lz)]$$

$|F(hkl)|$ and $\alpha(hkl)$ relationships as for No. 143.

$-h+k+l = 3n$ $\quad A = 3[\cos 2\pi(hx+ky+lz) + \cos 2\pi(kx+iy+lz) + \cos 2\pi(ix+hy+lz)]$

$B = 3[\sin 2\pi(hx+ky+lz) + \sin 2\pi(kx+iy+lz) + \sin 2\pi(ix+hy+lz)]$

$-h+k+l = 3n \pm 1$ $\quad A = B = 0$

$\rho(XYZ)$ as for No. 143.

No. 147 $P\bar{3}$ C_{3i}^1

Origin at centre ($\bar{3}$). $\pm\ |\ x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z\ |$

$A = 2[\cos 2\pi(hx+ky+lz) + \cos 2\pi(kx+iy+lz) + \cos 2\pi(ix+hy+lz)]$; $B = 0$

$F(hkl) = F(\bar{h}\bar{k}\bar{l}) = F(kil) \neq F(\bar{h}kl) \neq F(h\bar{k}l) \neq F(hk\bar{l}) \neq F(khl)$

$$\rho(XYZ) = \frac{2}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{F(hkl)\cos 2\pi(hX+kY+lZ) + F(\bar{h}kl)\cos 2\pi(-hX+kY+lZ) + F(h\bar{k}l)\cos 2\pi(hX-kY+lZ) + F(hk\bar{l})\cos 2\pi(hX+kY-lZ)\}$$

No. 148 $R\bar{3}$ C_{3i}^2

Origin at centre ($\bar{3}$). Rhombohedral co-ordinates: $\pm\ |\ x,y,z;\ y,z,x;\ z,x,y\ |$

$A = 2[\cos 2\pi(\mathrm{hx+ky+lz}) + \cos 2\pi(\mathrm{kx+ly+hz}) + \cos 2\pi(\mathrm{lx+hy+kz})]$; $B = 0$

$F(hkl) = F(\bar{h}\bar{k}\bar{l}) = F(klh) \neq F(\bar{h}kl) \neq F(h\bar{k}l) \neq F(hkl)$

Hexagonal co-ordinates: $(0,0,0;\ \frac{1}{3},\frac{2}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3},\frac{1}{3}) \pm |\ x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z\ |$

$$A = 2\left(1 + 2\cos 2\pi\frac{-h+k+l}{3}\right)[\cos 2\pi(hx+ky+lz) + \cos 2\pi(kx+iy+lz) + \cos 2\pi(ix+hy+lz)]; \quad B = 0$$

$F(hkl)$ relationships as for No. 147.

$-h+k+l = 3n$ $\quad A = 6[\cos 2\pi(hx+ky+lz) + \cos 2\pi(kx+iy+lz) + \cos 2\pi(ix+hy+lz)]$

$-h+k+l = 3n \pm 1$ $\quad A = B = 0$

$\rho(XYZ)$ as for No. 147.

$P312$ D_3^1

No. 149

Origin at 312. | $x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ \bar{y},\bar{x},\bar{z};\ x,x-y,\bar{z};\ y-x,y,\bar{z}$ |

$A=2\{\cos\pi[h(x+y)-2lz]\cos\pi(k-i)(x-y)+\cos\pi[k(x+y)-2lz]\cos\pi(i-h)(x-y)+$
$\cos\pi[i(x+y)-2lz]\cos\pi(h-k)(x-y)\}$

$B=2\{\cos\pi[h(x+y)-2lz]\sin\pi(k-i)(x-y)+\cos\pi[k(x+y)-2lz]\sin\pi(i-h)(x-y)+$
$\cos\pi[i(x+y)-2lz]\sin\pi(h-k)(x-y)\}$

$B=0$ if $h=k$ or $k=i$ or $i=h$. $|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(kil)|=|F(khl)|\neq|F(\bar{h}kl)|\neq|F(h\bar{k}l)|\neq|F(hk\bar{l})|$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(kil)=-\alpha(khl)\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})$

$\rho(XYZ)$ as for No. 143.

$P321$ D_3^2

No. 150

Origin at 321. | $x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ y,x,\bar{z};\ \bar{x},y-x,\bar{z};\ x-y,\bar{y},\bar{z}$ |

$A=2\{\cos\pi h(x+y)\cos\pi[(k-i)(x-y)+2lz]+\cos\pi k(x+y)\cos\pi[(i-h)(x-y)+2lz]+$
$\cos\pi i(x+y)\cos\pi[(h-k)(x-y)+2lz]\}$

$B=-2\{\sin\pi h(x+y)\cos\pi[(k-i)(x-y)+2lz]+\sin\pi k(x+y)\cos\pi[(i-h)(x-y)+2lz]+$
$\sin\pi i(x+y)\cos\pi[(h-k)(x-y)+2lz]\}$

$B=0$ if $h=-k$ or $k=-i$ or $i=-h$ $|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(kil)|\neq|F(\bar{h}kl)|\neq|F(h\bar{k}l)|\neq|F(hk\bar{l})|=|F(khl)|$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})=\alpha(khl)$

$\rho(XYZ)$ as for No. 143.

$P3_112$ D_3^3

No. 151

Enantiomorphous to $P3_212$; Origin at 3_112.

| $x,y,z;\ \bar{y},x-y,\frac{1}{3}+z;\ y-x,\bar{x},\frac{2}{3}+z;\ \bar{y},\bar{x},\bar{z};\ x,x-y,\frac{1}{3}-z;\ y-x,y,\frac{2}{3}-z$ |

$$A=2\left\{\cos\pi[i(x+y)-2lz]\cos\pi(h-k)(x-y)+\cos\pi[h(x+y)-2lz]\cos\pi\left[(k-i)(x-y)+2\frac{l}{3}\right]+\cos\pi[k(x+y)-2lz]\cos\pi\left[(i-h)(x-y)-2\frac{l}{3}\right]\right\}$$

$$B=2\left\{\cos\pi[i(x+y)-2lz]\sin\pi(h-k)(x-y)+\cos\pi[h(x+y)-2lz]\sin\pi\left[(k-i)(x-y)+2\frac{l}{3}\right]+\cos\pi[k(x+y)-2lz]\sin\pi\left[(i-h)(x-y)-2\frac{l}{3}\right]\right\}$$

$B=0$ if $l=3n$ and $h=k$ (or $k=i$ or $i=h$). $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(khl)\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})$

$A=B=0$ if $l=3n\pm1$ and $h=k=0$

$l=3n$	$\alpha(hkl)=\alpha(kil)$
$l=3n\pm1$	$\alpha(hkl)=\alpha(kil)\pm\frac{2}{3}\pi$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 149 (above).

No. 152

$P3_121$
D_3^4

Enantiomorphous to $P3_221$; Origin at 3_121.

$| \; x,y,z;\; \bar{y},x-y,\tfrac{1}{3}+z;\; y-x,\bar{x},\tfrac{2}{3}+z;\; y,x,\bar{z};\; \bar{x},y-x,\tfrac{1}{3}-z;\; x-y,\bar{y},\tfrac{2}{3}-z \; |$

$$A=2\Big\{\cos\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\cos\pi[(k-i)(x-y)+2lz]\cos\pi\Big[h(x+y)-2\frac{l}{3}\Big]+$$
$$\cos\pi[(i-h)(x-y)+2lz]\cos\pi\Big[k(x+y)+2\frac{l}{3}\Big]\Big\}$$

$$B=-2\Big\{\cos\pi[(h-k)(x-y)+2lz]\sin\pi i(x+y)+\cos\pi[(k-i)(x-y)+2lz]\sin\pi\Big[h(x+y)-2\frac{l}{3}\Big]+$$
$$\cos\pi[(i-h)(x-y)+2lz]\sin\pi\Big[k(x+y)+2\frac{l}{3}\Big]\Big\}$$

$B=0$ if $l=3n$ and $h=-k$ (*or* $k=-i$ or $i=-h$)

$A=B=0$ if $l=3n\pm1$ and $h=k=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})=\alpha(khl)$

$l=3n$	$\alpha(hkl)=\alpha(kil)$
$l=3n\pm1$	$\alpha(hkl)=\alpha(kil)\pm\frac{2}{3}\pi$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 150.

No. 153

$P3_212$
D_3^5

Enantiomorphous to $P3_112$; Origin at 3_212.

$| \; x,y,z;\; \bar{y},x-y,\tfrac{2}{3}+z;\; y-x,\bar{x},\tfrac{1}{3}+z;\; \bar{y},\bar{x},\bar{z};\; x,x-y,\tfrac{2}{3}-z;\; y-x,y,\tfrac{1}{3}-z \; |$

$$A=2\Big\{\cos\pi[i(x+y)-2lz]\cos\pi(h-k)(x-y)+\cos\pi[h(x+y)-2lz]\cos\pi\Big[(k-i)(x-y)-2\frac{l}{3}\Big]+$$
$$\cos\pi[k(x+y)-2lz]\cos\pi\Big[(i-h)(x-y)+2\frac{l}{3}\Big]\Big\}$$

$$B=2\Big\{\cos\pi[i(x+y)-2lz]\sin\pi(h-k)(x-y)+\cos\pi[h(x+y)-2lz]\sin\pi\Big[(k-i)(x-y)-2\frac{l}{3}\Big]+$$
$$\cos\pi[k(x+y)-2lz]\sin\pi\Big[(i-h)(x-y)+2\frac{l}{3}\Big]\Big\}$$

$B=0$ if $l=3n$ and $h=k$ (or $k=i$ or $i=h$)

$A=B=0$ if $l=3n\pm1$ and $h=k=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(khl)\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})$

$l=3n$	$\alpha(hkl)=\alpha(kil)$
$l=3n\pm1$	$\alpha(hkl)=\alpha(kil)\mp\frac{2}{3}\pi$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 149.

$P3_221$ D_3^6

No. 154

Enantiomorphous to $P3_121$; Origin at 3_221.

$| x,y,z;\ \bar{y},x-y,\frac{2}{3}+z;\ y-x,\bar{x},\frac{1}{3}+z;\ y,x,\bar{z};\ \bar{x},y-x,\frac{2}{3}-z;\ x-y,\bar{y},\frac{1}{3}-z |$

$$A=2\Big\{\cos\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\cos\pi[(k-i)(x-y)+2lz]\cos\pi\Big[h(x+y)+2\frac{l}{3}\Big]+$$
$$\cos\pi[(i-h)(x-y)+2lz]\cos\pi\Big[k(x+y)-2\frac{l}{3}\Big]\Big\}$$

$$B=-2\Big\{\cos\pi[(h-k)(x-y)+2lz]\sin\pi i(x+y)+\cos\pi[(k-i)(x-y)+2lz]\sin\pi\Big[h(x+y)+2\frac{l}{3}\Big]+$$
$$\cos\pi[(i-h)(x-y)+2lz]\sin\pi\Big[k(x+y)-2\frac{l}{3}\Big]\Big\}$$

$B=0$ if $l=3n$ and $h=-k$ (or $k=-i$ or $i=-h$) $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})=\alpha(khl)$

$A=B=0$ if $l=3n\pm1$ and $h=k=0$

$l=3n$	$\alpha(hkl)=\alpha(kil)$
$l=3n\pm1$	$\alpha(hkl)=\alpha(kil)\mp\frac{2}{3}\pi$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 150.

$R32$ D_3^7

No. 155

Origin at 32. Rhombohedral co-ordinates: $|$ x,y,z; y,z,x; z,x,y; $\bar{y},\bar{x},\bar{z}$; $\bar{x},\bar{z},\bar{y}$; $\bar{z},\bar{y},\bar{x}$ $|$

$$A=2\{\cos\pi(h-k)(x-y)\cos\pi[(h+k)(x+y)+2lz]+\cos\pi(k-l)(x-y)\cos\pi[(k+l)(x+y)+2hz]+$$
$$\cos\pi(l-h)(x-y)\cos\pi[(l+h)(x+y)+2kz]\}$$

$$B=2\{\sin\pi(h-k)(x-y)\cos\pi[(h+k)(x+y)+2lz]+\sin\pi(k-l)(x-y)\cos\pi[(k+l)(x+y)+2hz]+$$
$$\sin\pi(l-h)(x-y)\cos\pi[(l+h)(x+y)+2kz]\}$$

$B=0$ if $h=k$ or $k=l$ or $l=h$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(klh)|=|F(khl)|\neq|F(\bar{h}kl)|\neq|F(h\bar{k}l)|\neq|F(hk\bar{l})|$$
$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(klh)=-\alpha(khl)\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})$$

Hexagonal co-ordinates: $(0,0,0;\ \frac{1}{3},\frac{2}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3},\frac{1}{3})+$ $| x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ y,x,\bar{z};\ \bar{x},y-x,\bar{z};\ x-y,\bar{y},\bar{z} |$

$$A=2\Big(1+2\cos 2\pi\frac{-h+k+l}{3}\Big)\{\cos\pi i(x+y)\cos\pi[(h-k)(x-y)+2lz]+$$
$$\cos\pi h(x+y)\cos\pi[(k-i)(x-y)+2lz]+\cos\pi k(x+y)\cos\pi[(i-h)(x-y)+2lz]\}$$

$$B=-2\Big(1+2\cos 2\pi\frac{-h+k+l}{3}\Big)\{\sin\pi i(x+y)\cos\pi[(h-k)(x-y)+2lz]+$$
$$\sin\pi h(x+y)\cos\pi[(k-i)(x-y)+2lz]+\sin\pi k(x+y)\cos\pi[(i-h)(x-y)+2lz]\}$$

$|F(hkl)|$ and $\alpha(hkl)$ relationships as for No. 150.

$-h+k+l=3n$

$$A=6\{\cos\pi i(x+y)\cos\pi[(h-k)(x-y)+2lz]+$$
$$\cos\pi h(x+y)\cos\pi[(k-i)(x-y)+2lz]+\cos\pi k(x+y)\cos\pi[(i-h)(x-y)+2lz]\}$$

$$B=-6\{\sin\pi i(x+y)\cos\pi[(h-k)(x-y)+2lz]+$$
$$\sin\pi h(x+y)\cos\pi[(k-i)(x-y)+2lz]+\sin\pi k(x+y)\cos\pi[(i-h)(x-y)+2lz]\}$$

$B=0$ if $h=-k$ or $k=-i$ or $i=-h$

$-h+k+l=3n\pm1$ $A=B=0$

$\rho(XYZ)$ as for No. 143.

No. 156 $P3m1$ C_{3v}^{1}

Origin on $3m1$. | $x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ \bar{y},\bar{x},z;\ x,x-y,z;\ y-x,y,z$ |

$$A=2\{\cos\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\cos\pi[(k-i)(x-y)+2lz]\cos\pi h(x+y)+\cos\pi[(i-h)(x-y)+2lz]\cos\pi k(x+y)\}$$

$$B=2\{\sin\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\sin\pi[(k-i)(x-y)+2lz]\cos\pi h(x+y)+\sin\pi[(i-h)(x-y)+2lz]\cos\pi k(x+y)\}$$

$B=0$ if $l=0$ and $h=k$ (or $k=i$ or $i=h$)

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(kil)|\neq|F(\bar{h}kl)|\neq|F(h\bar{k}l)|\neq|F(hk\bar{l})|=|F(khl)|$$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})=-\alpha(khl)$$

$\rho(XYZ)$ as for No. 143.

No. 157 $P31m$ C_{3v}^{2}

Origin on $31m$. | $x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ y,x,z;\ \bar{x},y-x,z;\ x-y,\bar{y},z$ |

$$A=2\{\cos\pi[i(x+y)-2lz]\cos\pi(h-k)(x-y)+\cos\pi[h(x+y)-2lz]\cos\pi(k-i)(x-y)+\cos\pi[k(x+y)-2lz]\cos\pi(i-h)(x-y)\}$$

$$B=-2\{\sin\pi[i(x+y)-2lz]\cos\pi(h-k)(x-y)+\sin\pi[h(x+y)-2lz]\cos\pi(k-i)(x-y)+\sin\pi[k(x+y)-2lz]\cos\pi(i-h)(x-y)\}$$

$B=0$ if $l=0$ and $h=-k$ (or $k=-i$ or $i=-h$)

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(kil)|=|F(khl)|\neq|F(\bar{h}kl)|\neq|F(h\bar{k}l)|\neq|F(hk\bar{l})|$$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(kil)=\alpha(khl)\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})$$

$\rho(XYZ)$ as for No. 143.

No. 158 $P3c1$ C_{3v}^{3}

Origin on 3. | $x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ \bar{y},\bar{x},\frac{1}{2}+z;\ x,x-y,\frac{1}{2}+z;\ y-x,y,\frac{1}{2}+z$ |

$$A=2\left\{\cos\pi\left[(h-k)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[i(x+y)+\frac{l}{2}\right]+\cos\pi\left[(k-i)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[h(x+y)+\frac{l}{2}\right]+\cos\pi\left[(i-h)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[k(x+y)+\frac{l}{2}\right]\right\}$$

$$B=2\left\{\sin\pi\left[(h-k)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[i(x+y)+\frac{l}{2}\right]+\sin\pi\left[(k-i)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[h(x+y)+\frac{l}{2}\right]+\sin\pi\left[(i-h)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[k(x+y)+\frac{l}{2}\right]\right\}$$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})$$

$l = 2n$ $\quad A=2\{\cos \pi[(h-k)(x-y)+2lz] \cos \pi i(x+y)+ \cos \pi[(k-i)(x-y)+2lz] \cos \pi h(x+y)+ \cos \pi[(i-h)(x-y)+2lz] \cos \pi k(x+y)\}$

$B=2\{\sin \pi[(h-k)(x-y)+2lz] \cos \pi i(x+y)+ \sin \pi[(k-i)(x-y)+2lz] \cos \pi h(x+y)+ \sin \pi[(i-h)(x-y)+2lz] \cos \pi k(x+y)\}$

$B=0$ if $l=0$ and $h=k$ (or $k=i$ or $i=h$) $\quad \alpha(khl)=-\alpha(hk\bar{l})$

$l = 2n + 1$ $\quad A=2\{\sin \pi[(h-k)(x-y)+2lz] \sin \pi i(x+y)+ \sin \pi[(k-i)(x-y)+2lz] \sin \pi h(x+y)+ \sin \pi[(i-h)(x-y)+2lz] \sin \pi k(x+y)\}$

$B=-2\{\cos \pi[(h-k)(x-y)+2lz] \sin \pi i(x+y)+ \cos \pi[(k-i)(x-y)+2lz] \sin \pi h(x+y)+ \cos \pi[(i-h)(x-y)+2lz] \sin \pi k(x+y)\}$

$A=B=0$ if $h=-k$ (or $k=-i$ or $i=-h$) $\quad \alpha(khl)=\pi-\alpha(hk\bar{l})$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 156.

$P31c$
C_{3v}^{4}

No. 159

Origin on 3. $\quad | \; x,y,z;\; \bar{y},x-y,z;\; y-x,\bar{x},z;\; y,x,\tfrac{1}{2}+z;\; \bar{x},y-x,\tfrac{1}{2}+z;\; x-y,\bar{y},\tfrac{1}{2}+z \; |$

$$A=2\left\{\cos \pi\left[i(x+y)-2lz+\frac{l}{2}\right] \cos \pi\left[(h-k)(x-y)+\frac{l}{2}\right]+ \cos \pi\left[h(x+y)-2lz+\frac{l}{2}\right] \cos \pi\left[(k-i)(x-y)+\frac{l}{2}\right]+ \cos \pi\left[k(x+y)-2lz+\frac{l}{2}\right] \cos \pi\left[(i-h)(x-y)+\frac{l}{2}\right]\right\}$$

$$B=-2\left\{\sin \pi\left[i(x+y)-2lz+\frac{l}{2}\right] \cos \pi\left[(h-k)(x-y)+\frac{l}{2}\right]+ \sin \pi\left[h(x+y)-2lz+\frac{l}{2}\right] \cos \pi\left[(k-i)(x-y)+\frac{l}{2}\right]+ \sin \pi\left[k(x+y)-2lz+\frac{l}{2}\right] \cos \pi\left[(i-h)(x-y)+\frac{l}{2}\right]\right\}$$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})$

$l = 2n$ $\quad A=2\{\cos \pi[i(x+y)-2lz] \cos \pi(h-k)(x-y)+ \cos \pi[h(x+y)-2lz] \cos \pi(k-i)(x-y)+ \cos \pi[k(x+y)-2lz] \cos \pi(i-h)(x-y)\}$

$B=-2\{\sin \pi[i(x+y)-2lz] \cos \pi(h-k)(x-y)+ \sin \pi[h(x+y)-2lz] \cos \pi(k-i)(x-y)+ \sin \pi[k(x+y)-2lz] \cos \pi(i-h)(x-y)\}$

$B=0$ if $l=0$ and $h=-k$ (or $k=-i$ or $i=-h$) $\quad \alpha(hkl)=\alpha(khl)$

$l = 2n + 1$ $\quad A=2\{\sin \pi[i(x+y)-2lz] \sin \pi(h-k)(x-y)+ \sin \pi[h(x+y)-2lz] \sin \pi(k-i)(x-y)+ \sin \pi[k(x+y)-2lz] \sin \pi(i-h)(x-y)\}$

$B=2\{\cos \pi[i(x+y)-2lz] \sin \pi(h-k)(x-y)+ \cos \pi[h(x+y)-2lz] \sin \pi(k-i)(x-y)+ \cos \pi[k(x+y)-2lz] \sin \pi(i-h)(x-y)\}$

$A=B=0$ if $h=k$ (or $k=i$ or $i=h$) $\quad \alpha(hkl)=\pi+\alpha(khl)$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 157.

No. 160 $R3m$ C_{3v}^{5}

Origin on $3m$. Rhombohedral co-ordinates: | x,y,z; y,z,x; z,x,y; y,x,z; z,y,x; x,z,y |

$$A=2\{\cos\pi[(h+k)(x+y)+2lz]\cos\pi(h-k)(x-y)+\cos\pi[(k+l)(x+y)+2hz]\cos\pi(k-l)(x-y)+\cos\pi[(l+h)(x+y)+2kz]\cos\pi(l-h)(x-y)\}$$

$$B=2\{\sin\pi[(h+k)(x+y)+2lz]\cos\pi(h-k)(x-y)+\sin\pi[(k+l)(x+y)+2hz]\cos\pi(k-l)(x-y)+\sin\pi[(l+h)(x+y)+2kz]\cos\pi(l-h)(x-y)\}$$

$B=0$ if $l=0$ and $h=-k$ (or $h=0$ and $k=-l$, or $k=0$ and $l=-h$)

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(klh)|=|F(khl)|\neq|F(\bar{h}kl)|\neq|F(h\bar{k}l)|\neq|F(hk\bar{l})|$$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(klh)=\alpha(khl)\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})$$

Hexagonal co-ordinates: $(0,0,0;\ \frac{1}{3},\frac{2}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3},\frac{1}{3})$ + | $x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ \bar{y},\bar{x},z;\ x,x-y,z;\ y-x,y,z$ |

$$A=2\left(1+2\cos 2\pi\frac{-h+k+l}{3}\right)\{\cos\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\cos\pi[(k-i)(x-y)+2lz]\cos\pi h(x+y)+\cos\pi[(i-h)(x-y)+2lz]\cos\pi k(x+y)\}$$

$$B=2\left(1+2\cos 2\pi\frac{-h+k+l}{3}\right)\{\sin\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\sin\pi[(k-i)(x-y)+2lz]\cos\pi h(x+y)+\sin\pi[(i-h)(x-y)+2lz]\cos\pi k(x+y)\}$$

$|F(hkl)|$ and $\alpha(hkl)$ relationships as for No. 156.

$-h+k+l=3n$

$$A=6\{\cos\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\cos\pi[(k-i)(x-y)+2lz]\cos\pi h(x+y)+\cos\pi[(i-h)(x-y)+2lz]\cos\pi k(x+y)\}$$

$$B=6\{\sin\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\sin\pi[(k-i)(x-y)+2lz]\cos\pi h(x+y)+\sin\pi[(i-h)(x-y)+2lz]\cos\pi k(x+y)\}$$

$B=0$ if $l=0$ and $h=k$ (or $k=i$ or $i=h$)

$-h+k+l=3n\pm1$ $\quad A=B=0$

$\rho(XYZ)$ as for No. 143.

No. 161 $R3c$ C_{3v}^{6}

Origin on 3.

Rhombohedral co-ordinates: | x,y,z; y,z,x; z,x,y; $\frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z$; $\frac{1}{2}+z,\frac{1}{2}+y,\frac{1}{2}+x$; $\frac{1}{2}+x,\frac{1}{2}+z,\frac{1}{2}+y$ |

$$A=2\left\{\cos\pi\left[(h+k)(x+y)+2lz-\frac{h+k+l}{2}\right]\cos\pi\left[(h-k)(x-y)+\frac{h+k+l}{2}\right]+\cos\pi\left[(k+l)(x+y)+2hz-\frac{h+k+l}{2}\right]\cos\pi\left[(k-l)(x-y)+\frac{h+k+l}{2}\right]+\cos\pi\left[(l+h)(x+y)+2kz-\frac{h+k+l}{2}\right]\cos\pi\left[(l-h)(x-y)+\frac{h+k+l}{2}\right]\right\}$$

$$B=2\left\{\sin\pi\left[(h+k)(x+y)+2lz-\frac{h+k+l}{2}\right]\cos\pi\left[(h-k)(x-y)+\frac{h+k+l}{2}\right]+\sin\pi\left[(k+l)(x+y)+2hz-\frac{h+k+l}{2}\right]\cos\pi\left[(k-l)(x-y)+\frac{h+k+l}{2}\right]+\sin\pi\left[(l+h)(x+y)+2kz-\frac{h+k+l}{2}\right]\cos\pi\left[(l-h)(x-y)+\frac{h+k+l}{2}\right]\right\}$$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(klh)|=|F(khl)|\neq|F(\bar{h}kl)|\neq|F(h\bar{k}l)|\neq|F(hk\bar{l})|$$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(klh)\neq\alpha(\bar{h}kl)\neq\alpha(h\bar{k}l)\neq\alpha(hk\bar{l})$$

$h + k + l = 2n$

$$A=2\{\cos\pi[(h+k)(x+y)+2lz]\cos\pi(h-k)(x-y)+\cos\pi[(k+l)(x+y)+2hz]x$$
$$\cos\pi(k-l)(x-y)+\cos\pi[(l+h)(x+y)+2kz]\cos\pi(l-h)(x-y)\}$$
$$B=2\{\sin\pi[(h+k)(x+y)+2lz]\cos\pi(h-k)(x-y)+\sin\pi[(k+l)(x+y)+2hz]x$$
$$\cos\pi(k-l)(x-y)+\sin\pi[(l+h)(x+y)+2kz]\cos\pi(l-h)(x-y)\}$$

$B=0$ if $l=0$ and $h=-k$ (or $k=-i$ or $i=-h$) $\qquad \alpha(hkl)=\alpha(khl)$

$h + k + l = 2n + 1$

$$A=-2\{\sin\pi[(h+k)(x+y)+2lz]\sin\pi(h-k)(x-y)+\sin\pi[(k+l)(x+y)+2hz]x$$
$$\sin\pi(k-l)(x-y)+\sin\pi[(l+h)(x+y)+2kz]\sin\pi(l-h)(x-y)\}$$
$$B=2\{\cos\pi[(h+k)(x+y)+2lz]\sin\pi(h-k)(x-y)+\cos\pi[(k+l)(x+y)+2hz]x$$
$$\sin\pi(k-l)(x-y)+\cos\pi[(l+h)(x+y)+2kz]\sin\pi(l-h)(x-y)\}$$

$A=B=0$ if $h=k$ (or $k=l$ or $l=h$) $\qquad \alpha(hkl)=\pi+\alpha(khl)$

Hexagonal co-ordinates:

$$(0,0,0;\ \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3};\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3}) + \ |\ x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ \bar{y},\bar{x},\tfrac{1}{2}+z;\ x,x-y,\tfrac{1}{2}+z;\ y-x,y,\tfrac{1}{2}+z\ |$$

$$A=2\left(1+2\cos 2\pi\frac{-h+k+l}{3}\right)\left\{\cos\pi\left[(h-k)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[i(x+y)+\frac{l}{2}\right]+\right.$$
$$\left.\cos\pi\left[(k-i)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[h(x+y)+\frac{l}{2}\right]+\cos\pi\left[(i-h)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[k(x+y)+\frac{l}{2}\right]\right\}$$
$$B=2\left(1+2\cos 2\pi\frac{-h+k+l}{3}\right)\left\{\sin\pi\left[(h-k)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[i(x+y)+\frac{l}{2}\right]+\right.$$
$$\left.\sin\pi\left[(k-i)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[h(x+y)+\frac{l}{2}\right]+\sin\pi\left[(i-h)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[k(x+y)+\frac{l}{2}\right]\right\}$$

$|F(hkl)|$ and $\alpha(hkl)$ relationships as for No. 158.

$\begin{cases} -h+k+l=3n \\ l=2n \end{cases}$

$$A=6\{\cos\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\cos\pi[(k-i)(x-y)+2lz]\cos\pi h(x+y)+$$
$$\cos\pi[(i-h)(x-y)+2lz]\cos\pi k(x+y)\}$$
$$B=6\{\sin\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\sin\pi[(k-i)(x-y)+2lz]\cos\pi h(x+y)+$$
$$\sin\pi[(i-h)(x-y)+2lz]\cos\pi k(x+y)\}$$

$B=0$ if $l=0$ and $h=k$ (or $k=i$ or $i=h$)

$\begin{cases} -h+k+l=3n \\ l=2n+1 \end{cases}$

$$A=6\{\sin\pi[(h-k)(x-y)+2lz]\sin\pi i(x+y)+\sin\pi[(k-i)(x-y)+2lz]\sin\pi h(x+y)+$$
$$\sin\pi[(i-h)(x-y)+2lz]\sin\pi k(x+y)\}$$
$$B=-6\{\cos\pi[(h-k)(x-y)+2lz]\sin\pi i(x+y)+\cos\pi[(k-i)(x-y)+2lz]\sin\pi h(x+y)+$$
$$\cos\pi[(i-h)(x-y)+2lz]\sin\pi k(x+y)\}$$

$A=B=0$ if $h=-k$ (or $k=-i$ or $i=-h$)

$-h+k+l=3n\pm 1$ $\quad A=B=0$

$\rho(XYZ)$ as for No. 143.

No. 162 $P\bar{3}1m$ D_{3d}^{1}

Origin at centre ($\bar{3}1m$). $\pm\ |\ x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ y,x,z;\ \bar{x},y-x,z;\ x-y,\bar{y},z\ |$

$$A=4\{\cos\pi[i(x+y)-2lz]\cos\pi(h-k)(x-y)+\cos\pi[h(x+y)-2lz]\cos\pi(k-i)(x-y)+\cos\pi[k(x+y)-2lz]\cos\pi(i-h)(x-y)\}$$

$B=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(kil)=F(khl)\neq F(\bar{h}kl)\neq F(h\bar{k}l)\neq F(hk\bar{l})$

$\rho(XYZ)$ as for No. 147.

No. 163 $P\bar{3}1c$ D_{3d}^{2}

Origin at centre ($\bar{3}$). $\pm\ |\ x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ y,x,\tfrac{1}{2}+z;\ \bar{x},y-x,\tfrac{1}{2}+z;\ x-y,\bar{y},\tfrac{1}{2}+z\ |$

$$A=4\left\{\cos\pi\left[i(x+y)-2lz+\frac{l}{2}\right]\cos\pi\left[(h-k)(x-y)+\frac{l}{2}\right]+\cos\pi\left[h(x+y)-2lz+\frac{l}{2}\right]\cos\pi\left[(k-i)(x-y)+\frac{l}{2}\right]+\cos\pi\left[k(x+y)-2lz+\frac{l}{2}\right]\cos\pi\left[(i-h)(x-y)+\frac{l}{2}\right]\right\}$$

$B=0$;

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(kil)\neq F(\bar{h}kl)\neq F(h\bar{k}l)\neq F(hk\bar{l})$

$l=2n$ $\quad A=4\{\cos\pi[i(x+y)-2lz]\cos\pi(h-k)(x-y)+\cos\pi[h(x+y)-2lz]\cos\pi(k-i)(x-y)+\cos\pi[k(x+y)-2lz]\cos\pi(i-h)(x-y)\}$

$F(hkl)=F(khl)$

$l=2n+1$ $\quad A=4\{\sin\pi[i(x+y)-2lz]\sin\pi(h-k)(x-y)+\sin\pi[h(x+y)-2lz]\sin\pi(k-i)(x-y)+\sin\pi[k(x+y)-2lz]\sin\pi(i-h)(x-y)\}$

$F(hkl)=-F(khl)$

$A=B=0$ if $h=k$ (or $k=i$ or $i=h$)

$\rho(XYZ)$ as for No. 147.

No. 164 $P\bar{3}m1$ D_{3d}^{3}

Origin at centre ($\bar{3}m1$). $\pm\ |\ x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ \bar{y},\bar{x},z;\ x,x-y,z;\ y-x,y,z\ |$

$$A=4\{\cos\pi i(x+y)\cos\pi[(h-k)(x-y)+2lz]+\cos\pi h(x+y)\cos\pi[(k-i)(x-y)+2lz]+\cos\pi k(x+y)\cos\pi[(i-h)(x-y)+2lz]\}$$

$B=0$

$F(hkl)=F(\bar{h}k\bar{l})=F(kil)\neq F(\bar{h}kl)\neq F(h\bar{k}l)\neq F(hk\bar{l})=F(khl)$

$\rho(XYZ)$ as for No. 147.

$P\bar{3}c1$ D_{3d}^{4}

No. 165

Origin at centre ($\bar{3}$). $\pm$ | x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{y},\bar{x},\frac{1}{2}+z$; $x,x-y,\frac{1}{2}+z$; $y-x,y,\frac{1}{2}+z$ |

$A=4\{\cos\pi\left[i(x+y)+\frac{l}{2}\right]\cos\pi\left[(h-k)(x-y)+2lz+\frac{l}{2}\right]+\cos\pi\left[h(x+y)+\frac{l}{2}\right]\cos\pi\left[(k-i)(x-y)+2lz+\frac{l}{2}\right]+$

$B=0$; $\cos\pi\left[k(x+y)+\frac{l}{2}\right]\cos\pi\left[(i-h)(x-y)+2lz+\frac{l}{2}\right]\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(kil)\neq F(\bar{h}kl)\neq F(h\bar{k}l)\neq F(hk\bar{l})$

$l=2n$ $A=4\{\cos\pi i(x+y)\cos\pi[(h-k)(x-y)+2lz]+\cos\pi h(x+y)\cos\pi[(k-i)(x-y)+2lz]+$

$F(hk\bar{l})=F(khl)$ $\cos\pi k(x+y)\cos\pi[(i-h)(x-y)+2lz]\}$

$l=2n+1$ $A=4\{\sin\pi i(x+y)\sin\pi[(h-k)(x-y)+2lz]+\sin\pi h(x+y)\sin\pi[(k-i)(x-y)+2lz]+$

$F(hk\bar{l})=-F(khl)$ $\sin\pi k(x+y)\sin\pi[(i-h)(x-y)+2lz]\}$

$A=0$ if $h=-k$ (or $k=-i$ or $i=-h$)

$\rho(XYZ)$ as for No. 147.

$R\bar{3}m$ D_{3d}^{5}

No. 166

Origin at centre ($\bar{3}m$).

Rhombohedral co-ordinates: $\pm$ | x,y,z; y,z,x; z,x,y; y,x,z; z,y,x; x,z,y |

$A=4\{\cos\pi[(h+k)(x+y)+2lz]\cos\pi(h-k)(x-y)+\cos\pi[(k+l)(x+y)+2hz]\cos\pi(k-l)(x-y)+$

$B=0$; $\cos\pi[(l+h)(x+y)+2kz]\cos\pi(l-h)(x-y)\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(klh)=F(khl)\neq F(\bar{h}kl)\neq F(h\bar{k}l)\neq F(hk\bar{l})$

Hexagonal co-ordinates: $(0,0,0;\ \frac{1}{3},\frac{2}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3},\frac{1}{3})\ \pm$ | x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{y},\bar{x},z$; $x,x-y,z$; $y-x,y,z$ |

$A=4\left(1+2\cos 2\pi\frac{-h+k+l}{3}\right)\{\cos\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\cos\pi[(k-i)(x-y)+2lz]\cos\pi h(x+y)+$

$B=0$; $\cos\pi[(i-h)(x-y)+2lz]\cos\pi k(x+y)\}$

$F(hkl)$ relationships as for No. 164.

$-h+k+l=3n$ $A=12\{\cos\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\cos\pi[(k-i)(x-y)+2lz]\cos\pi h(x+y)+$

$\cos\pi[(i-h)(x-y)+2lz]\cos\pi k(x+y)\}$

$-h+k+l=3n\pm 1$ $A=B=0$

$\rho(XYZ)$ as for No. 147.

No. 167 $R\bar{3}c$ D_{3d}^{6}

Origin at centre ($\bar{3}$).

Rhombohedral co-ordinates: $\pm$ | x,y,z; y,z,x; z,x,y; $\frac{1}{2}$+y,$\frac{1}{2}$+x,$\frac{1}{2}$+z; $\frac{1}{2}$+z,$\frac{1}{2}$+y,$\frac{1}{2}$+x; $\frac{1}{2}$+x,$\frac{1}{2}$+z,$\frac{1}{2}$+y |

$$A=4\left\{\cos\pi\left[(h+k)(x+y)+2lz+\frac{h+k+l}{2}\right]\cos\pi\left[(h-k)(x-y)-\frac{h+k+l}{2}\right]+\right.$$
$$\cos\pi\left[(k+l)(x+y)+2hz+\frac{h+k+l}{2}\right]\cos\pi\left[(k-l)(x-y)-\frac{h+k+l}{2}\right]+$$
$$\left.\cos\pi\left[(l+h)(x+y)+2kz+\frac{h+k+l}{2}\right]\cos\pi\left[(l-h)(x-y)-\frac{h+k+l}{2}\right]\right\}$$

$B=0$ $\quad F(hkl)=F(\bar{h}k\bar{l})=F(klh)\neq F(\bar{h}kl)\neq F(h\bar{k}l)\neq F(hk\bar{l})$

$h+k+l=2n$	$A=4\{\cos\pi[(h+k)(x+y)+2lz]\cos\pi(h-k)(x-y)+\cos\pi[(k+l)(x+y)+2hz]$
	$F(hkl)=F(khl)$ $\quad\cos\pi(k-l)(x-y)+\cos\pi[(l+h)(x+y)+2kz]\cos\pi(l-h)(x-y)\}$
$h+k+l=2n+1$	$A=-4\{\sin\pi[(h+k)(x+y)+2lz]\sin\pi(h-k)(x-y)+\sin\pi[(k+l)(x+y)+2hz]$
	$F(hkl)=-F(khl)$ $\quad\sin\pi(k-l)(x-y)+\sin\pi[(l+h)(x+y)+2kz]\sin\pi(l-h)(x-y)\}$
	$A=0$ if $h=k$ (or $k=l$ or $l=h$)

Hexagonal co-ordinates:

(0,0,0; $\frac{1}{3},\frac{2}{3},\frac{2}{3}$; $\frac{2}{3},\frac{1}{3},\frac{1}{3}$) $\pm$ | x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{y},\bar{x},\frac{1}{2}+z$; $x,x-y,\frac{1}{2}+z$; $y-x,y,\frac{1}{2}+z$ |

$$A=4\left(1+2\cos 2\pi\frac{-h+k+l}{3}\right)\left\{\cos\pi\left[(h-k)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[i(x+y)+\frac{l}{2}\right]+\right.$$
$$\left.\cos\pi\left[(k-i)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[h(x+y)+\frac{l}{2}\right]+\cos\pi\left[(i-h)(x-y)+2lz+\frac{l}{2}\right]\cos\pi\left[k(x+y)+\frac{l}{2}\right]\right\}$$

$B=0$

$F(hkl)$ relationships as for No. 165.

$\begin{cases}-h+k+l=3n\\ l=2n\end{cases}$	$A=12\{\cos\pi[(h-k)(x-y)+2lz]\cos\pi i(x+y)+\cos\pi[(k-i)(x-y)+2lz]\cos\pi h(x+y)+$
	$\cos\pi[(i-h)(x-y)+2lz]\cos\pi k(x+y)\}$
$\begin{cases}-h+k+l=3n\\ l=2n+1\end{cases}$	$A=12\{\sin\pi[(h-k)(x-y)+2lz]\sin\pi i(x+y)+\sin\pi[(k-i)(x-y)+2lz]\sin\pi h(x+y)+$
	$\sin\pi[(i-h)(x-y)+2lz]\sin\pi k(x+y)\}$
	$A=B=0$ if $h=-k$ (or $k=-i$ or $i=-h$)
$-h+k+l=3n\pm 1$	$A=B=0$

$\rho(XYZ)$ as for No. 147.

No. 168 $P6$ C_{6}^{1}

Origin on 6. | x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},z$; $y,y-x,z$; $x-y,x,z$ |

$A=2\cos 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)\}$

$B=2\sin 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)\}$ $=0$ if $l=0$

$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(h\bar{k}\bar{l})|=|F(kil)|\neq|F(\bar{h}kl)|\neq|F(khl)|$; $\quad|F(\bar{h}kl)|=|F(h\bar{k}l)|$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(h\bar{k}\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)\neq\alpha(khl)$; $\quad\alpha(\bar{h}kl)=(h\bar{k}l)$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^{\infty}\sum_0^{\infty}\sum_0^{\infty}\{|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\}$$

$P6_1$
C_6^2

No. 169

Enantiomorphous to $P6_5$; Origin on 6_1.

$|\ x,y,z;\ \bar{y},x-y,\tfrac{1}{3}+z;\ y-x,\bar{x},\tfrac{2}{3}+z;\ \bar{x},\bar{y},\tfrac{1}{2}+z;\ y,y-x,\tfrac{5}{6}+z;\ x-y,x,\tfrac{1}{3}+z\ |$

$$A=2\left\{\cos 2\pi\left(hx+ky+\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{l}{4}\right)+\cos 2\pi\left(kx+iy+\frac{l}{4}\right)\cos 2\pi\left(lz+\frac{l}{12}\right)+\cos 2\pi\left(ix+hy-\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{l}{12}\right)\right\}$$

$$B=2\left\{\cos 2\pi\left(hx+ky+\frac{l}{4}\right)\sin 2\pi\left(lz-\frac{l}{4}\right)+\cos 2\pi\left(kx+iy+\frac{l}{4}\right)\sin 2\pi\left(lz+\frac{l}{12}\right)+\cos 2\pi\left(ix+hy-\frac{l}{4}\right)\sin 2\pi\left(lz-\frac{l}{12}\right)\right\}$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|=|F(kil)|\neq|F(\bar{h}kl)|\neq|F(khl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|$$

$l=6n$

$A=2\cos 2\pi lz[\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)]$

$B=2\sin 2\pi lz[\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)]$ $=0$ if $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l=6n+1$

$A=-2\{\sin 2\pi(hx+ky)\sin 2\pi lz+\sin 2\pi(kx+iy)\sin 2\pi(lz+\tfrac{1}{3})+\sin 2\pi(ix+hy)\sin 2\pi(lz-\tfrac{1}{3})\}$

$B=2\{\sin 2\pi(hx+ky)\cos 2\pi lz+\sin 2\pi(kx+iy)\cos 2\pi(lz+\tfrac{1}{3})+\sin 2\pi(ix+hy)\cos 2\pi(lz-\tfrac{1}{3})\}$

$A=B=0$ if $h=k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)+\tfrac{2}{3}\pi\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$

$l=6n+2$

$A=2\{\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(kx+iy)\cos 2\pi(lz-\tfrac{1}{3})+\cos 2\pi(ix+hy)\cos 2\pi(lz+\tfrac{1}{3})\}$

$B=2\{\cos 2\pi(hx+ky)\sin 2\pi lz+\cos 2\pi(kx+iy)\sin 2\pi(lz-\tfrac{1}{3})+\cos 2\pi(ix+hy)\sin 2\pi(lz+\tfrac{1}{3})\}$

$A=B=0$ if $h=k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)-\tfrac{2}{3}\pi\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l=6n+3$

$A=-2\sin 2\pi lz[\sin 2\pi(hx+ky)+\sin 2\pi(kx+iy)+\sin 2\pi(ix+hy)]$

$B=2\cos 2\pi lz[\sin 2\pi(hx+ky)+\sin 2\pi(kx+iy)+\sin 2\pi(ix+hy)]$

$A=B=0$ if $h=k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$

$l=6n+4$

$A=2\{\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(kx+iy)\cos 2\pi(lz+\tfrac{1}{3})+\cos 2\pi(ix+hy)\cos 2\pi(lz-\tfrac{1}{3})\}$

$B=2\{\cos 2\pi(hx+ky)\sin 2\pi lz+\cos 2\pi(kx+iy)\sin 2\pi(lz+\tfrac{1}{3})+\cos 2\pi(ix+hy)\sin 2\pi(lz-\tfrac{1}{3})\}$

$A=B=0$ if $h=k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)+\tfrac{2}{3}\pi\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l=6n+5$

$A=-2\{\sin 2\pi(hx+ky)\sin 2\pi lz+\sin 2\pi(kx+iy)\sin 2\pi(lz-\tfrac{1}{3})+\sin 2\pi(ix+hy)\sin 2\pi(lz+\tfrac{1}{3})\}$

$B=2\{\sin 2\pi(hx+ky)\cos 2\pi lz+\sin 2\pi(kx+iy)\cos 2\pi(lz-\tfrac{1}{3})+\sin 2\pi(ix+hy)\cos 2\pi(lz+\tfrac{1}{3})\}$

$A=B=0$ if $h=k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)-\tfrac{2}{3}\pi\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos 2\pi(hX+kY)\cos[2\pi lZ-\alpha(hkl)]+|F(\bar{h}kl)|\cos 2\pi(hX-kY)\cos[2\pi lZ-\alpha(\bar{h}kl)]\}^{l=2n}-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\sin 2\pi(hX+kY)\sin[2\pi lZ-\alpha(hkl)]-|F(\bar{h}kl)|\sin 2\pi(hX-kY)\sin[2\pi lZ-\alpha(\bar{h}kl)]\}^{l=2n+1}\right\}$$

No. 170

$P6_5$
C_6^3

Enantiomorphous to $P6_1$; Origin on 6_5.

| x,y,z; $\bar{y},x-y,\frac{2}{3}+z$; $y-x,\bar{x},\frac{1}{3}+z$; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,y-x,\frac{1}{6}+z$; $x-y,x,\frac{5}{6}+z$ |

$$A=2\left\{\cos 2\pi\left(hx+ky+\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{l}{4}\right)+\cos 2\pi\left(kx+iy-\frac{l}{4}\right)\cos 2\pi\left(lz-\frac{l}{12}\right)+\cos 2\pi\left(ix+hy+\frac{l}{4}\right)\cos 2\pi\left(lz+\frac{l}{12}\right)\right\}$$

$$B=2\left\{\cos 2\pi\left(hx+ky+\frac{l}{4}\right)\sin 2\pi\left(lz-\frac{l}{4}\right)+\cos 2\pi\left(kx+iy-\frac{l}{4}\right)\sin 2\pi\left(lz-\frac{l}{12}\right)+\cos 2\pi\left(ix+hy+\frac{l}{4}\right)\sin 2\pi\left(lz+\frac{l}{12}\right)\right\}$$

$l=6n$ $\quad A=2\cos 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)\}$

$B=2\sin 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy\}$ $=0$ if $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)$; $\alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l=6n+1$ $\quad A=-2\{\sin 2\pi(hx+ky)\sin 2\pi lz+\sin 2\pi(kx+iy)\sin 2\pi(lz-\frac{1}{3})+\sin 2\pi(ix+hy)\sin 2\pi(lz+\frac{1}{3})\}$

$B=2\{\sin 2\pi(hx+ky)\cos 2\pi lz+\sin 2\pi(kx+iy)\cos 2\pi(lz-\frac{1}{3})+\sin 2\pi(ix+hy)\cos 2\pi(lz+\frac{1}{3})\}$

$A=B=0$ if $h=k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)-\frac{2}{3}\pi\neq\alpha(\bar{h}kl)$; $\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$

$l=6n+2$ $\quad A=2\{\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(kx+iy)\cos 2\pi(lz+\frac{1}{3})+\cos 2\pi(ix+hy)\cos 2\pi(lz-\frac{1}{3})\}$

$B=2\{\cos 2\pi(hx+ky)\sin 2\pi lz+\cos 2\pi(kx+iy)\sin 2\pi(lz+\frac{1}{3})+\cos 2\pi(ix+hy)\sin 2\pi(lz-\frac{1}{3})\}$

$A=B=0$ if $h=k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)+\frac{2}{3}\pi\neq\alpha(\bar{h}kl)$; $\alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l=6n+3$ $\quad A=-2\sin 2\pi lz\{\sin 2\pi(hx+ky)+\sin 2\pi(kx+iy)+\sin 2\pi(ix+hy)\}$

$B=2\cos 2\pi lz\{\sin 2\pi(hx+ky)+\sin 2\pi(kx+iy)+\sin 2\pi(ix+hy)\}$

$A=B=0$ if $h=k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)$; $\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$

$l=6n+4$ $\quad A=2\{\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(kx+iy)\cos 2\pi(lz-\frac{1}{3})+\cos 2\pi(ix+hy)\cos 2\pi(lz+\frac{1}{3})\}$

$B=2\{\cos 2\pi(hx+ky)\sin 2\pi lz+\cos 2\pi(kx+iy)\sin 2\pi(lz-\frac{1}{3})+\cos 2\pi(ix+hy)\sin 2\pi(lz+\frac{1}{3})\}$

$A=B=0$ if $h=k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)-\frac{2}{3}\pi\neq\alpha(\bar{h}kl)$; $\alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l=6n+5$ $\quad A=-2\{\sin 2\pi(hx+ky)\sin 2\pi lz+\sin 2\pi(kx+iy)\sin 2\pi(lz+\frac{1}{3})+\sin 2\pi(ix+hy)\sin 2\pi(lz-\frac{1}{3})\}$

$B=2\{\sin 2\pi(hx+ky)\cos 2\pi lz+\sin 2\pi(kx+iy)\cos 2\pi(lz+\frac{1}{3})+\sin 2\pi(ix+hy)\cos 2\pi(lz-\frac{1}{3})\}$

$A=B=0$ if $h=k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)+\frac{2}{3}\pi\neq\alpha(\bar{h}kl)$; $\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$

$|F(hkl)|$ relationships and $\rho(XYZ)$ as for No. 169.

$P6_2$ C_6^4

No. 171

Enantiomorphous to $P6_4$; Origin on 6_2.

| $x,y,z;\ \bar{y},x-y,\frac{2}{3}+z;\ y-x,\bar{x},\frac{1}{3}+z;\ \bar{x},\bar{y},z;\ y,y-x,\frac{2}{3}+z;\ x-y,x,\frac{1}{3}+z$ |

$$A=2\left\{\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(kx+iy)\cos 2\pi\left(lz-\frac{l}{3}\right)+\cos 2\pi(ix+hy)\cos 2\pi\left(lz+\frac{l}{3}\right)\right\}$$

$$B=2\left\{\cos 2\pi(hx+ky)\sin 2\pi lz+\cos 2\pi(kx+iy)\sin 2\pi\left(lz-\frac{l}{3}\right)+\cos 2\pi(ix+hy)\sin 2\pi\left(lz+\frac{l}{3}\right)\right\}$$

$l=3n$ $\quad A=2\cos 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)\}$

$B=2\sin 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)\}$ $=0$ if $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)$; $\quad\alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l=3n\pm 1$ $\quad A=2\{\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(kx+iy)\cos 2\pi(lz\mp\frac{1}{3})+\cos 2\pi(ix+hy)\cos 2\pi(lz\pm\frac{1}{3})\}$

$B=2\{\cos 2\pi(hx+ky)\sin 2\pi lz+\cos 2\pi(kx+iy)\sin 2\pi(lz\mp\frac{1}{3})+\cos 2\pi(ix+hy)\sin 2\pi(lz\pm\frac{1}{3})\}$

$A=B=0$ if $h=k=0$ $\quad\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)\mp\frac{2}{3}\pi\neq\alpha(\bar{h}kl)$; $\quad\alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$|F(hkl)|$ relationships and $\rho(XYZ)$ as for No. 168.

$P6_4$ C_6^5

No. 172

Enantiomorphous to $P6_2$; Origin on 6_4.

| $x,y,z;\ \bar{y},x-y,\frac{1}{3}+z;\ y-x,\bar{x},\frac{2}{3}+z;\ \bar{x},\bar{y},z;\ y,y-x,\frac{1}{3}+z;\ x-y,x,\frac{2}{3}+z$ |

$$A=2\left\{\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(kx+iy)\cos 2\pi\left(lz+\frac{l}{3}\right)+\cos 2\pi(ix+hy)\cos 2\pi\left(lz-\frac{l}{3}\right)\right\}$$

$$B=2\left\{\cos 2\pi(hx+ky)\sin 2\pi lz+\cos 2\pi(kx+iy)\sin 2\pi\left(lz+\frac{l}{3}\right)+\cos 2\pi(ix+hy)\sin 2\pi\left(lz-\frac{l}{3}\right)\right\}$$

$l=3n$ $\quad A=2\cos 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)\}$

$B=2\sin 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)\}$ $=0$ if $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)$; $\quad\alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l=3n\pm 1$ $\quad A=2\{\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(kx+iy)\cos 2\pi(lz\pm\frac{1}{3})+\cos 2\pi(ix+hy)\cos 2\pi(lz\mp\frac{1}{3})\}$

$B=2\{\cos 2\pi(hx+ky)\sin 2\pi lz+\cos 2\pi(kx+iy)\sin 2\pi(lz\pm\frac{1}{3})+\cos 2\pi(ix+hy)\sin 2\pi(lz\mp\frac{1}{3})\}$

$A=B=0$ if $h=k=0$ $\quad\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)\pm\frac{2}{3}\pi\neq\alpha(\bar{h}kl)$; $\quad\alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$|F(hkl)|$ relationships and $\rho(XYZ)$ as for No. 168.

No. 173 $P6_3$ C_6^6

Origin on 6_3. | x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,y-x,\frac{1}{2}+z$; $x-y,x,\frac{1}{2}+z$ |

$$A=2\cos 2\pi\left(lz-\frac{l}{4}\right)\left\{\cos 2\pi\left(hx+ky+\frac{l}{4}\right)+\cos 2\pi\left(kx+iy+\frac{l}{4}\right)+\cos 2\pi\left(ix+hy+\frac{l}{4}\right)\right\}$$

$$B=2\sin 2\pi\left(lz-\frac{l}{4}\right)\left\{\cos 2\pi\left(hx+ky+\frac{l}{4}\right)+\cos 2\pi\left(kx+iy+\frac{l}{4}\right)+\cos 2\pi\left(ix+hy+\frac{l}{4}\right)\right\}$$

$l=2n$ $\quad A=2\cos 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)\}$

$B=2\sin 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)\}$ $=0$ if $l=0$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)$; $\quad\alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l=2n+1$ $\quad A=-2\sin 2\pi lz\{\sin 2\pi(hx+ky)+\sin 2\pi(kx+iy)+\sin 2\pi(ix+hy)\}$

$B=2\cos 2\pi lz\{\sin 2\pi(hx+ky)+\sin 2\pi(kx+iy)+\sin 2\pi(ix+hy)\}$

$A=B=0$ if $h=k=0$ $\quad\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)$; $\quad\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$

$|F(hkl)|$ relationships and $\rho(XYZ)$ as for No. 169.

No. 174 $P\bar{6}$ C_{3h}^1

Origin at $\bar{6}$ $(=3/m)$. | x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $x,y,\bar{z}$; $\bar{y},x-y,\bar{z}$; $y-x,\bar{x},\bar{z}$ |

$A=2\cos 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)\}$

$B=2\cos 2\pi lz\{\sin 2\pi(hx+ky)+\sin 2\pi(kx+iy)+\sin 2\pi(ix+hy)\}$ $=0$ if $h=k=0$

$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|=|F(kil)|\neq|F(\bar{h}kl)|\neq|F(khl)|$; $\quad|F(\bar{h}kl)|=|F(h\bar{k}l)|$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(hk\bar{l})=\alpha(kil)\neq\alpha(\bar{h}kl)\neq\alpha(khl)$; $\quad\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{|F(hkl)|\cos[2\pi(hX+kY)-\alpha(hkl)]+|F(\bar{h}kl)|\cos[2\pi(hX-kY)+\alpha(\bar{h}kl)]\}\cos 2\pi lZ$$

No. 175 $P6/m$ C_{6h}^1

Origin at centre on 6 (6/m). $\pm$ | x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},z$; $y,y-x,z$; $x-y,x,z$ |

$A=4\cos 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)\}$; $\quad B=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})=F(kil)\neq F(\bar{h}kl)\neq F(khl)$; $\quad F(\bar{h}kl)=F(h\bar{k}l)$

$$\rho(XYZ)=\frac{4}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty\{F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(hX-kY)\}\cos 2\pi lZ$$

$P6_3/m$ C_{6h}^2

No. 176

Origin at centre on 6_3 ($\bar{3}$). $\pm$ | x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,y-x,\frac{1}{2}+z$; $x-y,x,\frac{1}{2}+z$ |

$$A=4\cos 2\pi\left(lz-\frac{l}{4}\right)\left\{\cos 2\pi\left(hx+ky+\frac{l}{4}\right)+\cos 2\pi\left(kx+iy+\frac{l}{4}\right)+\cos 2\pi\left(ix+hy+\frac{l}{4}\right)\right\};\quad B=0$$

$l=2n$ $\quad A=4\cos 2\pi lz\{\cos 2\pi(hx+ky)+\cos 2\pi(kx+iy)+\cos 2\pi(ix+hy)\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})=F(kil)\neq F(\bar{h}kl)\neq F(khl)$; $\quad F(\bar{h}kl)=F(h\bar{k}l)$

$l=2n+1$ $\quad A=-4\sin 2\pi lz\{\sin 2\pi(hx+ky)+\sin 2\pi(kx+iy)+\sin 2\pi(ix+hy)\}$

$A=B=0$ if $h=k=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(hk\bar{l})=F(kil)\neq F(\bar{h}kl)\neq F(khl)$; $\quad F(\bar{h}kl)=-F(h\bar{k}l)$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}[F(hkl)\cos 2\pi(hX+kY)+F(\bar{h}kl)\cos 2\pi(hX-kY)]\cos 2\pi lZ+\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}[F(\bar{h}kl)\sin 2\pi(hX-kY)-F(hkl)\sin 2\pi(hX+kY)]\sin 2\pi lZ\right\}$$

$P622$ D_6^1

No. 177

Origin at 622.

x,y,z; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{x},\bar{y},z$; $y,y-x,z$; $x-y,x,z$;
$y,x,\bar{z}$; $\bar{x},y-x,\bar{z}$; $x-y,\bar{y},\bar{z}$; $\bar{y},\bar{x},\bar{z}$; $x,x-y,\bar{z}$; $y-x,y,\bar{z}$

$$A=4\cos 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+$$
$$\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$$
$$B=4\sin 2\pi lz\{\sin \pi i(x+y)\sin \pi(h-k)(x-y)+\sin \pi h(x+y)\sin \pi(k-i)(x-y)+\sin \pi k(x+y)\sin \pi(i-h)(x-y)\}$$

$B=0$ if $l=0$ or $h=\pm k$ (or $k=\pm i$ or $i=\pm h$)

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|=|F(kil)|=|F(khl)|\neq|F(\bar{h}kl)|;$$
$$|F(\bar{h}kl)|=|F(h\bar{k}l)|$$
$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)=-\alpha(khl)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$$

$\rho(XYZ)$ as for No. 168.

$P6_122$ D_6^2

No. 178

Enantiomorphous to $P6_522$; Origin at 6_121.

x,y,z;	$\bar{y},x-y,\frac{1}{3}+z$;	$y-x,\bar{x},\frac{2}{3}+z$;	$\bar{x},\bar{y},\frac{1}{2}+z$;	$y,y-x,\frac{5}{6}+z$;	$x-y,x,\frac{1}{6}+z$;
$y,x,\frac{1}{3}-z$;	$\bar{x},y-x,\frac{2}{3}-z$;	$x-y,\bar{y},\bar{z}$;	$\bar{y},\bar{x},\frac{5}{6}-z$;	$x,x-y,\frac{1}{6}-z$;	$y-x,y,\frac{1}{2}-z$

$$A=4\left\{\cos 2\pi\left(lz+\frac{l}{4}\right)\cos \pi\left[(i-k)y+\frac{l}{2}\right]\cos \pi h(2x-y)+\cos 2\pi\left(lz+\frac{l}{12}\right)\cos \pi\left[(i-k)(y-x)+\frac{l}{2}\right]\cos \pi h(x+y)+\right.$$
$$\left.\cos 2\pi\left(lz-\frac{l}{12}\right)\cos \pi\left[(i-k)x-\frac{l}{2}\right]\cos \pi h(x-2y)\right\}$$
$$B=4\left\{\sin 2\pi\left(lz+\frac{l}{4}\right)\sin \pi\left[(i-k)y+\frac{l}{2}\right]\sin \pi h(2x-y)+\sin 2\pi\left(lz+\frac{l}{12}\right)\sin \pi\left[(i-k)(y-x)+\frac{l}{2}\right]\sin \pi h(x+y)+\right.$$
$$\left.\sin 2\pi\left(lz-\frac{l}{12}\right)\sin \pi\left[(i-k)x-\frac{l}{2}\right]\sin \pi h(x-2y)\right\}$$

or

$$A=2\left\{\cos 2\pi\left(lz+\frac{l}{4}\right)\left[\cos 2\pi\left(hx+ky-\frac{l}{4}\right)+\cos 2\pi\left(hx+iy+\frac{l}{4}\right)\right]+\right.$$
$$\cos 2\pi\left(lz+\frac{7l}{12}\right)\left[\cos 2\pi\left(kx+iy-\frac{l}{4}\right)+\cos 2\pi\left(ix+ky+\frac{l}{4}\right)\right]+$$
$$\left.\cos 2\pi\left(lz-\frac{l}{12}\right)\left[\cos 2\pi\left(ix+hy-\frac{l}{4}\right)+\cos 2\pi\left(kx+hy+\frac{l}{4}\right)\right]\right\}$$

$$B=2\left\{\sin 2\pi\left(lz+\frac{l}{4}\right)\left[\cos 2\pi\left(hx+ky-\frac{l}{4}\right)-\cos 2\pi\left(hx+iy+\frac{l}{4}\right)\right]+\right.$$
$$\sin 2\pi\left(lz+\frac{7l}{12}\right)\left[\cos 2\pi\left(kx+iy-\frac{l}{4}\right)-\cos 2\pi\left(ix+ky+\frac{l}{4}\right)\right]+$$
$$\left.\sin 2\pi\left(lz-\frac{l}{12}\right)\left[\cos 2\pi\left(ix+hy-\frac{l}{4}\right)-\cos 2\pi\left(kx+hy+\frac{l}{4}\right)\right]\right\}$$

$|F(hkl)|$ relationships as for No. 177.

$l=6n$

$$A=4\cos 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$$

$$B=4\sin 2\pi lz\{\sin \pi i(x+y)\sin \pi(h-k)(x-y)+\sin \pi h(x+y)\sin \pi(k-i)(x-y)+\sin \pi k(x+y)\sin \pi(i-h)(x-y)\}$$

$B=0$ if $l=0$ or $h=\pm k$ (or $k=\pm i$ or $i=\pm h$) $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)=-\alpha(khl)\neq\alpha(\bar{h}kl)$; $\alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l=6n+1$

$$A=-2\{\sin 2\pi lz[\sin 2\pi(hx+ky)-\sin 2\pi(hx+iy)]+\sin 2\pi(lz+\tfrac{1}{3})[\sin 2\pi(kx+iy)-\sin 2\pi(ix+ky)]+\sin 2\pi(lz-\tfrac{1}{3})[\sin 2\pi(ix+hy)-\sin 2\pi(kx+hy)]\}$$

$$B=2\{\cos 2\pi lz[\sin 2\pi(hx+ky)+\sin 2\pi(hx+iy)]+\cos 2\pi(lz+\tfrac{1}{3})[\sin 2\pi(kx+iy)+\sin 2\pi(ix+ky)]+\cos 2\pi(lz-\tfrac{1}{3})[\sin 2\pi(ix+hy)+\sin 2\pi(kx+hy)]\}$$

$A=0$ if $k=i$; $\quad B=0$ if $k=-i$ (i.e. if $h=0$)

$A=B=0$ if $h=k=0$ (Note. If $l=6n+1$, $-l=6n+5$)

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)+\tfrac{2}{3}\pi=-\alpha(khl)-\frac{\pi}{3}\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$$

$l=6n+2$

$$A=2\{\cos 2\pi lz[\cos 2\pi(hx+ky)+\cos 2\pi(hx+iy)]+\cos 2\pi(lz-\tfrac{1}{3})[\cos 2\pi(kx+iy)+\cos 2\pi(ix+ky)]+\cos 2\pi(lz+\tfrac{1}{3})[\cos 2\pi(ix+hy)+\cos 2\pi(kx+hy)]\}$$

$$B=2\{\sin 2\pi lz[\cos 2\pi(hx+ky)-\cos 2\pi(hx+iy)]+\sin 2\pi(lz-\tfrac{1}{3})[\cos 2\pi(kx+iy)-\cos 2\pi(ix+ky)]+\sin 2\pi(lz+\tfrac{1}{3})[\cos 2\pi(ix+hy)-\cos 2\pi(kx+hy)]\}$$

$B=0$ if $k=\pm i$; $\quad A=B=0$ if $h=k=0$ (Note. $-l=6n+4$)

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)-\tfrac{2}{3}\pi=-\alpha(khl)-\tfrac{2}{3}\pi\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$$

$l=6n+3$

$$A=-4\sin 2\pi lz\{\cos \pi i(x+y)\sin \pi(h-k)(x-y)+\cos \pi h(x+y)\sin \pi(k-i)(x-y)+\cos \pi k(x+y)\sin \pi(i-h)(x-y)\}$$

$$B=-4\cos 2\pi lz\{\sin \pi i(x+y)\cos \pi(h-k)(x-y)+\sin \pi h(x+y)\cos \pi(k-i)(x-y)+\sin \pi k(x+y)\cos \pi(i-h)(x-y)\}$$

$A=0$ if $h=k$ (etc.); $\quad B=0$ if $h=-k$ (etc.)

$A=B=0$ if $h=k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)=\pi-\alpha(khl)\neq\alpha(\bar{h}kl)$; $\quad \alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$

$l = 6n + 4$ $A=2\{\cos 2\pi lz[\cos 2\pi(hx+ky)+\cos 2\pi(hx+iy)]+\cos 2\pi(lz+\frac{1}{3})[\cos 2\pi(kx+iy)+\cos 2\pi(ix+ky)]+$
$\cos 2\pi(lz-\frac{1}{3})[\cos 2\pi(ix+hy)+\cos 2\pi(kx+hy)]\}$

$B=2\{\sin 2\pi lz[\cos 2\pi(hx+ky)-\cos 2\pi(hx+iy)]+\sin 2\pi(lz+\frac{1}{3})[\cos 2\pi(kx+iy)-\cos 2\pi(ix+ky)]+$
$\sin 2\pi(lz-\frac{1}{3})[\cos 2\pi(ix+hy)-\cos 2\pi(kx+hy)]\}$

$B=0$ if $k=\pm i$; $A=B=0$ if $h=k=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\frac{2}{3}\pi+\alpha(kil)=\frac{2}{3}\pi-\alpha(khl)\neq\alpha(\bar{h}kl)$;
$\alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l = 6n + 5$ $A=-2\{\sin 2\pi lz[\sin 2\pi(hx+ky)-\sin 2\pi(hx+iy)]+\sin 2\pi(lz-\frac{1}{3})[\sin 2\pi(kx+iy)-\sin 2\pi(ix+ky)]+$
$\sin 2\pi(lz+\frac{1}{3})[\sin 2\pi(ix+hy)-\sin 2\pi(kx+hy)]\}$

$B=2\{\cos 2\pi lz[\sin 2\pi(hx+ky)+\sin 2\pi(hx+iy)]+\cos 2\pi(lz-\frac{1}{3})[\sin 2\pi(kx+iy)+\sin 2\pi(ix+ky)]+$
$\cos 2\pi(lz+\frac{1}{3})[\sin 2\pi(ix+hy)+\sin 2\pi(kx+hy)]\}$

$A=0$ if $k=i$; $B=0$ if $k=-i$;

$A=B=0$ if $h=k=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)-\frac{2}{3}\pi=\frac{\pi}{3}-\alpha(khl)\neq\alpha(\bar{h}kl)$; $\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$

$\rho(XYZ)$ as for No. 169.

$P6_522$ D_6^3

No. 179

Enantiomorphous to $P6_122$; Origin at 6_521.

x,y,z;	$\bar{y},x-y,\frac{2}{3}+z$;	$y-x,\bar{x},\frac{1}{3}+z$;	$y,x,\frac{2}{3}-z$;	$\bar{x},y-x,\frac{1}{3}-z$;	$x-y,\bar{y},\bar{z}$;
$\bar{x},\bar{y},\frac{1}{2}+z$;	$y,y-x,\frac{1}{6}+z$;	$x-y,x,\frac{5}{6}+z$;	$\bar{y},\bar{x},\frac{1}{6}-z$;	$x,x-y,\frac{5}{6}-z$;	$y-x,y,\frac{1}{2}-z$

$$A=2\left\{\cos 2\pi\left(lz+\frac{l}{4}\right)\left[\cos 2\pi\left(hx+ky-\frac{l}{4}\right)+\cos 2\pi\left(hx+iy+\frac{l}{4}\right)\right]+\right.$$
$$\cos 2\pi\left(lz-\frac{l}{12}\right)\left[\cos 2\pi\left(kx+iy-\frac{l}{4}\right)+\cos 2\pi\left(ix+ky+\frac{l}{4}\right)\right]+$$
$$\left.\cos 2\pi\left(lz+\frac{7l}{12}\right)\left[\cos 2\pi\left(ix+hy-\frac{l}{4}\right)+\cos 2\pi\left(kx+hy+\frac{l}{4}\right)\right]\right\}$$

$$B=2\left\{\sin 2\pi\left(lz+\frac{l}{4}\right)\left[\cos 2\pi\left(hx+ky-\frac{l}{4}\right)-\cos 2\pi\left(hx+iy+\frac{l}{4}\right)\right]+\right.$$
$$\sin 2\pi\left(lz-\frac{l}{12}\right)\left[\cos 2\pi\left(kx+iy-\frac{l}{4}\right)-\cos 2\pi\left(ix+ky+\frac{l}{4}\right)\right]+$$
$$\left.\sin 2\pi\left(lz+\frac{7l}{12}\right)\left[\cos 2\pi\left(ix+hy-\frac{l}{4}\right)-\cos 2\pi\left(kx+hy+\frac{l}{4}\right)\right]\right\}$$

$l = 6n$ As for $P6_122$, $l = 6n$

$l = 6n + 1$ As for $P6_122$, $l = 6n + 5$

$l = 6n + 2$ As for $P6_122$, $l = 6n + 4$

$l = 6n + 3$ As for $P6_122$, $l = 6n + 3$

$l = 6n + 4$ As for $P6_122$, $l = 6n + 2$

$l = 6n + 5$ As for $P6_122$, $l = 6n + 1$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 178.

No. 180

$P6_222$
D_6^4

Enantiomorphous to $P6_422$; Origin at 6_222.

x,y,z; $\bar{y},x-y,\frac{2}{3}+z$; $y-x,\bar{x},\frac{1}{3}+z$; $y,x,\frac{2}{3}-z$; $x,x-y,\frac{1}{3}-z$; $x-y,\bar{y},\bar{z}$;	
$\bar{x},\bar{y},z$; $y,y-x,\frac{2}{3}+z$; $x-y,x,\frac{1}{3}+z$; $\bar{y},\bar{x},\frac{2}{3}-z$; $\bar{x},y-x,\frac{1}{3}-z$; $y-x,y,\bar{z}$	

$$A=2\left\{\cos 2\pi lz[\cos 2\pi(hx+ky)+\cos 2\pi(hx+iy)]+\cos 2\pi\left(lz-\frac{l}{3}\right)[\cos 2\pi(kx+iy)+\cos 2\pi(ix+ky)]+\right.$$
$$\left.\cos 2\pi\left(lz+\frac{l}{3}\right)[\cos 2\pi(ix+hy)+\cos 2\pi(kx+hy)]\right\}$$

$$B=2\left\{\sin 2\pi lz[\cos 2\pi(hx+ky)-\cos 2\pi(hx+iy)]+\sin 2\pi\left(lz-\frac{l}{3}\right)[\cos 2\pi(kx+iy)-\cos 2\pi(ix+ky)]+\right.$$
$$\left.\sin 2\pi\left(lz+\frac{l}{3}\right)[\cos 2\pi(ix+hy)-\cos 2\pi(kx+hy)]\right\}$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|=|F(kil)|=|F(khl)|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|.$$
$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$$

$l=3n$

$$A=4\cos 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+$$
$$\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$$
$$B=4\sin 2\pi lz\{\sin \pi i(x+y)\sin \pi(h-k)(x-y)+\sin \pi h(x+y)\sin \pi(k-i)(x-y)+$$
$$\sin \pi k(x+y)\sin \pi(i-h)(x-y)\}$$

$B=0$ if $l=0$ or $h=\pm k$ (or $k=\pm i$ or $i=\pm h$) $\qquad \alpha(hkl)=\alpha(kil)=-\alpha(khl)$

$l=3n\pm 1$

$$A=4\{\cos 2\pi lz\cos \pi h(2x-y)\cos \pi(i-k)y+\cos 2\pi(lz\mp\tfrac{1}{3})\cos \pi h(x+y)\cos \pi(i-k)(y-x)+$$
$$\cos 2\pi(lz\pm\tfrac{1}{3})\cos \pi h(x-2y)\cos \pi(i-k)x\}$$
$$B=4\{\sin 2\pi lz\sin \pi h(2x-y)\sin \pi(i-k)y-\sin 2\pi(lz\mp\tfrac{1}{3})\sin \pi h(x+y)\sin \pi(i-k)(y-x)+$$
$$\sin 2\pi(lz\pm\tfrac{1}{3})\sin \pi h(x-2y)\sin \pi(i-k)x\}$$

$B=0$ if $k=\pm i$; $A=B=0$ if $h=k=0$ $\qquad \alpha(hkl)=\alpha(kil)\mp\frac{2}{3}\pi=-\alpha(khl)\mp\frac{2}{3}\pi$

$\rho(XYZ)$ as for No. 168.

No. 181

$P6_422$
D_6^5

Enantiomorphous to $P6_222$; Origin at 6_422.

x,y,z; $\bar{y},x-y,\frac{1}{3}+z$; $y-x,\bar{x},\frac{2}{3}+z$; $y,x,\frac{1}{3}-z$; $x,x-y,\frac{2}{3}-z$; $x-y,\bar{y},\bar{z}$;	
$\bar{x},\bar{y},z$; $y,y-x,\frac{1}{3}+z$; $x-y,x,\frac{2}{3}+z$; $\bar{y},\bar{x},\frac{1}{3}-z$; $\bar{x},y-x,\frac{2}{3}-z$; $y-x,y,\bar{z}$	

$$A=2\left\{\cos 2\pi lz[\cos 2\pi(hx+ky)+\cos 2\pi(hx+iy)]+\cos 2\pi\left(lz+\frac{l}{3}\right)[\cos 2\pi(kx+iy)+\cos 2\pi(ix+ky)]+\right.$$
$$\left.\cos 2\pi\left(lz-\frac{l}{3}\right)[\cos 2\pi(ix+hy)+\cos 2\pi(kx+hy)]\right\}$$

$$B=2\left\{\sin 2\pi lz[\cos 2\pi(hx+ky)-\cos 2\pi(hx+iy)]+\sin 2\pi\left(lz+\frac{l}{3}\right)[\cos 2\pi(kx+iy)-\cos 2\pi(ix+ky)]+\right.$$
$$\left.\sin 2\pi\left(lz-\frac{l}{3}\right)[\cos 2\pi(ix+hy)-\cos 2\pi(kx+hy)]\right\}$$

$l = 3n$	As for $P6_222$, $l = 3n$
$l = 3n \pm 1$	As for $P6_222$, $l = 3n \mp 1$

$|F(hkl)|$ and $\alpha(hkl)$ relationships, and $\rho(XYZ)$ as for No. 180.

$P6_322$ D_6^6

No. 182

Origin at 6_321.

$x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ \bar{x},\bar{y},\frac{1}{2}+z;\ y,y-x,\frac{1}{2}+z;\ x-y,x,\frac{1}{2}+z;$
$y,x,\bar{z};\ \bar{x},y-x,\bar{z};\ x-y,\bar{y},\bar{z};\ \bar{y},\bar{x},\frac{1}{2}-z;\ x,x-y,\frac{1}{2}-z;\ y-x,y,\frac{1}{2}-z$

$$A=4\cos 2\pi\left(lz+\frac{l}{4}\right)\left\{\cos \pi i(x+y)\cos \pi\left[(h-k)(x-y)-\frac{l}{2}\right]+\cos \pi h(x+y)\cos \pi\left[(k-i)(x-y)-\frac{l}{2}\right]+\cos \pi k(x+y)\cos \pi\left[(i-h)(x-y)-\frac{l}{2}\right]\right\}$$

$$B=4\sin 2\pi\left(lz+\frac{l}{4}\right)\left\{\sin \pi i(x+y)\sin \pi\left[(h-k)(x-y)-\frac{l}{2}\right]+\sin \pi h(x+y)\sin \pi\left[(k-i)(x-y)-\frac{l}{2}\right]+\sin \pi k(x+y)\sin \pi\left[(i-h)(x-y)-\frac{l}{2}\right]\right\}$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|=|F(kil)|=|F(khl)|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|$$

$l = 2n$

$$A=4\cos 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$$

$$B=4\sin 2\pi lz\{\sin \pi i(x+y)\sin \pi(h-k)(x-y)+\sin \pi h(x+y)\sin \pi(k-i)(x-y)+\sin \pi k(x+y)\sin \pi(i-h)(x-y)\}$$

$B=0$ if $l=0$ or $h=\pm k$ (or $k=\pm i$ or $i=\pm h$)

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)=-\alpha(khl)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$$

$l = 2n + 1$

$$A=-4\sin 2\pi lz\{\cos \pi i(x+y)\sin \pi(h-k)(x-y)+\cos \pi h(x+y)\sin \pi(k-i)(x-y)+\cos \pi k(x+y)\sin \pi(i-h)(x-y)\}$$

$$B=-4\cos 2\pi lz\{\sin \pi i(x+y)\cos \pi(h-k)(x-y)+\sin \pi h(x+y)\cos \pi(k-i)(x-y)+\sin \pi k(x+y)\cos \pi(i-h)(x-y)\}$$

$A=0$ if $h=k$ (etc.); $B=0$ if $h=-k$ (etc.)

$A=B=0$ if $h=k=0$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)=\pi-\alpha(khl)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$$

$\rho(XYZ)$ as for No. 169.

No. 183 $P6mm$ C_{6v}^{1}

Origin on $6mm$.

$$\left|\begin{array}{l} x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ \bar{x},\bar{y},z;\ y,y-x,z;\ x-y,x,z; \\ y,x,z;\ \bar{x},y-x,z;\ x-y,\bar{y},z;\ \bar{y},\bar{x},z;\ x,x-y,z;\ y-x,y,z \end{array}\right|$$

$$A=4\cos 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$$

$$B=4\sin 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$$

$B=0$ if $l=0$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|$$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)=\alpha(khl)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$$

$|F(hkl)|$ relationships and $\rho(XYZ)$ as for No. 177.

No. 184 $P6cc$ C_{6v}^{2}

Origin on 6.

$$\left|\begin{array}{l} x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ y,x,\tfrac{1}{2}+z;\ \bar{x},y-x,\tfrac{1}{2}+z;\ x-y,\bar{y},\tfrac{1}{2}+z; \\ \bar{x},\bar{y},z;\ y,y-x,z;\ x-y,x,z;\ \bar{y},\bar{x},\tfrac{1}{2}+z;\ x,x-y,\tfrac{1}{2}+z;\ y-x,y,\tfrac{1}{2}+z \end{array}\right|$$

$$A=4\cos 2\pi lz\left\{\cos \pi\left[i(x+y)+\frac{l}{2}\right]\cos \pi\left[(h-k)(x-y)+\frac{l}{2}\right]+\cos \pi\left[h(x+y)+\frac{l}{2}\right]\cos \pi\left[(k-i)(x-y)+\frac{l}{2}\right]+\cos \pi\left[k(x+y)+\frac{l}{2}\right]\cos \pi\left[(i-h)(x-y)+\frac{l}{2}\right]\right\}$$

$$B=4\sin 2\pi lz\left\{\cos \pi\left[i(x+y)+\frac{l}{2}\right]\cos \pi\left[(h-k)(x-y)+\frac{l}{2}\right]+\cos \pi\left[h(x+y)+\frac{l}{2}\right]\cos \pi\left[(k-i)(x-y)+\frac{l}{2}\right]+\cos \pi\left[k(x+y)+\frac{l}{2}\right]\cos \pi\left[(i-h)(x-y)+\frac{l}{2}\right]\right\}$$

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)$$

$l=2n$

$$A=4\cos 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$$

$$B=4\sin 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$$

$B=0$ if $l=0$ $\qquad \alpha(hkl)=\alpha(khl)$

$l=2n+1$

$$A=4\cos 2\pi lz\{\sin \pi i(x+y)\sin \pi(h-k)(x-y)+\sin \pi h(x+y)\sin \pi(k-i)(x-y)+\sin \pi k(x+y)\sin \pi(i-h)(x-y)\}$$

$$B=4\sin 2\pi lz\{\sin \pi i(x+y)\sin \pi(h-k)(x-y)+\sin \pi h(x+y)\sin \pi(k-i)(x-y)+\sin \pi k(x+y)\sin \pi(i-h)(x-y)\}$$

$A=B=0$ if $h=\pm k$ (or $k=\pm i$ or $i=\pm h$) $\qquad \alpha(hkl)=\pi+\alpha(khl)$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 177.

$P6_3cm$ C_{6v}^3

No. 185

Origin on 6_3 $(3m)$.

$x,y,z;$ $\bar{y},x-y,z;$ $y-x,\bar{x},z;$ $\bar{x},\bar{y},\frac{1}{2}+z;$ $y,y-x,\frac{1}{2}+z;$ $x-y,x,\frac{1}{2}+z;$
$y,x,z;$ $\bar{x},y-x,z;$ $x-y,\bar{y},z;$ $\bar{y},\bar{x},\frac{1}{2}+z;$ $x,x-y,\frac{1}{2}+z;$ $y-x,y,\frac{1}{2}+z$

$$A=4\cos 2\pi\left(lz+\frac{l}{4}\right)\left\{\cos\pi\left[i(x+y)+\frac{l}{2}\right]\cos\pi(h-k)(x-y)+\cos\pi\left[h(x+y)+\frac{l}{2}\right]\cos\pi(k-i)(x-y)+\cos\pi\left[k(x+y)+\frac{l}{2}\right]\cos\pi(i-h)(x-y)\right\}$$

$$B=4\sin 2\pi\left(lz+\frac{l}{4}\right)\left\{\cos\pi\left[i(x+y)+\frac{l}{2}\right]\cos\pi(h-k)(x-y)+\cos\pi\left[h(x+y)+\frac{l}{2}\right]\cos\pi(k-i)(x-y)+\cos\pi\left[k(x+y)+\frac{l}{2}\right]\cos\pi(i-h)(x-y)\right\}$$

$$|F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|=|F(kil)|=|F(khl)|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|$$

$l=2n$

$$A=4\cos 2\pi lz\{\cos\pi i(x+y)\cos\pi(h-k)(x-y)+\cos\pi h(x+y)\cos\pi(k-i)(x-y)+\cos\pi k(x+y)\cos\pi(i-h)(x-y)\}$$

$$B=4\sin 2\pi lz\{\cos\pi i(x+y)\cos\pi(h-k)(x-y)+\cos\pi h(x+y)\cos\pi(k-i)(x-y)+\cos\pi k(x+y)\cos\pi(i-h)(x-y)\}$$

$B=0$ if $l=0$ $\qquad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)=\alpha(khl)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l=2n+1$

$$A=4\sin 2\pi lz\{\sin\pi i(x+y)\cos\pi(h-k)(x-y)+\sin\pi h(x+y)\cos\pi(k-i)(x-y)+\sin\pi k(x+y)\cos\pi(i-h)(x-y)\}$$

$$B=-4\cos 2\pi lz\{\sin\pi i(x+y)\cos\pi(h-k)(x-y)+\sin\pi h(x+y)\cos\pi(k-i)(x-y)+\sin\pi k(x+y)\cos\pi(i-h)(x-y)\}$$

$A=B=0$ if $h=-k$ (or $k=-i$ or $i=-h$); $\qquad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)=\alpha(khl)\neq\alpha(\bar{h}kl);$

$\alpha(\bar{h}kl)=\pi+\alpha(h\bar{k}l)$

$\rho(XYZ)$ as for No. 169.

No. 186

$P6_3mc$ C_{6v}^4

Origin on 6_3 ($3m$).

$$\left|\begin{matrix} x,y,z; & \bar{y},x-y,z; & y-x,\bar{x},z; & \bar{x},\bar{y},\tfrac{1}{2}+z; & y,y-x,\tfrac{1}{2}+z; & x-y,x,\tfrac{1}{2}+z; \\ y,x,z; & x,x-y,z; & y-x,y,z; & y,x,\tfrac{1}{2}+z; & \bar{x},y-x,\tfrac{1}{2}+z; & x-y,\bar{y},\tfrac{1}{2}+z \end{matrix}\right|$$

$$A=4\cos 2\pi\left(lz-\frac{l}{4}\right)\left\{\cos \pi i(x+y)\cos \pi\left[(h-k)(x-y)+\frac{l}{2}\right]+\cos \pi h(x+y)\cos \pi\left[(k-i)(x-y)+\frac{l}{2}\right]+\cos \pi k(x+y)\cos \pi\left[(i-h)(x-y)+\frac{l}{2}\right]\right\}$$

$$B=4\sin 2\pi\left(lz-\frac{l}{4}\right)\left\{\cos \pi i(x+y)\cos \pi\left[(h-k)(x-y)+\frac{l}{2}\right]+\cos \pi h(x+y)\cos \pi\left[(k-i)(x-y)+\frac{l}{2}\right]+\cos \pi k(x+y)\cos \pi\left[(i-h)(x-y)+\frac{l}{2}\right]\right\}$$

$$|F(hkl)|=|F(\bar{h}\bar{k}l)|=|F(hk\bar{l})|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(h\bar{k}l)|$$

$l=2n$

$$A=4\cos 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$$

$$B=4\sin 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$$

$B=0$ if $l=0$ $\qquad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(hk\bar{l})=\alpha(kil)=\alpha(khl)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\alpha(h\bar{k}l)$

$l=2n+1$

$$A=-4\sin 2\pi lz\{\cos \pi i(x+y)\sin \pi(h-k)(x-y)+\cos \pi h(x+y)\sin \pi(k-i)(x-y)+\cos \pi k(x+y)\sin \pi(i-h)(x-y)\}$$

$$B=4\cos 2\pi lz\{\cos \pi i(x+y)\sin \pi(h-k)(x-y)+\cos \pi h(x+y)\sin \pi(k-i)(x-y)+\cos \pi k(x+y)\sin \pi(i-h)(x-y)\}$$

$A=B=0$ if $h=k$ (or $k=i$ or $i=h$) $\qquad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(hk\bar{l})=\alpha(kil)=\pi+\alpha(khl)\neq\alpha(\bar{h}kl);$
$\alpha(hkl)=\pi+\alpha(h\bar{k}l)$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 178.

No. 187

$P\bar{6}m2$ D_{3h}^1

Origin at $\bar{6}m2$.

$$\left|\begin{matrix} x,y,z; & \bar{y},x-y,z; & y-x,\bar{x},z; & x,y,\bar{z}; & \bar{y},x-y,\bar{z}; & y-x,\bar{x},\bar{z}; \\ \bar{y},\bar{x},z; & x,x-y,z; & y-x,y,z; & \bar{y},\bar{x},\bar{z}; & x,x-y,\bar{z}; & y-x,y,\bar{z} \end{matrix}\right|$$

$$A=4\cos 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$$

$$B=4\cos 2\pi lz\{\cos \pi i(x+y)\sin \pi(h-k)(x-y)+\cos \pi h(x+y)\sin \pi(k-i)(x-y)+\cos \pi k(x+y)\sin \pi(i-h)(x-y)\}$$

$B=0$ if $h=k$ (or $k=i$ or $i=h$) $\qquad |F(hkl)|=|F(\bar{h}\bar{k}\bar{l})|=|F(hk\bar{l})|=|F(kil)|=|F(khl)|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|Fh\bar{k}l)|$
$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(hkl)=\alpha(kil)=-\alpha(khl)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=-\alpha(h\bar{k}l)$

$\rho(XYZ)$ as for No. 174.

$P\bar{6}c2$ D_{3h}^{2}

No. 188

Origin at 312.

$x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ x,y,\frac{1}{2}-z;\ \bar{y},x-y,\frac{1}{2}-z;\ y-x,\bar{x},\frac{1}{2}-z;$
$\bar{y},\bar{x},\bar{z};\ x,x-y,\bar{z};\ y-x,y,\bar{z};\ \bar{y},\bar{x},\frac{1}{2}+z;\ x,x-y,\frac{1}{2}+z;\ y-x,y,\frac{1}{2}+z$

$$A=4\cos 2\pi\left(lz+\frac{l}{4}\right)\left\{\cos\pi\left[i(x+y)+\frac{l}{2}\right]\cos\pi(h-k)(x-y)+\cos\pi\left[h(x+y)+\frac{l}{2}\right]\cos\pi(k-i)(x-y)+\cos\pi\left[k(x+y)+\frac{l}{2}\right]\cos\pi(i-h)(x-y)\right\}$$

$$B=4\cos 2\pi\left(lz+\frac{l}{4}\right)\left\{\cos\pi\left[i(x+y)+\frac{l}{2}\right]\sin\pi(h-k)(x-y)+\cos\pi\left[h(x+y)+\frac{l}{2}\right]\sin\pi(k-i)(x-y)+\cos\pi\left[k(x+y)+\frac{l}{2}\right]\sin\pi(i-h)(x-y)\right\}$$

$$|F(hkl)|=|F(\bar{h}k\bar{l})|=|F(hk\bar{l})|=|F(kil)|=|F(khl)|\neq|F(\bar{h}kl)|;\quad |F(\bar{h}kl)|=|F(hk\bar{l})|$$

$l=2n$

$$A=4\cos 2\pi lz\{\cos\pi i(x+y)\cos\pi(h-k)(x-y)+\cos\pi h(x+y)\cos\pi(k-i)(x-y)+\cos\pi k(x+y)\cos\pi(i-h)(x-y)\}$$

$$B=4\cos 2\pi lz\{\cos\pi i(x+y)\sin\pi(h-k)(x-y)+\cos\pi h(x+y)\sin\pi(k-i)(x-y)+\cos\pi k(x+y)\sin\pi(i-h)(x-y)\}$$

$B=0$ if $h=k$ (or $k=i$ or $i=h$) $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(hk\bar{l})=\alpha(kil)=\alpha(khl)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=-\alpha(h\bar{k}l)$

$l=2n+1$

$$A=4\sin 2\pi lz\{\sin\pi i(x+y)\cos\pi(h-k)(x-y)+\sin\pi h(x+y)\cos\pi(k-i)(x-y)+\sin\pi k(x+y)\cos\pi(i-h)(x-y)\}$$

$$B=4\sin 2\pi lz\{\sin\pi i(x+y)\sin\pi(h-k)(x-y)+\sin\pi h(x+y)\sin\pi(k-i)(x-y)+\sin\pi k(x+y)\sin\pi(i-h)(x-y)\}$$

$B=0$ if $h=k$ (etc.); $\quad A=B=0$ if $h=-k$ (etc.)

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi+\alpha(hk\bar{l})=\alpha(kil)=-\alpha(khl)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)$$

$$\rho(XYZ)=\frac{4}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n}[|F(hkl)|\cos(2\pi hX+2\pi kY-\alpha(hkl))+|F(\bar{h}kl)|\cos(2\pi hX-2\pi kY+\alpha(\bar{h}kl))]\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{l=2n+1}[|F(hkl)|\sin(2\pi hX+2\pi kY-\alpha(hkl))-|F(\bar{h}kl)|\sin(2\pi hX-2\pi kY+\alpha(\bar{h}kl))]\sin 2\pi lZ\right\}$$

$P\bar{6}2m$ D_{3h}^{3}

No. 189

Origin at $\bar{6}2m$.

$x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ x,y,\bar{z};\ \bar{y},x-y,\bar{z};\ y-x,\bar{x},\bar{z};$
$y,x,z;\ \bar{x},y-x,z;\ x-y,\bar{y},z;\ y,x,\bar{z};\ \bar{x},y-x,\bar{z};\ x-y,\bar{y},\bar{z}$

$$A=4\cos 2\pi lz\{\cos\pi i(x+y)\cos\pi(h-k)(x-y)+\cos\pi h(x+y)\cos\pi(k-i)(x-y)+\cos\pi k(x+y)\cos\pi(i-h)(x-y)\}$$

$$B=-4\cos 2\pi lz\{\sin\pi i(x+y)\cos\pi(h-k)(x-y)+\sin\pi h(x+y)\cos\pi(k-i)(x-y)+\sin\pi k(x+y)\cos\pi(i-h)(x-y)\}$$

$B=0$ if $h=-k$ (or $k=-i$ or $i=-h$)

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\alpha(hk\bar{l})=\alpha(kil)=\alpha(khl)\neq\alpha(\bar{h}kl);\quad \alpha(\bar{h}kl)=-\alpha(h\bar{k}l)$$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 187.

No. 190 $P\bar{6}2c$ D_{3h}^{4}

Origin at 321.

$$\left|\begin{array}{lllll} x,y,z; & \bar{y},x-y,z; & y-x,\bar{x},z; & x,y,\tfrac{1}{2}-z; & \bar{y},x-y,\tfrac{1}{2}-z; \quad y-x,\bar{x},\tfrac{1}{2}-z; \\ y,x,\bar{z}; & \bar{x},y-x,\bar{z}; & x-y,\bar{y},\bar{z}; & y,x,\tfrac{1}{2}+z; & \bar{x},y-x,\tfrac{1}{2}+z; \quad x-y,\bar{y},\tfrac{1}{2}+z \end{array}\right|$$

$$A=4\cos 2\pi\left(lz-\frac{l}{4}\right)\left\{\cos \pi i(x+y)\cos \pi\left[(h-k)(x-y)+\frac{l}{2}\right]+\cos \pi h(x+y)\cos \pi\left[(k-i)(x-y)+\frac{l}{2}\right]+\cos \pi k(x+y)\cos \pi\left[(i-h)(x-y)+\frac{l}{2}\right]\right\}$$

$$B=-4\cos 2\pi\left(lz-\frac{l}{4}\right)\left\{\sin \pi i(x+y)\cos \pi\left[(h-k)(x-y)+\frac{l}{2}\right]+\sin \pi h(x+y)\cos \pi\left[(k-i)(x-y)+\frac{l}{2}\right]+\sin \pi k(x+y)\cos \pi\left[(i-h)(x-y)+\frac{l}{2}\right]\right\}$$

$l=2n$ $\quad A=4\cos 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$

$B=-4\cos 2\pi lz\{\sin \pi i(x+y)\cos \pi(h-k)(x-y)+\sin \pi h(x+y)\cos \pi(k-i)(x-y)+\sin \pi k(x+y)\cos \pi(i-h)(x-y)\}$

$B=0$ if $h=-k$ (or $k=-i$ or $i=-k$) $\quad \alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(hk\bar{l})=\alpha(kil)=\alpha(khl)\neq\alpha(\bar{h}kl)$; $\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)$

$l=2n+1$ $\quad A=-4\sin 2\pi lz\{\cos \pi i(x+y)\sin \pi(h-k)(x-y)+\cos \pi h(x+y)\sin \pi(k-i)(x-y)+\cos \pi k(x+y)\sin \pi(i-h)(x-y)\}$

$B=4\sin 2\pi lz\{\sin \pi i(x+y)\sin \pi(h-k)(x-y)+\sin \pi h(x+y)\sin \pi(k-i)(x-y)+\sin \pi k(x+y)\sin \pi(i-h)(x-y)\}$

$B=0$ if $h=-k$ (etc.); $\quad A=B=0$ if $h=k$ (etc.)

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi+\alpha(hk\bar{l})=\alpha(kil)=\pi+\alpha(khl)\neq\alpha(\bar{h}kl)$; $\quad \alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)$

$|F(hkl)|$ relationships and $\rho(XYZ)$ as for No. 188.

No. 191 $P6/mmm$ D_{6h}^{1}

Origin at centre ($6/mmm$). $\pm$

$$\left|\begin{array}{lllll} x,y,z; & \bar{y},x-y,z; & y-x,\bar{x},z; & \bar{x},\bar{y},z; & y,y-x,z; \quad x-y,x,z; \\ y,x,\bar{z}; & \bar{x},y-x,\bar{z}; & x-y,\bar{y},\bar{z}; & \bar{y},\bar{x},\bar{z}; & x,x-y,\bar{z}; \quad y-x,y,\bar{z} \end{array}\right|$$

$A=8\cos 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$

$B=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})=F(kil)=F(khl)\neq F(\bar{h}kl)$; $\quad F(\bar{h}kl)=F(h\bar{k}l)$

$\rho(XYZ)$ as for No. 175.

$P6/mcc$ D_{6h}^{2} No. 192

Origin at centre $(6/m)$. $\pm$ $\left|\begin{array}{lllll} x,y,z; & \bar{y},x-y,z; & y-x,\bar{x},z; & y,x,\frac{1}{2}-z; & \bar{x},y-x,\frac{1}{2}-z; \quad x-y,\bar{y},\frac{1}{2}-z; \\ \bar{x},\bar{y},z; & y,y-x,z; & x-y,x,z; & \bar{y},\bar{x},\frac{1}{2}-z; & x,x-y,\frac{1}{2}-z; \quad y-x,y,\frac{1}{2}-z \end{array}\right|$

$$A=8\cos 2\pi lz\left\{\cos\pi\left[i(x+y)+\frac{l}{2}\right]\cos\pi\left[(h-k)(x-y)+\frac{l}{2}\right]+\cos\pi\left[h(x+y)+\frac{l}{2}\right]\cos\pi\left[(k-i)(x-y)+\frac{l}{2}\right]+\cos\pi\left[k(x+y)+\frac{l}{2}\right]\cos\pi\left[(i-h)(x-y)+\frac{l}{2}\right]\right\}$$

$B=0$ $\qquad F(hkl)=F(\bar{h}k\bar{l})=F(hk\bar{l})=F(kil)\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(h\bar{k}l)$

$l=2n$ $\qquad A=8\cos 2\pi lz\{\cos\pi i(x+y)\cos\pi(h-k)(x-y)+\cos\pi h(x+y)\cos\pi(k-i)(x-y)+\cos\pi k(x+y)\cos\pi(i-h)(x-y)\}$

$F(hkl)=F(khl)$

$l=2n+1$ $\qquad A=8\cos 2\pi lz\{\sin\pi i(x+y)\sin\pi(h-k)(x-y)+\sin\pi h(x+y)\sin\pi(k-i)(x-y)+\sin\pi k(x+y)\sin\pi(i-h)(x-y)\}$

$A=B=0$ if $h=\pm k$ (or $k=\pm i$ or $i=\pm h$) $\qquad F(hkl)=-F(khl)$

$\rho(XYZ)$ as for No. 175.

$P6_3/mcm$ D_{6h}^{3} No. 193

Origin at centre $(\bar{3}1m)$. $\pm$ $\left|\begin{array}{lllll} x,y,z; & \bar{y},x-y,z; & y-x,\bar{x},z; & \bar{x},\bar{y},\frac{1}{2}+z; & y,y-x,\frac{1}{2}+z; \quad x-y,x,\frac{1}{2}+z; \\ \bar{y},\bar{x},\bar{z}; & x,x-y,\bar{z}; & y-x,y,\bar{z}; & y,x,\frac{1}{2}-z; & \bar{x},y-x,\frac{1}{2}-z; \quad x-y,\bar{y},\frac{1}{2}-z \end{array}\right|$

$$A=8\cos 2\pi\left(lz+\frac{l}{4}\right)\left\{\cos\pi\left[i(x+y)+\frac{l}{2}\right]\cos\pi(h-k)(x-y)+\cos\pi\left[h(x+y)+\frac{l}{2}\right]\cos\pi(k-i)(x-y)+\cos\pi\left[k(x+y)+\frac{l}{2}\right]\cos\pi(i-h)(x-y)\right\}$$

$B=0$

$l=2n$ $\qquad A=8\cos 2\pi lz\{\cos\pi i(x+y)\cos\pi(h-k)(x-y)+\cos\pi h(x+y)\cos\pi(k-i)(x-y)+\cos\pi k(x+y)\cos\pi(i-h)(x-y)\}$

$F(hkl)=F(\bar{h}k\bar{l})=F(hk\bar{l})=F(kil)=F(khl)\neq F(\bar{h}kl);\quad F(\bar{h}kl)=F(h\bar{k}l)$

$l=2n+1$ $\qquad A=8\sin 2\pi lz\{\sin\pi i(x+y)\cos\pi(h-k)(x-y)+\sin\pi h(x+y)\cos\pi(k-i)(x-y)+\sin\pi k(x+y)\cos\pi(i-h)(x-y)\}$

$A=B=0$ if $h=-k$ (or $k=-i$ or $i=-h$) $\qquad F(hkl)=F(\bar{h}k\bar{l})=-F(hk\bar{l})=F(kil)=(khl)\neq F(\bar{h}kl);$

$F(\bar{h}kl)=-F(h\bar{k}l)$

$\rho(XYZ)$ as for No. 176.

No. 194 $P6_3/mmc$ D_{6h}^4

Origin at centre ($\bar{3}m1$). $\pm$ $\left|\begin{array}{l} x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ \bar{x},\bar{y},\frac{1}{2}+z;\ y,y-x,\frac{1}{2}+z;\ x-y,x,\frac{1}{2}+z; \\ y,x,\bar{z};\ \bar{x},y-x,\bar{z};\ x-y,\bar{y},\bar{z};\ \bar{y},\bar{x},\frac{1}{2}-z;\ x,x-y,\frac{1}{2}-z;\ y-x,y,\frac{1}{2}-z \end{array}\right|$

$$A=8\cos 2\pi\left(lz+\frac{l}{4}\right)\left\{\cos \pi i(x+y)\cos \pi\left[(h-k)(x-y)-\frac{l}{2}\right]+\cos \pi h(x+y)\cos \pi\left[(k-i)(x-y)-\frac{l}{2}\right]+\cos \pi k(x+y)\cos \pi\left[(i-h)(x-y)-\frac{l}{2}\right]\right\}$$

$B=0$

$l=2n$ $\quad A=8\cos 2\pi lz\{\cos \pi i(x+y)\cos \pi(h-k)(x-y)+\cos \pi h(x+y)\cos \pi(k-i)(x-y)+\cos \pi k(x+y)\cos \pi(i-h)(x-y)\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(hk\bar{l})=F(kil)=F(khl)\neq F(\bar{h}kl)$; $\quad F(\bar{h}kl)=F(h\bar{k}l)$

$l=2n+1$ $\quad A=-8\sin 2\pi lz\{\cos \pi i(x+y)\sin \pi(h-k)(x-y)+\cos \pi h(x+y)\sin \pi(k-i)(x-y)+\cos \pi k(x+y)\sin \pi(i-h)(x-y)\}$

$A=B=0$ if $h=k$ (or $k=i$ or $i=h$)

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(hk\bar{l})=F(kil)=-F(khl)\neq F(hkl)$; $\quad F(\bar{h}kl)=-F(h\bar{k}l)$

$\rho(XYZ)$ as for No. 176.

No. 195 $P23$ T^1

Origin at 23.

$\left|\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ y,z,x;\ y,\bar{z},\bar{x};\ \bar{y},z,\bar{x};\ \bar{y},\bar{z},x;\ z,x,y;\ z,\bar{x},\bar{y};\ \bar{z},x,\bar{y};\ \bar{z},\bar{x},y\ \right|$

$$A=4\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz\}$$

$$B=-4\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz+\sin 2\pi lx\sin 2\pi hy\sin 2\pi kz\}$$

$B=0$ if $h=0$ (or $k=0$ or $l=0$) $\quad |F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|\neq|F(khl)|$

$\alpha(hkl)=\alpha(klh)=\alpha(lhk)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty|F(hkl)|\{\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin \alpha(hkl)\}$$

$F23$ T^2

No. 196

Origin at 23.

$$(0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0)+\left|\begin{matrix} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; \\ y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; \\ z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y \end{matrix}\right|$$

$$A=16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz\}$$

$$B=-16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz+\sin 2\pi lx\sin 2\pi hy\sin 2\pi kz\}$$

$h+k=2n$ and $k+l=2n$: $A=16\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz\}$

$B=-16\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz+\sin 2\pi lx\sin 2\pi hy\sin 2\pi kz\}$

$B=0$ if $h=0$ (or $k=0$ or $l=0$) [h, k, l all even or all odd]

h, k, l mixed even and odd: $A=B=0$

$|F(hkl)|$ and $\alpha(hkl)$ relationships, and $\rho(XYZ)$ as for No. 195.

$I23$ T^3

No. 197

Origin at 23.

$$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+\left|\begin{matrix} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y \end{matrix}\right|$$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz\}$$

$$B=-8\cos^2 2\pi\frac{h+k+l}{4}\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz+\sin 2\pi lx\sin 2\pi hy\sin 2\pi kz\}$$

$h+k+l=2n$: $A=8\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz\}$

$B=-8\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz+\sin 2\pi lx\sin 2\pi hy\sin 2\pi kz\}$

$B=0$ if $h=0$ (or $k=0$ or $l=0$)

$h+k+l=2n+1$: $A=B=0$

$|F(hkl)|$ and $\alpha(hkl)$ relationships, and $\rho(XYZ)$ as for No. 195.

Origin on 3, at mid-point of three pairs of non-intersecting 2_1-axes.

$x,y,z;$	$\frac{1}{2}+x,\frac{1}{2}-y,\bar{z};$	$\bar{x},\frac{1}{2}+y,\frac{1}{2}-z;$	$\frac{1}{2}-x,\bar{y},\frac{1}{2}+z;$
$y,z,x;$	$\frac{1}{2}+y,\frac{1}{2}-z,\bar{x};$	$\bar{y},\frac{1}{2}+z,\frac{1}{2}-x;$	$\frac{1}{2}-y,\bar{z},\frac{1}{2}+x;$
$z,x,y;$	$\frac{1}{2}+z,\frac{1}{2}-x,\bar{y};$	$\bar{z},\frac{1}{2}+x,\frac{1}{2}-y;$	$\frac{1}{2}-z,\bar{x},\frac{1}{2}+y$

$$A=4\left\{\cos 2\pi\left(hx+\frac{k-h}{4}\right)\cos 2\pi\left(ky+\frac{l-k}{4}\right)\cos 2\pi\left(lz+\frac{h-l}{4}\right)+\right.$$
$$\cos 2\pi\left(kx+\frac{l-k}{4}\right)\cos 2\pi\left(ly+\frac{h-l}{4}\right)\cos 2\pi\left(hz+\frac{k-h}{4}\right)+$$
$$\left.\cos 2\pi\left(lx+\frac{h-l}{4}\right)\cos 2\pi\left(hy+\frac{k-h}{4}\right)\cos 2\pi\left(kz+\frac{l-k}{4}\right)\right\}$$

$$B=-4\left\{\sin 2\pi\left(hx+\frac{k-h}{4}\right)\sin 2\pi\left(ky+\frac{l-k}{4}\right)\sin 2\pi\left(lz+\frac{h-l}{4}\right)+\right.$$
$$\sin 2\pi\left(kx+\frac{l-k}{4}\right)\sin 2\pi\left(ly+\frac{h-l}{4}\right)\sin 2\pi\left(hz+\frac{k-h}{4}\right)+$$
$$\left.\sin 2\pi\left(lx+\frac{h-l}{4}\right)\sin 2\pi\left(hy+\frac{k-h}{4}\right)\sin 2\pi\left(kz+\frac{l-k}{4}\right)\right\}$$

$$|F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|\neq|F(khl)|$$
$$\alpha(hkl)=\alpha(klh)=\alpha(lhk)$$

$\begin{cases} h+k=2n \\ k+l=2n \end{cases}$ $A=4\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz\}$

$B=-4\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz+\sin 2\pi lx\sin 2\pi hy\sin 2\pi kz\}$

$B=0$ if $h=0$ (or $k=0$ or $l=0$) $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$\begin{cases} h+k=2n \\ k+l=2n+1 \end{cases}$ $A=-4\{\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi ly\cos 2\pi hz+\sin 2\pi lx\cos 2\pi hy\sin 2\pi kz\}$

$B=4\{\sin 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\sin 2\pi hz+\cos 2\pi lx\sin 2\pi hy\cos 2\pi kz\}$

$A=0$ if $k=0$ or $l=0$; $B=0$ if $h=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$

$\begin{cases} h+k=2n+1 \\ k+l=2n \end{cases}$ $A=-4\{\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz+\cos 2\pi kx\sin 2\pi ly\sin 2\pi hz+\sin 2\pi lx\sin 2\pi hy\cos 2\pi kz\}$

$B=4\{\cos 2\pi hx\sin 2\pi ky\cos 2\pi lz+\sin 2\pi kx\cos 2\pi ly\cos 2\pi hz+\cos 2\pi lx\cos 2\pi hy\sin 2\pi kz\}$

$A=0$ if $h=0$ or $l=0$; $B=0$ if $k=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$

$\begin{cases} h+k=2n+1 \\ k+l=2n+1 \end{cases}$ $A=-4\{\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz+\sin 2\pi kx\cos 2\pi ly\sin 2\pi hz+\cos 2\pi lx\sin 2\pi hy\sin 2\pi kz\}$

$B=4\{\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz+\cos 2\pi kx\sin 2\pi ly\cos 2\pi hz+\sin 2\pi lx\cos 2\pi hy\cos 2\pi kz\}$

$A=0$ if $h=0$ or $k=0$; $B=0$ if $l=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)]+\right.$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n+1}|F(hkl)|[\sin 2\pi hX\cos 2\pi kY\cos 2\pi lZ\sin\alpha(hkl)-\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos\alpha(hkl)]+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n}|F(hkl)|[\cos 2\pi hX\sin 2\pi kY\cos 2\pi lZ\sin\alpha(hkl)-\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\cos\alpha(hkl)]+$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n+1}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\sin 2\pi lZ\sin\alpha(hkl)-\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\cos\alpha(hkl)]\right\}$$

$I2_13$
T^5

No. 199

Origin on 3, at mid-point of three pairs of non-intersecting 2-axes.

$$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) + \left|\begin{array}{llll} x,y,z; & \tfrac{1}{2}+x,\tfrac{1}{2}-y,\bar{z}; & \bar{x},\tfrac{1}{2}+y,\tfrac{1}{2}-z; & \tfrac{1}{2}-x,\bar{y},\tfrac{1}{2}+z; \\ y,z,x; & \tfrac{1}{2}+y,\tfrac{1}{2}-z,\bar{x}; & \bar{y},\tfrac{1}{2}+z,\tfrac{1}{2}-x; & \tfrac{1}{2}-y,\bar{z},\tfrac{1}{2}+x; \\ z,x,y; & \tfrac{1}{2}+z,\tfrac{1}{2}-x,\bar{y}; & \bar{z},\tfrac{1}{2}+x,\tfrac{1}{2}-y; & \tfrac{1}{2}-z,\bar{x},\tfrac{1}{2}+y \end{array}\right|$$

$$A=8\cos 2\pi\frac{h+k+l}{4}\left\{\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{h}{4}\right)\cos 2\pi\left(lz+\frac{k}{4}\right)+\cos 2\pi\left(kx+\frac{h}{4}\right)\cos 2\pi\left(ly+\frac{k}{4}\right)\cos 2\pi\left(hz+\frac{l}{4}\right)+\right.$$
$$\left.\cos 2\pi\left(lx+\frac{k}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\cos 2\pi\left(kz+\frac{h}{4}\right)\right\}$$

$$B=-8\cos 2\pi\frac{h+k+l}{4}\left\{\sin 2\pi\left(hx+\frac{l}{4}\right)\sin 2\pi\left(ky+\frac{h}{4}\right)\sin 2\pi\left(lz+\frac{k}{4}\right)+\sin 2\pi\left(kx+\frac{h}{4}\right)\sin 2\pi\left(ly+\frac{k}{4}\right)\sin 2\pi\left(hz+\frac{l}{4}\right)+\right.$$
$$\left.\sin 2\pi\left(lx+\frac{k}{4}\right)\sin 2\pi\left(hy+\frac{l}{4}\right)\sin 2\pi\left(kz+\frac{h}{4}\right)\right\}$$

$$|F(hkl)|=|F(khl)|=|F(lhk)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|\neq|F(khl)|$$

$$\alpha(hkl)=\alpha(klh)=\alpha(lhk)$$

$\begin{cases} h+k+l=2n \\ h=2n \\ k=2n \end{cases}$ $A=8\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz\}$

$B=-8\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz+\sin 2\pi lx\sin 2\pi hy\sin 2\pi kz\}$

$B=0$ if $h=0$ (or $k=0$ or $l=0$) $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$\begin{cases} h+k+l=2n \\ h=2n+1 \\ k=2n+1 \end{cases}$ $A=-8\{\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi ly\cos 2\pi hz+\sin 2\pi lx\cos 2\pi hy\sin 2\pi kz\}$

$B=8\{\sin 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\sin 2\pi hz+\cos 2\pi lx\sin 2\pi hy\cos 2\pi kz\}$

$A=0$ if $l=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$

$\begin{cases} h+k+l=2n \\ h=2n \\ k=2n+1 \end{cases}$ $A=-8\{\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz+\cos 2\pi kx\sin 2\pi ly\sin 2\pi hz+\sin 2\pi lx\sin 2\pi hy\cos 2\pi kz\}$

$B=8\{\cos 2\pi hx\sin 2\pi ky\cos 2\pi lz+\sin 2\pi kx\cos 2\pi ly\cos 2\pi hz+\cos 2\pi lx\cos 2\pi hy\sin 2\pi kz\}$

$A=0$ if $h=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$

$\begin{cases} h+k+l=2n \\ h=2n+1 \\ k=2n \end{cases}$ $A=-8\{\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz+\sin 2\pi kx\cos 2\pi ly\sin 2\pi hz+\cos 2\pi lx\sin 2\pi hy\sin 2\pi kz\}$

$B=8\{\cos 2\pi hx\cos 2\pi ky\sin 2\pi lz+\cos 2\pi kx\sin 2\pi ly\cos 2\pi hz+\sin 2\pi lx\cos 2\pi hy\cos 2\pi kz\}$

$A=0$ if $k=0$ $\quad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

$h+k+l=2n+1$ $\quad A=B=0$

$\rho(XYZ)$ as for No. 198.

No. 200

$Pm3$ T_h^1

Origin at centre ($m3$).

$\pm$	$x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ y,z,x;\ y,\bar{z},\bar{x};\ \bar{y},z,\bar{x};\ \bar{y},\bar{z},x;\ z,x,y;\ z,\bar{x},\bar{y};\ \bar{z},x,\bar{y};\ \bar{z},\bar{x},y$

$A=8\{\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz+ \cos 2\pi kx \cos 2\pi ly \cos 2\pi hz+ \cos 2\pi lx \cos 2\pi hy \cos 2\pi kz\}$

$B=0$ $\qquad F(hkl)=F(klh)=F(lhk)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})\neq F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty F(hkl) \cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ$$

No. 201

$Pn3$ T_h^2

Origin at 23 (at $\bar{1}\frac{1}{4},\bar{1}\frac{1}{4},\bar{1}\frac{1}{4}$ from centre at $\bar{3}$).

	$x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ \frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z;\ \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z;\ \frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z;$
	$y,z,x;\ y,\bar{z},\bar{x};\ \bar{y},z,\bar{x};\ \bar{y},\bar{z},x;\ \frac{1}{2}-y,\frac{1}{2}-z,\frac{1}{2}-x;\ \frac{1}{2}-y,\frac{1}{2}+z,\frac{1}{2}+x;\ \frac{1}{2}+y,\frac{1}{2}-z,\frac{1}{2}+x;\ \frac{1}{2}+y,\frac{1}{2}+z,\frac{1}{2}-x;$
	$z,x,y;\ z,\bar{x},\bar{y};\ \bar{z},x,\bar{y};\ \bar{z},\bar{x},y;\ \frac{1}{2}-z,\frac{1}{2}-x,\frac{1}{2}-y;\ \frac{1}{2}-z,\frac{1}{2}+x,\frac{1}{2}+y;\ \frac{1}{2}+z,\frac{1}{2}-x,\frac{1}{2}+y;\ \frac{1}{2}+z,\frac{1}{2}+x,\frac{1}{2}-y$

$A=8 \cos^2 2\pi\frac{h+k+l}{4}\{\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz+ \cos 2\pi kx \cos 2\pi ly \cos 2\pi hz+ \cos 2\pi lx \cos 2\pi hy \cos 2\pi kz\}$

$B=-8 \sin^2 2\pi\frac{h+k+l}{4}\{\sin 2\pi hx \sin 2\pi ky \sin 2\pi lz+ \sin 2\pi kx \sin 2\pi ly \sin 2\pi hz+ \sin 2\pi lx \sin 2\pi hy \sin 2\pi kz\}$

$|F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|\neq|F(khl)|$

$\alpha(hkl)=\alpha(klh)=\alpha(lhk)$

$h+k+l=2n$ $\qquad A=8\{\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz+ \cos 2\pi kx \cos 2\pi ly \cos 2\pi hz+ \cos 2\pi lx \cos 2\pi hy \cos 2\pi kz\}$

$B=0$ $\qquad \alpha(hkl)=\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\mathrm{m}\pi$

$h+k+l=2n+1$ $\qquad A=0$

$B=-8\{\sin 2\pi hx \sin 2\pi ky \sin 2\pi lz+ \sin 2\pi kx \sin 2\pi ly \sin 2\pi hz+ \sin 2\pi lx \sin 2\pi hy \sin 2\pi kz\}$

$A=B=0$ if $h=0$ or $k=0$ or $l=0$

$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{2}$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)| \cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ \cos \mathrm{m}\pi-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)| \sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ \cos \mathrm{m}\pi\Big\}$$

where m=0 or 1 according as A or B is positive or negative.

$Pn3$ T_h^2

No. 201

Origin at centre ($\bar{3}$).

$$\pm\left|\begin{array}{llll} x,y,z; & x,\tfrac{1}{2}-y,\tfrac{1}{2}-z; & \tfrac{1}{2}-x,y,\tfrac{1}{2}-z; & \tfrac{1}{2}-x,\tfrac{1}{2}-y,z; \\ y,z,x; & y,\tfrac{1}{2}-z,\tfrac{1}{2}-x; & \tfrac{1}{2}-y,z,\tfrac{1}{2}-x; & \tfrac{1}{2}-y,\tfrac{1}{2}-z,x; \\ z,x,y; & z,\tfrac{1}{2}-x,\tfrac{1}{2}-y; & \tfrac{1}{2}-z,x,\tfrac{1}{2}-y; & \tfrac{1}{2}-z,\tfrac{1}{2}-x,y \end{array}\right|$$

$$A=8\left\{\cos 2\pi\left(hx+\frac{l-k}{4}\right)\cos 2\pi\left(ky+\frac{h-l}{4}\right)\cos 2\pi\left(lz+\frac{k-h}{4}\right)+\right.$$
$$\cos 2\pi\left(hy+\frac{l-k}{4}\right)\cos 2\pi\left(kz+\frac{h-l}{4}\right)\cos 2\pi\left(lx+\frac{k-h}{4}\right)+$$
$$\left.\cos 2\pi\left(hz+\frac{l-k}{4}\right)\cos 2\pi\left(kx+\frac{h-l}{4}\right)\cos 2\pi\left(ly+\frac{k-h}{4}\right)\right\}$$

$B=0$ $\qquad F(hkl)=F(klh)=F(lhk)\neq F(khl)$

$\begin{cases} h+k=2n \\ k+l=2n \end{cases}$ $\quad A=8\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi hy\cos 2\pi kz\cos 2\pi lx+\cos 2\pi hz\cos 2\pi kx\cos 2\pi ly\}$

$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=2n \\ k+l=2n+1 \end{cases}$ $\quad A=-8\{\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz+\sin 2\pi hy\sin 2\pi kz\cos 2\pi lx+\sin 2\pi hz\sin 2\pi kx\cos 2\pi ly\}$

$A=B=0$ if $h=0$ or $k=0$ $\qquad F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=2n+1 \\ k+l=2n \end{cases}$ $\quad A=-8\{\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz+\cos 2\pi hy\sin 2\pi kz\sin 2\pi lx+\cos 2\pi hz\sin 2\pi kx\sin 2\pi ly\}$

$A=B=0$ if $k=0$ or $l=0$ $\qquad F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h+k=2n+1 \\ k+l=2n+1 \end{cases}$ $\quad A=-8\{\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz+\sin 2\pi hy\cos 2\pi kz\sin 2\pi lx+\sin 2\pi hz\cos 2\pi kx\sin 2\pi ly\}$

$A=B=0$ if $h=0$ or $l=0$ $\qquad F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ k+l=2n}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ k+l=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\right\}$$

$Fm3$ T_h^3

No. 202

Origin at centre ($m3$). $\quad (0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0)\ \pm$

$$\left|\ x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ y,z,x;\ y,\bar{z},\bar{x};\ \bar{y},z,\bar{x};\ \bar{y},\bar{z},x;\ z,x,y;\ z,\bar{x},\bar{y};\ \bar{z},x,\bar{y};\ \bar{z},\bar{x},y\ \right|$$

$$A=32\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi hy\cos 2\pi kz\cos 2\pi lx+\cos 2\pi hz\cos 2\pi kx\cos 2\pi ly\}$$

$B=0$

$\begin{cases} h+k=2n \\ k+l=2n \end{cases}$ $\quad A=32\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi hy\cos 2\pi kz\cos 2\pi lx+\cos 2\pi hz\cos 2\pi kx\cos 2\pi ly\}$

$F(hkl)=F(klh)=F(lhk)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})\neq F(khl)$ [h, k, l all even or all odd]

$h+k=2n+1$ or $k+l=2n+1$; $\quad A=B=0$ $\qquad$ [h, k, l mixed even and odd]

$\rho(XYZ)$ as for No. 200.

Origin at 23 (at $\bar{\frac{1}{8}},\bar{\frac{1}{8}},\bar{\frac{1}{8}}$ from centre, $\bar{3}$). $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)$ +

$x,y,z;$	$x,\bar{y},\bar{z};$	$\bar{x},y,\bar{z};$	$\bar{x},\bar{y},z;$	$\frac{1}{4}-x,\frac{1}{4}-y,\frac{1}{4}-z;$	$\frac{1}{4}-x,\frac{1}{4}+y,\frac{1}{4}+z;$	$\frac{1}{4}+x,\frac{1}{4}-y,\frac{1}{4}+z;$	$\frac{1}{4}+x,\frac{1}{4}+y,\frac{1}{4}-z;$
$y,z,x;$	$y,\bar{z},\bar{x};$	$\bar{y},z,\bar{x};$	$\bar{y},\bar{z},x;$	$\frac{1}{4}-y,\frac{1}{4}-z,\frac{1}{4}-x;$	$\frac{1}{4}-y,\frac{1}{4}+z,\frac{1}{4}+x;$	$\frac{1}{4}+y,\frac{1}{4}-z,\frac{1}{4}+x;$	$\frac{1}{4}+y,\frac{1}{4}+z,\frac{1}{4}-x;$
$z,x,y;$	$z,\bar{x},\bar{y};$	$\bar{z},x,\bar{y};$	$\bar{z},\bar{x},y;$	$\frac{1}{4}-z,\frac{1}{4}-x,\frac{1}{4}-y;$	$\frac{1}{4}-z,\frac{1}{4}+x,\frac{1}{4}+y;$	$\frac{1}{4}+z,\frac{1}{4}-x,\frac{1}{4}+y;$	$\frac{1}{4}+z,\frac{1}{4}+x,\frac{1}{4}-y$

$A=32\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\cos 2\pi\frac{h+k+l}{8}.G;$

$B=32\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\sin 2\pi\frac{h+k+l}{8}.G;$ where

$$G=\cos 2\pi\frac{h+k+l}{8}\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi hy\cos 2\pi kz\cos 2\pi lx+\cos 2\pi hz\cos 2\pi kx\cos 2\pi ly\}-$$
$$\sin 2\pi\frac{h+k+l}{8}\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi hy\sin 2\pi kz\sin 2\pi lx+\sin 2\pi hz\sin 2\pi kx\sin 2\pi ly\}$$

$\alpha(hkl)=\alpha(klh)=\alpha(lhk);$ $|F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|\neq|F(khl)|$

$\begin{cases} h+k=2n \\ k+l=2n \\ h+k+l=4n \end{cases}$ $A=32\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi hy\cos 2\pi kz\cos 2\pi lx+\cos 2\pi hz\cos 2\pi kx\cos 2\pi ly\}$

$B=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\mathrm{m}\pi$

$\begin{cases} h+k=2n \\ k+l=2n \\ h+k+l=4n+1 \end{cases}$ $A=B=16\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz-\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+$
$\cos 2\pi hy\cos 2\pi kz\cos 2\pi lx-\sin 2\pi hy\sin 2\pi kz\sin 2\pi lx+$
$\cos 2\pi hz\cos 2\pi kx\cos 2\pi ly-\sin 2\pi hz\sin 2\pi kx\sin 2\pi ly\}$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{4}$

$\begin{cases} h+k=2n \\ k+l=2n \\ h+k+l=4n+2 \end{cases}$ $A=0$

$B=-32\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi hy\sin 2\pi kz\sin 2\pi lx+$
$\sin 2\pi hz\sin 2\pi kx\sin 2\pi ly\}$

$A=B=0$ if $h=0$ (or $k=0$ or $l=0$)

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{2}$

$\begin{cases} h+k=2n \\ k+l=2n \\ h+k+l=4n+3 \end{cases}$ $A=-B=16\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+$
$\cos 2\pi hy\cos 2\pi kz\cos 2\pi lx+\sin 2\pi hy\sin 2\pi kz\sin 2\pi lx+$
$\cos 2\pi hz\cos 2\pi kx\cos 2\pi ly+\sin 2\pi hz\sin 2\pi kx\sin 2\pi ly\}$

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi-\frac{\pi}{4}$

$h+k=2n+1$ or $k+l=2n+1;$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi+$$
$$\frac{1}{\sqrt{2}}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n+1}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ]\cos \mathrm{m}\pi-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n+2}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi+$$
$$\frac{1}{\sqrt{2}}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n+3}|F(hkl)|[\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ+\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ]\cos \mathrm{m}\pi\Big\}$$

where m=0 or 1 according as A (or if $A=0$, then B) is positive or negative.

$Fd3$
T_h^4

No. 203

Origin at centre ($\bar{3}$). $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)\ \pm$

$$\left|\begin{array}{llll} x,y,z; & x,\frac{1}{4}-y,\frac{1}{4}-z; & \frac{1}{4}-x,y,\frac{1}{4}-z; & \frac{1}{4}-x,\frac{1}{4}-y,z; \\ y,z,x; & y,\frac{1}{4}-z,\frac{1}{4}-x; & \frac{1}{4}-y,z,\frac{1}{4}-x; & \frac{1}{4}-y,\frac{1}{4}-z,x; \\ z,x,y; & z,\frac{1}{4}-x,\frac{1}{4}-y; & \frac{1}{4}-z,x,\frac{1}{4}-y; & \frac{1}{4}-z,\frac{1}{4}-x,y \end{array}\right|$$

$$A=8\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\times$$
$$\Big\{\cos 2\pi(hx+ky+lz)+\cos 2\pi\Big(hx+ky-lz-\frac{h+k}{4}\Big)+\cos 2\pi\Big(hx-ky+lz-\frac{l+h}{4}\Big)+\cos 2\pi\Big(-hx+ky+lz-\frac{k+l}{4}\Big)+$$
$$\cos 2\pi(hy+kz+lx)+\cos 2\pi\Big(hy+kz-lx-\frac{h+k}{4}\Big)+\cos 2\pi\Big(hy-kz+lx-\frac{l+h}{4}\Big)+\cos 2\pi\Big(-hy+kz+lx-\frac{k+l}{4}\Big)+$$
$$\cos 2\pi(hz+kx+ly)+\cos 2\pi\Big(hz+kx-ly-\frac{h+k}{4}\Big)+\cos 2\pi\Big(hz-kx+ly-\frac{l+h}{4}\Big)+\cos 2\pi\Big(-hz+kx+ly-\frac{k+l}{4}\Big)\Big\}$$

$B=0$ $\qquad F(hkl)=F(klh)=F(lhk)\neq F(khl)$

$\begin{cases} h+k=4n \\ k+l=4n \\ l+h=4n \end{cases}$ $\quad A=32\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi hy\cos 2\pi kz\cos 2\pi lx+\cos 2\pi hz\cos 2\pi kx\cos 2\pi ly\}$

$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=4n \\ k+l=4n+2 \\ l+h=4n+2 \end{cases}$ $\quad A=-32\{\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz+\sin 2\pi hy\sin 2\pi kz\cos 2\pi lx+\sin 2\pi hz\sin 2\pi kx\cos 2\pi ly\}$

$A=B=0$ if $h=0$ or $k=0$ $\qquad F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=4n+2 \\ k+l=4n \\ l+h=4n+2 \end{cases}$ $\quad A=-32\{\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz+\cos 2\pi hy\sin 2\pi kz\sin 2\pi lx+\cos 2\pi hz\sin 2\pi kx\sin 2\pi ly\}$

$A=B=0$ if $k=0$ or $l=0$ $\qquad F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h+k=4n+2 \\ k+l=4n+2 \\ l+h=4n \end{cases}$ $\quad A=-32\{\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz+\sin 2\pi hy\cos 2\pi kz\sin 2\pi lx+\sin 2\pi hz\cos 2\pi kx\sin 2\pi ly\}$

$A=B=0$ if $h=0$ or $l=0$ $\qquad F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h+k=4n \\ k+l=4n \\ l+h=4n+2 \end{cases}$ $\quad A=16\{\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(hy+kz)\cos 2\pi lx+\cos 2\pi(hz-kx)\cos 2\pi ly+$
$\sin 2\pi(hx-ky)\sin 2\pi lz+\sin 2\pi(hy-kz)\sin 2\pi lx+\sin 2\pi(hz-kx)\sin 2\pi ly\}$

$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=4n \\ k+l=4n+2 \\ l+h=4n \end{cases}$ $\quad A=16\{\cos 2\pi(hx+ky)\cos 2\pi lz+\cos 2\pi(hy+kz)\cos 2\pi lx+\cos 2\pi(hz+kx)\cos 2\pi ly-$
$\sin 2\pi(hx-ky)\sin 2\pi lz-\sin 2\pi(hy-kz)\sin 2\pi lx-\sin 2\pi(hz-kx)\sin 2\pi ly\}$

$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=4n+2 \\ k+l=4n \\ l+h=4n \end{cases}$ $\quad A=16\{\cos 2\pi(hx-ky)\cos 2\pi lz+\cos 2\pi(hy-kz)\cos 2\pi lx+\cos 2\pi(hz-kx)\cos 2\pi ly-$
$\sin 2\pi(hx+ky)\sin 2\pi lz-\sin 2\pi(hy+kz)\sin 2\pi lx-\sin 2\pi(hz+kx)\sin 2\pi ly\}$

$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h+k=4n+2 \\ k+l=4n+2 \\ l+h=4n+2 \end{cases}$ $\quad A=-16\{\cos 2\pi(hx-ky)\cos 2\pi lz+\cos 2\pi(hy-kz)\cos 2\pi lx+\cos 2\pi(hz-kx)\cos 2\pi ly+$
$\sin 2\pi(hx+ky)\sin 2\pi lz+\sin 2\pi(hy+kz)\sin 2\pi lx+\sin 2\pi(hz+kx)\sin 2\pi ly\}$

$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$h+k=2n+1$ or $k+l=2n+1$ [indices mixed even and odd]; $\quad A=B=0$

$\rho(XYZ)$ as for No. 70.

No. 204

$Im3$ T_h^5

Origin at centre ($m3$).

$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm \left| x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ y,z,x;\ y,\bar{z},\bar{x};\ \bar{y},z,\bar{x};\ \bar{y},\bar{z},x;\ z,x,y;\ z,\bar{x},\bar{y};\ \bar{z},x,\bar{y};\ \bar{z},\bar{x},y \right|$

$A=16\cos^2 2\pi\frac{h+k+l}{4}\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi hy\cos 2\pi kz\cos 2\pi lx+\cos 2\pi hz\cos 2\pi kx\cos 2\pi ly\}$

$B=0$ $\quad F(hkl)=F(klh)=F(lhk)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=Fhk\bar{l})\neq F(khl)$

$h+k+l=2n$ $\quad A=16\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi hy\cos 2\pi kz\cos 2\pi lx+\cos 2\pi hz\cos 2\pi kx\cos 2\pi ly\}$

$h+k+l=2n+1$ $\quad A=B=0$

$\rho(XYZ)$ as for No. 200.

No. 205

$Pa3$ T_h^6

Origin at centre ($\bar{3}$).

$$\pm\left|\begin{array}{llll} x,y,z; & \frac{1}{2}+x,\frac{1}{2}-y,\bar{z}; & \bar{x},\frac{1}{2}+y,\frac{1}{2}-z; & \frac{1}{2}-x,\bar{y},\frac{1}{2}+z; \\ y,z,x; & \frac{1}{2}+y,\frac{1}{2}-z,\bar{x}; & \bar{y},\frac{1}{2}+z,\frac{1}{2}-x; & \frac{1}{2}-y,\bar{z},\frac{1}{2}+x; \\ z,x,y; & \frac{1}{2}+z,\frac{1}{2}-x,\bar{y}; & \bar{z},\frac{1}{2}+x,\frac{1}{2}-y; & \frac{1}{2}-z,\bar{x},\frac{1}{2}+y \end{array}\right|$$

$$A=8\left\{\cos 2\pi\left(hx+\frac{k-h}{4}\right)\cos 2\pi\left(ky+\frac{l-k}{4}\right)\cos 2\pi\left(lz+\frac{h-l}{4}\right)+\cos 2\pi\left(hy+\frac{k-h}{4}\right)\cos 2\pi\left(kz+\frac{l-k}{4}\right)\cos 2\pi\left(lx+\frac{h-l}{4}\right)+\cos 2\pi\left(hz+\frac{k-h}{4}\right)\cos 2\pi\left(kx+\frac{l-k}{4}\right)\cos 2\pi\left(ly+\frac{h-l}{4}\right)\right\}$$

$B=0$ $\quad F(hkl)=F(klh)=F(lhk)\neq F(khl)$

$\begin{cases} h+k=2n \\ k+l=2n \end{cases}$ $\quad A=8\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi hy\cos 2\pi kz\cos 2\pi lx+\cos 2\pi hz\cos 2\pi kx\cos 2\pi ly\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

$\begin{cases} h+k=2n \\ k+l=2n+1 \end{cases}$ $\quad A=-8\{\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz+\cos 2\pi hy\sin 2\pi kz\sin 2\pi lx+\cos 2\pi hz\sin 2\pi kx\sin 2\pi ly\}$

$A=B=0$ if $k=0$ or $l=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h+k=2n+1 \\ k+l=2n \end{cases}$ $\quad A=-8\{\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz+\sin 2\pi hy\cos 2\pi kz\sin 2\pi lx+\sin 2\pi hz\cos 2\pi kx\sin 2\pi ly\}$

$A=B=0$ if $h=0$ or $l=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h+k=2n+1 \\ k+l=2n+1 \end{cases}$ $\quad A=-8\{\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz+\sin 2\pi hy\sin 2\pi kz\cos 2\pi lx+\sin 2\pi hz\sin 2\pi kx\cos 2\pi ly\}$

$A=B=0$ if $h=0$ or $k=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ k+l=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ k+l=2n}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ\right\}$$

$Ia3$ T_h^7

No. 206

Origin at centre ($\bar{3}$).

$$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})\ \pm \left|\begin{array}{llll} x,y,z; & \tfrac{1}{2}+x,\tfrac{1}{2}-y,\bar{z}; & \bar{x},\tfrac{1}{2}+y,\tfrac{1}{2}-z; & \tfrac{1}{2}-x,\bar{y},\tfrac{1}{2}+z; \\ y,z,x; & \tfrac{1}{2}+y,\tfrac{1}{2}-z,\bar{x}; & \bar{y},\tfrac{1}{2}+z,\tfrac{1}{2}-x; & \tfrac{1}{2}-y,\bar{z},\tfrac{1}{2}+x; \\ z,x,y; & \tfrac{1}{2}+z,\tfrac{1}{2}-x,\bar{y}; & \bar{z},\tfrac{1}{2}+x,\tfrac{1}{2}-y; & \tfrac{1}{2}-z,\bar{x},\tfrac{1}{2}+y \end{array}\right|$$

$$A=16\cos 2\pi\frac{h+k+l}{4}\left\{\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{h}{4}\right)\cos 2\pi\left(lz+\frac{k}{4}\right)+\cos 2\pi\left(hy+\frac{l}{4}\right)\cos 2\pi\left(kz+\frac{h}{4}\right)\cos 2\pi\left(lx+\frac{k}{4}\right)+\right.$$
$$\left.\cos 2\pi\left(hz+\frac{l}{4}\right)\cos 2\pi\left(kx+\frac{h}{4}\right)\cos 2\pi\left(ly+\frac{k}{4}\right)\right\}$$

$B=0$

$F(hkl)=F(klh)=F(lhk)\neq F(khl)$

$\begin{cases} h+k+l=2n \\ h=2n \\ k=2n \end{cases}$ $A=16\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi hy\cos 2\pi kz\cos 2\pi lx+\cos 2\pi hz\cos 2\pi kx\cos 2\pi ly\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$ [Indices all even]

$\begin{cases} h+k+l=2n \\ h=2n+1 \\ k=2n+1 \end{cases}$ $A=-16\{\cos 2\pi hx\sin 2\pi ky\sin 2\pi lz+\cos 2\pi hy\sin 2\pi kz\sin 2\pi lx+\cos 2\pi hz\sin 2\pi kx\sin 2\pi ly\}$

$A=B=0$ if $l=0$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h+k+l=2n \\ h=2n \\ k=2n+1 \end{cases}$ $A=-16\{\sin 2\pi hx\cos 2\pi ky\sin 2\pi lz+\sin 2\pi hy\cos 2\pi kz\sin 2\pi lx+\sin 2\pi hz\cos 2\pi kx\sin 2\pi ly\}$

$A=B=0$ if $h=0$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$\begin{cases} h+k+l=2n \\ h=2n+1 \\ k=2n \end{cases}$ $A=-16\{\sin 2\pi hx\sin 2\pi ky\cos 2\pi lz+\sin 2\pi hy\sin 2\pi kz\cos 2\pi lx+\sin 2\pi hz\sin 2\pi kx\cos 2\pi ly\}$

$A=B=0$ if $k=0$ $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

$h+k+l=2n+1$ $A=B=0$

$\rho(XYZ)$ as for No. 205.

$P432$ O^1

No. 207

Origin at 43.

$$\left|\begin{array}{llllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & \bar{y},\bar{x},\bar{z}; & \bar{y},x,z; & y,\bar{x},z; & y,x,\bar{z}; \\ y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & \bar{z},\bar{y},\bar{x}; & \bar{z},y,x; & z,\bar{y},x; & z,y,\bar{x}; \\ z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; & \bar{x},\bar{z},\bar{y}; & \bar{x},z,y; & x,\bar{z},y; & x,z,\bar{y} \end{array}\right|$$

$A=4\{\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]+\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly+\cos 2\pi lx\cos 2\pi ky]+\cos 2\pi kz[\cos 2\pi lx\cos 2\pi hy+\cos 2\pi hx\cos 2\pi ly]\}$

$B=-4\{\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]+\sin 2\pi hz[\sin 2\pi kx\sin 2\pi ly-\sin 2\pi lx\sin 2\pi ky]+\sin 2\pi kz[\sin 2\pi lx\sin 2\pi hy-\sin 2\pi hx\sin 2\pi ly]\}$

$B=0$ if $h=0$ (or $k=0$ or $l=0$) or $h=\pm k$ (or $k=\pm l$ or $l=\pm h$)

$|F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|Fhk\bar{l})|=|F(khl)|$

$\alpha(hkl)=\alpha(klh)=\alpha(lhk)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(khl)$

$\rho(XYZ)$ as for No. 195.

No. 208

$P4_232$
O^2

Origin at 23.

$$\left|\begin{array}{llllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & \tfrac{1}{2}-y,\tfrac{1}{2}-x,\tfrac{1}{2}-z; & \tfrac{1}{2}-y,\tfrac{1}{2}+x,\tfrac{1}{2}+z; & \tfrac{1}{2}+y,\tfrac{1}{2}-x,\tfrac{1}{2}+z; & \tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}-z; \\ y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & \tfrac{1}{2}-z,\tfrac{1}{2}-y,\tfrac{1}{2}-x; & \tfrac{1}{2}-z,\tfrac{1}{2}+y,\tfrac{1}{2}+x; & \tfrac{1}{2}+z,\tfrac{1}{2}-y,\tfrac{1}{2}+x; & \tfrac{1}{2}+z,\tfrac{1}{2}+y,\tfrac{1}{2}-x; \\ z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; & \tfrac{1}{2}-x,\tfrac{1}{2}-z,\tfrac{1}{2}-y; & \tfrac{1}{2}-x,\tfrac{1}{2}+z,\tfrac{1}{2}+y; & \tfrac{1}{2}+x,\tfrac{1}{2}-z,\tfrac{1}{2}+y; & \tfrac{1}{2}+x,\tfrac{1}{2}+z,\tfrac{1}{2}-y \end{array}\right|$$

$$A=4\{\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz+ \cos 2\pi kx \cos 2\pi ly \cos 2\pi hz+ \cos 2\pi lx \cos 2\pi hy \cos 2\pi kz+ \cos \pi(h+k+l)[\cos 2\pi kx \cos 2\pi hy \cos 2\pi lz+ \cos 2\pi lx \cos 2\pi ky \cos 2\pi hz+ \cos 2\pi hx \cos 2\pi ly \cos 2\pi kz]\}$$

$$B=-4\{\sin 2\pi hx \sin 2\pi ky \sin 2\pi lz+ \sin 2\pi kx \sin 2\pi ly \sin 2\pi hz+ \sin 2\pi lx \sin 2\pi hy \sin 2\pi kz- \cos \pi(h+k+l)[\sin 2\pi kx \sin 2\pi hy \sin 2\pi lz+ \sin 2\pi lx \sin 2\pi ky \sin 2\pi hz+ \sin 2\pi hx \sin 2\pi ly \sin 2\pi kz]\}$$

$h+k+l=2n$ $\quad$ A, B as for No. 207 (page 498); $B=0$ if $h=0$ (etc.) or $h=\pm k$ (etc.) $\alpha(hkl)$ relationships as for No. 207.

$h+k+l=2n+1$ $\quad$ $A=4\{\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky- \cos 2\pi kx \cos 2\pi hy]+ \cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly- \cos 2\pi lx \cos 2\pi ky]+ \cos 2\pi kz[\cos 2\pi lx \cos 2\pi hy- \cos 2\pi hx \cos 2\pi ly]\}$ $=0$ if $h=\pm k$ (etc.)

$B=-4\{\sin 2\pi lz[\sin 2\pi hx \sin 2\pi ky+ \sin 2\pi kx \sin 2\pi hy]+ \sin 2\pi hz[\sin 2\pi kx \sin 2\pi ly+ \sin 2\pi lx \sin 2\pi ky]+ \sin 2\pi kz[\sin 2\pi lx \sin 2\pi hy+ \sin 2\pi hx \sin 2\pi ly]\}$ $=0$ if $h=0$ (etc.)

$A=B=0$ if $h=k=0$ (or $k=l=0$, or $l=h=0$)

$$\alpha(hkl)=\alpha(klh)=\alpha(lhk)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi-\alpha(khl)$$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 207.

No. 209

$F432$
O^3

Origin at 43.

$$(0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0)+\left|\begin{array}{lllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & \bar{y},\bar{x},\bar{z}; & \bar{y},x,z; & y,\bar{x},z; & y,x,\bar{z}; \\ y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & \bar{z},\bar{y},\bar{x}; & \bar{z},y,x; & z,\bar{y},x; & z,y,\bar{x}; \\ z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; & \bar{x},\bar{z},\bar{y}; & \bar{x},z,y; & x,\bar{z},y; & x,z,\bar{y} \end{array}\right|$$

$$A=16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\{\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky+ \cos 2\pi kx \cos 2\pi hy]+ \cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly+ \cos 2\pi lx \cos 2\pi ky]+ \cos 2\pi kz[\cos 2\pi lx \cos 2\pi hy+ \cos 2\pi hx \cos 2\pi ly]\}$$

$$B=-16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\{\sin 2\pi lz[\sin 2\pi hx \sin 2\pi ky- \sin 2\pi kx \sin 2\pi hy]+ \sin 2\pi hz[\sin 2\pi kx \sin 2\pi ly- \sin 2\pi lx \sin 2\pi ky]+ \sin 2\pi kz[\sin 2\pi lx \sin 2\pi hy- \sin 2\pi hx \sin 2\pi ly]\}$$

h, k, l all even or all odd; A, B as for No. 207 (page 498) but with numerical factor 16 instead of 4.

h, k, l mixed even and odd; $A=B=0$

$|F(hkl)|$ and $\alpha(hkl)$ relationships, and $\rho(XYZ)$ as for No. 207.

$F4_132$ O^4

No. 210

Origin at 23. $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$

$$\left|\begin{array}{lllllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & \frac{1}{4}-y,\frac{1}{4}-x,\frac{1}{4}-z; & \frac{1}{4}-y,\frac{1}{4}+x,\frac{1}{4}+z; & \frac{1}{4}+y,\frac{1}{4}-x,\frac{1}{4}+z; & \frac{1}{4}+y,\frac{1}{4}+x,\frac{1}{4}-z; \\ y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & \frac{1}{4}-z,\frac{1}{4}-y,\frac{1}{4}-x; & \frac{1}{4}-z,\frac{1}{4}+y,\frac{1}{4}+x; & \frac{1}{4}+z,\frac{1}{4}-y,\frac{1}{4}+x; & \frac{1}{4}+z,\frac{1}{4}+y,\frac{1}{4}-x; \\ z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; & \frac{1}{4}-x,\frac{1}{4}-z,\frac{1}{4}-y; & \frac{1}{4}-x,\frac{1}{4}+z,\frac{1}{4}+y; & \frac{1}{4}+x,\frac{1}{4}-z,\frac{1}{4}+y; & \frac{1}{4}+x,\frac{1}{4}+z,\frac{1}{4}-y \end{array}\right|$$

$$A=16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\Big\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+$$
$$\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz+\cos 2\pi\left(kx-\frac{k}{4}\right)\cos 2\pi\left(hy-\frac{h}{4}\right)\cos 2\pi\left(lz-\frac{l}{4}\right)+$$
$$\cos 2\pi\left(lx-\frac{l}{4}\right)\cos 2\pi\left(ky-\frac{k}{4}\right)\cos 2\pi\left(hz-\frac{h}{4}\right)+\cos 2\pi\left(hx-\frac{h}{4}\right)\cos 2\pi\left(ly-\frac{l}{4}\right)\cos 2\pi\left(kz-\frac{k}{4}\right)\Big\}$$

$$B=-16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\Big\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz+$$
$$\sin 2\pi lx\sin 2\pi hy\sin 2\pi kz-\sin 2\pi\left(kx-\frac{k}{4}\right)\sin 2\pi\left(hy-\frac{h}{4}\right)\sin 2\pi\left(lz-\frac{l}{4}\right)-$$
$$\sin 2\pi\left(lx-\frac{l}{4}\right)\sin 2\pi\left(ky-\frac{k}{4}\right)\sin 2\pi\left(hz-\frac{h}{4}\right)-\sin 2\pi\left(hx-\frac{h}{4}\right)\sin 2\pi\left(ly-\frac{l}{4}\right)\sin 2\pi\left(kz-\frac{k}{4}\right)\Big\}$$

$$\alpha(hkl)=\alpha(klh)=\alpha(lhk)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$$

$\begin{cases} h,k,l \text{ all even} \\ h+k+l=4n \end{cases}$ A, B as for No. 207 (page 498) but with numerical factor 16 instead of 4.

$B=0$ if $h=0$ (etc.) or $h=\pm k$ (etc.) $\alpha(hkl)=-\alpha(khl)$

$\begin{cases} h,k,l \text{ all odd} \\ h+k+l=4n+1 \end{cases}$

$$A=16\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz-\sin 2\pi hx\sin 2\pi ly\sin 2\pi kz+$$
$$\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz-\sin 2\pi kx\sin 2\pi hy\sin 2\pi lz+$$
$$\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz-\sin 2\pi lx\sin 2\pi ky\sin 2\pi hz\}$$
$$B=-16\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz-\cos 2\pi hx\cos 2\pi ly\cos 2\pi kz+$$
$$\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz-\cos 2\pi kx\cos 2\pi hy\cos 2\pi lz+$$
$$\sin 2\pi lx\sin 2\pi hy\sin 2\pi kz-\cos 2\pi lx\cos 2\pi ky\cos 2\pi hz\}$$

$\alpha(hkl)=\frac{\pi}{2}-\alpha(khl)$

$\begin{cases} h,k,l \text{ all even} \\ h+k+l=4n+2 \end{cases}$

$$A=16\{\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky-\cos 2\pi kx\cos 2\pi hy]+$$
$$\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly-\cos 2\pi lx\cos 2\pi ky]+$$
$$\cos 2\pi kz[\cos 2\pi lx\cos 2\pi hy-\cos 2\pi hx\cos 2\pi ly]\}$$ $=0$ if $h=\pm k$ (etc.)

$$B=-16\{\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi kx\sin 2\pi hy]+$$
$$\sin 2\pi hz[\sin 2\pi kx\sin 2\pi ly+\sin 2\pi lx\sin 2\pi ky]+$$
$$\sin 2\pi kz[\sin 2\pi lx\sin 2\pi hy+\sin 2\pi hx\sin 2\pi ly]\}$$ $=0$ if $h=0$ (etc.)

$A=B=0$ if $h=k=0$ (etc.) $\alpha(hkl)=\pi-\alpha(khl)$

$\begin{cases} h,k,l \text{ all odd} \\ h+k+l=4n+3 \end{cases}$

$$A=16\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\sin 2\pi hx\sin 2\pi ly\sin 2\pi kz+$$
$$\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+\sin 2\pi kx\sin 2\pi hy\sin 2\pi lz+$$
$$\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz+\sin 2\pi lx\sin 2\pi ky\sin 2\pi hz\}$$
$$B=-16\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\cos 2\pi hx\cos 2\pi ly\cos 2\pi kz+$$
$$\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz+\cos 2\pi kx\cos 2\pi hy\cos 2\pi lz+$$
$$\sin 2\pi lx\sin 2\pi hy\sin 2\pi kz+\cos 2\pi lx\cos 2\pi ky\cos 2\pi hz\}$$

$\alpha(hkl)=\frac{3\pi}{2}-\alpha(khl)$

h, k, l mixed even and odd: $A=B=0$

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 207.

Origin at 43. $(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}) + \left|\begin{array}{lllllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & \bar{y},\bar{x},\bar{z}; & \bar{y},x,z; & y,\bar{x},z; & y,x,\bar{z}; \\ y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & \bar{z},\bar{y},\bar{x}; & \bar{z},y,x; & z,\bar{y},x; & z,y,\bar{x}; \\ z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; & \bar{x},\bar{z},\bar{y}; & \bar{x},z,y; & x,\bar{z},y; & x,z,\bar{y} \end{array}\right|$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\{\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi kx\cos 2\pi hy]+$$
$$\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly+\cos 2\pi lx\cos 2\pi ky]+$$
$$\cos 2\pi kz[\cos 2\pi lx\cos 2\pi hy+\cos 2\pi hx\cos 2\pi ly]\}$$

$$B=-8\cos^2 2\pi\frac{h+k+l}{4}\{\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky-\sin 2\pi kx\sin 2\pi hy]+$$
$$\sin 2\pi hz[\sin 2\pi kx\sin 2\pi ly-\sin 2\pi lx\sin 2\pi ky]+$$
$$\sin 2\pi kz[\sin 2\pi lx\sin 2\pi hy-\sin 2\pi hx\sin 2\pi ly]\}$$

$h+k+l=2n$ A, B as for No. 207 (page 498) but with numerical factor 8 instead of 4.

$h+k+l=2n+1$ $A=B=0$

$|F(hkl)|$ and $\alpha(hkl)$ relationships, and $\rho(XYZ)$ as for No. 207.

Enantiomorphous to $P4_132$. Origin on 3, half-way between three pairs of non-intersecting 4_3-axes.

$$\left|\begin{array}{lllllllll} x,y,z; & \frac{1}{2}+x,\frac{1}{2}-y,\bar{z}; & \bar{x},\frac{1}{2}+y,\frac{1}{2}-z; & \frac{1}{2}-x,\bar{y},\frac{1}{2}+z; & \frac{1}{4}-y,\frac{1}{4}-x,\frac{1}{4}-z; & \frac{3}{4}-y,\frac{1}{4}+x,\frac{3}{4}+z; & \frac{3}{4}+y,\frac{3}{4}-x,\frac{1}{4}+z; & \frac{1}{4}+y,\frac{3}{4}+x,\frac{3}{4}-z; \\ y,z,x; & \frac{1}{2}+y,\frac{1}{2}-z,\bar{x}; & \bar{y},\frac{1}{2}+z,\frac{1}{2}-x; & \frac{1}{2}-y,\bar{z},\frac{1}{2}+x; & \frac{1}{4}-z,\frac{1}{4}-y,\frac{1}{4}-x; & \frac{3}{4}-z,\frac{1}{4}+y,\frac{3}{4}+x; & \frac{3}{4}+z,\frac{3}{4}-y,\frac{1}{4}+x; & \frac{1}{4}+z,\frac{3}{4}+y,\frac{3}{4}-x; \\ z,x,y; & \frac{1}{2}+z,\frac{1}{2}-x,\bar{y}; & \bar{z},\frac{1}{2}+x,\frac{1}{2}-y; & \frac{1}{2}-z,\bar{x},\frac{1}{2}+y; & \frac{1}{4}-x,\frac{1}{4}-z,\frac{1}{4}-y; & \frac{3}{4}-x,\frac{1}{4}+z,\frac{3}{4}+y; & \frac{3}{4}+x,\frac{3}{4}-z,\frac{1}{4}+y; & \frac{1}{4}+x,\frac{3}{4}+z,\frac{3}{4}-y \end{array}\right|$$

$$A=4\left\{\cos 2\pi\left(hx+\frac{k-h}{4}\right)\cos 2\pi\left(ky+\frac{l-k}{4}\right)\cos 2\pi\left(lz+\frac{h-l}{4}\right)+\cos 2\pi\left(kx-\frac{l}{4}\right)\cos 2\pi\left(hy-\frac{k}{4}\right)\cos 2\pi\left(lz-\frac{h}{4}\right)+\right.$$
$$\cos 2\pi\left(hy+\frac{k-h}{4}\right)\cos 2\pi\left(kz+\frac{l-k}{4}\right)\cos 2\pi\left(lx+\frac{h-l}{4}\right)+\cos 2\pi\left(ky-\frac{l}{4}\right)\cos 2\pi\left(hz-\frac{k}{4}\right)\cos 2\pi\left(lx-\frac{h}{4}\right)+$$
$$\left.\cos 2\pi\left(hz+\frac{k-h}{4}\right)\cos 2\pi\left(kx+\frac{l-k}{4}\right)\cos 2\pi\left(ly+\frac{h-l}{4}\right)+\cos 2\pi\left(kz-\frac{l}{4}\right)\cos 2\pi\left(hx-\frac{k}{4}\right)\cos 2\pi\left(ly-\frac{h}{4}\right)\right\}$$

$$B=-4\left\{\sin 2\pi\left(hx+\frac{k-h}{4}\right)\sin 2\pi\left(ky+\frac{l-k}{4}\right)\sin 2\pi\left(lz+\frac{h-l}{4}\right)-\sin 2\pi\left(kx-\frac{l}{4}\right)\sin 2\pi\left(hy-\frac{k}{4}\right)\sin 2\pi\left(lz-\frac{h}{4}\right)+\right.$$
$$\sin 2\pi\left(hy+\frac{k-h}{4}\right)\sin 2\pi\left(kz+\frac{l-k}{4}\right)\sin 2\pi\left(lx+\frac{h-l}{4}\right)-\sin 2\pi\left(ky-\frac{l}{4}\right)\sin 2\pi\left(hz-\frac{k}{4}\right)\sin 2\pi\left(lx-\frac{h}{4}\right)+$$
$$\left.\sin 2\pi\left(hz+\frac{k-h}{4}\right)\sin 2\pi\left(kx+\frac{l-k}{4}\right)\sin 2\pi\left(ly+\frac{h-l}{4}\right)-\sin 2\pi\left(kz-\frac{l}{4}\right)\sin 2\pi\left(hx-\frac{k}{4}\right)\sin 2\pi\left(ly-\frac{h}{4}\right)\right\}$$

$\alpha(hkl)=\alpha(klh)=\alpha(lhk)$; $|F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

(1) $\begin{cases} h, k, l \text{ all even} \\ h+k+l=4n \end{cases}$

$$A=4\{\cos 2\pi hx[\cos 2\pi ky \cos 2\pi lz+\cos 2\pi ly \cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz \cos 2\pi lx+\cos 2\pi lz \cos 2\pi kx]+$$
$$\cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly+\cos 2\pi lx \cos 2\pi ky]\}$$
$$B=-4\{\sin 2\pi hx[\sin 2\pi ky \sin 2\pi lz-\sin 2\pi ly \sin 2\pi kz]+$$
$$\sin 2\pi hy[\sin 2\pi kz \sin 2\pi lx-\sin 2\pi lz \sin 2\pi kx]+$$
$$\sin 2\pi hz[\sin 2\pi kx \sin 2\pi ly-\sin 2\pi lx \sin 2\pi ky]\} \quad =0 \text{ if } h=0 \text{ or } h=\pm k \text{ (etc.)}$$
$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$$
$$=-\alpha(khl)$$

(2) $\begin{cases} h, k, l \text{ all odd} \\ h+k+l=4n+1 \end{cases}$

$$A=4\{\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz-\sin 2\pi kx \sin 2\pi hy \sin 2\pi lz+$$
$$\cos 2\pi hy \cos 2\pi kz \cos 2\pi lx-\sin 2\pi ky \sin 2\pi hz \sin 2\pi lx+$$
$$\cos 2\pi hz \cos 2\pi kx \cos 2\pi ly-\sin 2\pi kz \sin 2\pi hx \sin 2\pi ly\}$$
$$B=-4\{\sin 2\pi hx \sin 2\pi ky \sin 2\pi lz-\cos 2\pi kx \cos 2\pi hy \cos 2\pi lz+$$
$$\sin 2\pi hy \sin 2\pi kz \sin 2\pi lx-\cos 2\pi ky \cos 2\pi hz \cos 2\pi lx+$$
$$\sin 2\pi hz \sin 2\pi kx \sin 2\pi ly-\cos 2\pi kz \cos 2\pi hx \cos 2\pi ly\}$$
$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$$
$$=\frac{\pi}{2}-\alpha(khl)$$

(3) $\begin{cases} h, k, l \text{ all even} \\ h+k+l=4n+2 \end{cases}$

$$A=4\{\cos 2\pi hx[\cos 2\pi ky \cos 2\pi lz-\cos 2\pi ly \cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz \cos 2\pi lx-\cos 2\pi lz \cos 2\pi kx]+$$
$$\cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly-\cos 2\pi lx \cos 2\pi ky]\} \quad =0 \text{ if } h=\pm k \text{ (etc.)}$$
$$B=-4\{\sin 2\pi hx[\sin 2\pi ky \sin 2\pi lz+\sin 2\pi ly \sin 2\pi kz]+$$
$$\sin 2\pi hy[\sin 2\pi kz \sin 2\pi lx+\sin 2\pi lz \sin 2\pi kx]+$$
$$\sin 2\pi hz[\sin 2\pi kx \sin 2\pi ly+\sin 2\pi lx \sin 2\pi ky]\} \quad =0 \text{ if } h=0 \text{ (etc.)}$$
$$A=B=0 \text{ if } h=k=0 \text{ (etc.)} \qquad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$$
$$=\pi-\alpha(khl)$$

(4) $\begin{cases} h, k, l \text{ all odd} \\ h+k+l=4n+3 \end{cases}$

$$A=4\{\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz+\sin 2\pi kx \sin 2\pi hy \sin 2\pi lz+$$
$$\cos 2\pi hy \cos 2\pi kz \cos 2\pi lx+\sin 2\pi ky \sin 2\pi hz \sin 2\pi lx+$$
$$\cos 2\pi hz \cos 2\pi kx \cos 2\pi ly+\sin 2\pi kz \sin 2\pi hx \sin 2\pi ly\}$$
$$B=-4\{\sin 2\pi hx \sin 2\pi ky \sin 2\pi lz+\cos 2\pi kx \cos 2\pi hy \cos 2\pi lz+$$
$$\sin 2\pi hy \sin 2\pi kz \sin 2\pi lx+\cos 2\pi ky \cos 2\pi hz \cos 2\pi lx+$$
$$\sin 2\pi hz \sin 2\pi kx \sin 2\pi ly+\cos 2\pi kz \cos 2\pi hx \cos 2\pi ly\}$$
$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$$
$$=\frac{3\pi}{2}-\alpha(khl)$$

(5) $\begin{cases} h=2n+1 \\ k=2n+1 \\ l=2n \\ h+k+l=4n \end{cases}$

$$A=-4\{\sin 2\pi lx[\cos 2\pi hy \sin 2\pi kz+\cos 2\pi ky \sin 2\pi hz]+$$
$$\sin 2\pi ly[\cos 2\pi hz \sin 2\pi kx+\cos 2\pi kz \sin 2\pi hx]+$$
$$\sin 2\pi lz[\cos 2\pi hx \sin 2\pi ky+\cos 2\pi kx \sin 2\pi hy]\} \quad =0 \text{ if } l=0 \text{ or } h=-k$$
$$B=4\{\cos 2\pi lx[\sin 2\pi hy \cos 2\pi kz-\sin 2\pi ky \cos 2\pi hz]+$$
$$\cos 2\pi ly[\sin 2\pi hz \cos 2\pi kx-\sin 2\pi kz \cos 2\pi hx]+$$
$$\cos 2\pi lz[\sin 2\pi hx \cos 2\pi ky-\sin 2\pi kx \cos 2\pi hy]\} \quad =0 \text{ if } h=k$$
$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$$
$$=-\alpha(khl)$$

$$(6)\quad \begin{cases} h = 2n \\ k = 2n \\ l = 2n+1 \\ h+k+l = 4n+1 \end{cases}$$

$$A=4\{\sin 2\pi kx[\cos 2\pi hy \cos 2\pi lz - \sin 2\pi ly \cos 2\pi hz]+ \sin 2\pi ky[\cos 2\pi hz \cos 2\pi lx - \sin 2\pi lz \cos 2\pi hx]+ \sin 2\pi kz[\cos 2\pi hx \cos 2\pi ly - \sin 2\pi lx \cos 2\pi hy]\} = 0 \text{ if } k=0$$

$$B=-4\{\cos 2\pi kx[\sin 2\pi hy \sin 2\pi lz - \cos 2\pi ly \sin 2\pi hz]+ \cos 2\pi ky[\sin 2\pi hz \sin 2\pi lx - \cos 2\pi lz \sin 2\pi hx]+ \cos 2\pi kz[\sin 2\pi hx \sin 2\pi ly - \cos 2\pi lx \sin 2\pi hy]\} = 0 \text{ if } h=0$$

$A=B=0$ if $h=k=0$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l}) = \frac{\pi}{2}-\alpha(khl)$$

$$(7)\quad \begin{cases} h = 2n+1 \\ k = 2n+1 \\ l = 2n \\ h+k+l = 4n+2 \end{cases}$$

$$A=-4\{\sin 2\pi lx[\cos 2\pi hy \sin 2\pi kz - \cos 2\pi ky \sin 2\pi hz]+ \sin 2\pi ly[\cos 2\pi hz \sin 2\pi kx - \cos 2\pi kz \sin 2\pi hx]+ \sin 2\pi lz[\cos 2\pi hx \sin 2\pi ky - \cos 2\pi kx \sin 2\pi hy]\} = 0 \text{ if } l=0 \text{ or } h=k$$

$$B=4\{\cos 2\pi lx[\sin 2\pi hy \cos 2\pi kz + \sin 2\pi ky \cos 2\pi hz]+ \cos 2\pi ly[\sin 2\pi hz \cos 2\pi kx + \sin 2\pi kz \cos 2\pi hx]+ \cos 2\pi lz[\sin 2\pi hx \cos 2\pi ky + \sin 2\pi kx \cos 2\pi hy]\} = 0 \text{ if } h=-k$$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l}) = \pi-\alpha(khl)$$

$$(8)\quad \begin{cases} h = 2n \\ k = 2n \\ l = 2n+1 \\ h+k+l = 4n+3 \end{cases}$$

$$A=-4\{\sin 2\pi kx[\cos 2\pi hy \cos 2\pi lz + \sin 2\pi ly \cos 2\pi hz]+ \sin 2\pi ky[\cos 2\pi hz \cos 2\pi lx + \sin 2\pi lz \cos 2\pi hx]+ \sin 2\pi kz[\cos 2\pi hx \cos 2\pi ly + \sin 2\pi lx \cos 2\pi hy]\} = 0 \text{ if } k=0$$

$$B=4\{\cos 2\pi kx[\sin 2\pi hy \sin 2\pi lz + \cos 2\pi ly \sin 2\pi hz]+ \cos 2\pi ky[\sin 2\pi hz \sin 2\pi lx + \cos 2\pi lz \sin 2\pi hx]+ \cos 2\pi kz[\sin 2\pi hx \sin 2\pi ly + \cos 2\pi lx \sin 2\pi hy]\} = 0 \text{ if } h=0$$

$A=B=0$ if $h=k=0$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l}) = \frac{3\pi}{2}-\alpha(khl)$$

$$(9)\quad \begin{cases} h = 2n \\ k = 2n+1 \\ l = 2n+1 \\ h+k+l = 4n \end{cases}$$

Change $h \to k \to l \to h$ in formulae (5)

$A=0$ if $h=0$ or $k=\pm l$; $B=0$ if $k=l$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l}) = -\alpha(khl)$$

$$(10)\quad \begin{cases} h = 2n+1 \\ k = 2n \\ l = 2n \\ h+k+l = 4n+1 \end{cases}$$

Change $h \to k \to l \to h$ in formulae (6)

$A=0$ if $l=0$; $B=0$ if $k=0$; $A=B=0$ if $k=l=0$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l}) = \frac{\pi}{2}-\alpha(khl)$$

$$(11)\begin{cases} h = 2n \\ k = 2n+1 \\ l = 2n+1 \\ h+k+l = 4n+2 \end{cases}$$

Change $h \to k \to l \to h$ in formulae (7)

$A=0$ if $h=0$ or $k=l$; $B=0$ if $k=-l$

$$\alpha(hkl) = -\alpha(\bar{h}k\bar{l}) = \pi - \alpha(\bar{h}kl) = -\alpha(h\bar{k}l) = \pi - \alpha(hk\bar{l}) = \pi - \alpha(khl)$$

$$(12)\begin{cases} h = 2n+1 \\ k = 2n \\ l = 2n \\ h+k+l = 4n+3 \end{cases}$$

Change $h \to k \to l \to h$ in formulae (8)

$A=0$ if $l=0$; $B=0$ if $k=0$; $A=B=0$ if $k=l=0$

$$\alpha(hkl) = -\alpha(\bar{h}k\bar{l}) = \pi - \alpha(\bar{h}kl) = -\alpha(h\bar{k}l) = \pi - \alpha(hk\bar{l}) = \frac{3\pi}{2} - \alpha(khl)$$

$$(13)\begin{cases} h = 2n+1 \\ k = 2n \\ l = 2n+1 \\ h+k+l = 4n \end{cases}$$

Change $h \to l \to k \to h$ in formulae (5)

$A=0$ if $k=0$ or $l=-h$; $B=0$ if $l=h$

$$\alpha(hkl) = -\alpha(\bar{h}k\bar{l}) = \pi - \alpha(\bar{h}kl) = \pi - \alpha(h\bar{k}l) = -\alpha(hk\bar{l}) = -\alpha(khl)$$

$$(14)\begin{cases} h = 2n \\ k = 2n+1 \\ l = 2n \\ h+k+l = 4n+1 \end{cases}$$

Change $h \to l \to k \to h$ in formulae (6)

$A=0$ if $h=0$; $B=0$ if $l=0$; $A=B=0$ if $l=h=0$

$$\alpha(hkl) = -\alpha(\bar{h}k\bar{l}) = \pi - \alpha(\bar{h}kl) = \pi - \alpha(h\bar{k}l) = -\alpha(hk\bar{l}) = \frac{\pi}{2} - \alpha(khl)$$

$$(15)\begin{cases} h = 2n+1 \\ k = 2n \\ l = 2n+1 \\ h+k+l = 4n+2 \end{cases}$$

Change $h \to l \to k \to h$ in formulae (7)

$A=0$ if $k=0$ or $l=h$; $B=0$ if $l=-h$

$$\alpha(hkl) = -\alpha(\bar{h}k\bar{l}) = \pi - \alpha(\bar{h}kl) = \pi - \alpha(h\bar{k}l) = -\alpha(hk\bar{l}) = \pi - \alpha(khl)$$

$$(16)\begin{cases} h = 2n \\ k = 2n+1 \\ l = 2n \\ h+k+l = 4n+3 \end{cases}$$

Change $h \to l \to k \to h$ in formulae (8)

$A=0$ if $h=0$; $B=0$ if $l=0$; $A=B=0$ if $l=h=0$

$$\alpha(hkl) = -\alpha(\bar{h}k\bar{l}) = \pi - \alpha(\bar{h}kl) = \pi - \alpha(h\bar{k}l) = -\alpha(hk\bar{l}) = \frac{3\pi}{2} - \alpha(khl)$$

$$\begin{aligned}\rho(XYZ) = \frac{8}{V_c}\Big\{ & \sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n} |F(hkl)|[\cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ \cos\alpha(hkl) - \sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ \sin\alpha(hkl)] + \\ & \sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n+1} |F(hkl)|[\sin 2\pi hX \cos 2\pi kY \cos 2\pi lZ \sin\alpha(hkl) - \cos 2\pi hX \sin 2\pi kY \sin 2\pi lZ \cos\alpha(hkl)] + \\ & \sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n} |F(hkl)|[\cos 2\pi hX \sin 2\pi kY \cos 2\pi lZ \sin\alpha(hkl) - \sin 2\pi hX \cos 2\pi kY \sin 2\pi lZ \cos\alpha(hkl)] + \\ & \sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n+1} |F(hkl)|[\cos 2\pi hX \cos 2\pi kY \sin 2\pi lZ \sin\alpha(hkl) - \sin 2\pi hX \sin 2\pi kY \cos 2\pi lZ \cos\alpha(hkl)]\Big\}\end{aligned}$$

$P4_132$ O^7

Enantiomorphous to $P4_332$. Origin on 3, half-way between three pairs of non-intersecting 4_1-axes.

x,y,z;	$\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$;	$\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$;	$\frac{1}{2}-x,\bar{y},\frac{1}{2}+z$;	$\frac{3}{4}-y,\frac{3}{4}-x,\frac{3}{4}-z$;	$\frac{1}{4}-y,\frac{3}{4}+x,\frac{1}{4}+z$;	$\frac{1}{4}+y,\frac{1}{4}-x,\frac{3}{4}+z$;	$\frac{3}{4}+y,\frac{1}{4}+x,\frac{1}{4}-z$;
y,z,x;	$\frac{1}{2}+y,\frac{1}{2}-z,\bar{x}$;	$\bar{y},\frac{1}{2}+z,\frac{1}{2}-x$;	$\frac{1}{2}-y,\bar{z},\frac{1}{2}+x$;	$\frac{3}{4}-z,\frac{3}{4}-y,\frac{3}{4}-x$;	$\frac{1}{4}-z,\frac{3}{4}+y,\frac{1}{4}+x$;	$\frac{1}{4}+z,\frac{1}{4}-y,\frac{3}{4}+x$;	$\frac{3}{4}+z,\frac{1}{4}+y,\frac{1}{4}-x$;
z,x,y;	$\frac{1}{2}+z,\frac{1}{2}-x,\bar{y}$;	$\bar{z},\frac{1}{2}+x,\frac{1}{2}-y$;	$\frac{1}{2}-z,\bar{x},\frac{1}{2}+y$;	$\frac{3}{4}-x,\frac{3}{4}-z,\frac{3}{4}-y$;	$\frac{1}{4}-x,\frac{3}{4}+z,\frac{1}{4}+y$;	$\frac{1}{4}+x,\frac{1}{4}-z,\frac{3}{4}+y$;	$\frac{3}{4}+x,\frac{1}{4}+z,\frac{1}{4}-y$

$$A=4\Big\{\cos 2\pi\Big(hx+\frac{k-h}{4}\Big)\cos 2\pi\Big(ky+\frac{l-k}{4}\Big)\cos 2\pi\Big(lz+\frac{h-l}{4}\Big)+\cos 2\pi\Big(kx+\frac{l}{4}\Big)\cos 2\pi\Big(hy+\frac{k}{4}\Big)\cos 2\pi\Big(lz+\frac{h}{4}\Big)+$$
$$\cos 2\pi\Big(hy+\frac{k-h}{4}\Big)\cos 2\pi\Big(kz+\frac{l-k}{4}\Big)\cos 2\pi\Big(lx+\frac{h-l}{4}\Big)+\cos 2\pi\Big(ky+\frac{l}{4}\Big)\cos 2\pi\Big(hz+\frac{k}{4}\Big)\cos 2\pi\Big(lx+\frac{h}{4}\Big)+$$
$$\cos 2\pi\Big(hz+\frac{k-h}{4}\Big)\cos 2\pi\Big(kx+\frac{l-k}{4}\Big)\cos 2\pi\Big(ly+\frac{h-l}{4}\Big)+\cos 2\pi\Big(kz+\frac{l}{4}\Big)\cos 2\pi\Big(hx+\frac{k}{4}\Big)\cos 2\pi\Big(ly+\frac{h}{4}\Big)\Big\}$$

$$B=-4\Big\{\sin 2\pi\Big(hx+\frac{k-h}{4}\Big)\sin 2\pi\Big(ky+\frac{l-k}{4}\Big)\sin 2\pi\Big(lz+\frac{h-l}{4}\Big)-\sin 2\pi\Big(kx+\frac{l}{4}\Big)\sin 2\pi\Big(hy+\frac{k}{4}\Big)\sin 2\pi\Big(lz+\frac{h}{4}\Big)+$$
$$\sin 2\pi\Big(hy+\frac{k-h}{4}\Big)\sin 2\pi\Big(kz+\frac{l-k}{4}\Big)\sin 2\pi\Big(lx+\frac{h-l}{4}\Big)-\sin 2\pi\Big(ky+\frac{l}{4}\Big)\sin 2\pi\Big(hz+\frac{k}{4}\Big)\sin 2\pi\Big(lx+\frac{h}{4}\Big)+$$
$$\sin 2\pi\Big(hz+\frac{k-h}{4}\Big)\sin 2\pi\Big(kx+\frac{l-k}{4}\Big)\sin 2\pi\Big(ly+\frac{h-l}{4}\Big)-\sin 2\pi\Big(kz+\frac{l}{4}\Big)\sin 2\pi\Big(hx+\frac{k}{4}\Big)\sin 2\pi\Big(ly+\frac{h}{4}\Big)\Big\}$$

$\alpha(hkl)=\alpha(klh)=\alpha(lhk)$; $\quad |F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

h, k, l all even;	$h+k+l=4n$	As for $P4_332$	(1)
h, k, l all odd;	$h+k+l=4n+1$	As for $P4_332$	(4)
h, k, l all even;	$h+k+l=4n+2$	As for $P4_332$	(3)
h, k, l all odd;	$h+k+l=4n+3$	As for $P4_332$	(2)
h, k odd, l even;	$h+k+l=4n$	As for $P4_332$	(5)
h, k even, l odd;	$h+k+l=4n+1$	As for $P4_332$	(8)
h, k odd, l even;	$h+k+l=4n+2$	As for $P4_332$	(7)
h, k even, l odd;	$h+k+l=4n+3$	As for $P4_332$	(6)
h, l odd, k even;	$h+k+l=4n$	As for $P4_332$	(13)
h, l even, k odd;	$h+k+l=4n+1$	As for $P4_332$	(16)
h, l odd, k even;	$h+k+l=4n+2$	As for $P4_332$	(15)
h, l even, k odd;	$h+k+l=4n+3$	As for $P4_332$	(14)
k, l odd, h even;	$h+k+l=4n$	As for $P4_332$	(9)
k, l even, h odd;	$h+k+l=4n+1$	As for $P4_332$	(12)
k, l odd, h even;	$h+k+l=4n+2$	As for $P4_332$	(11)
k, l even, h odd;	$h+k+l=4n+3$	As for $P4_332$	(10)

$\rho(XYZ)$ as for No. 212.

$I4_132$
O^8

No. 214

Origin on 3, half-way between three pairs of non-intersecting 2-axes.

$$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+\left|\begin{array}{lllll}
x,y,z; & y,z,x; & z,x,y; & \tfrac{1}{4}-y,\tfrac{1}{4}-x,\tfrac{1}{4}-z; & \tfrac{1}{4}-z,\tfrac{1}{4}-y,\tfrac{1}{4}-x; \\
\tfrac{1}{2}+x,\tfrac{1}{2}-y,\bar{z}; & \tfrac{1}{2}+y,\tfrac{1}{2}-z,\bar{x}; & \tfrac{1}{2}+z,\tfrac{1}{2}-x,\bar{y}; & \tfrac{3}{4}-y,\tfrac{1}{4}+x,\tfrac{3}{4}+z; & \tfrac{3}{4}-z,\tfrac{1}{4}+y,\tfrac{3}{4}+x; \\
\bar{x},\tfrac{1}{2}+y,\tfrac{1}{2}-z; & \bar{y},\tfrac{1}{2}+z,\tfrac{1}{2}-x; & \bar{z},\tfrac{1}{2}+x,\tfrac{1}{2}-y; & \tfrac{3}{4}+y,\tfrac{3}{4}-x,\tfrac{1}{4}+z; & \tfrac{3}{4}+z,\tfrac{3}{4}-y,\tfrac{1}{4}+x; \\
\tfrac{1}{2}-x,\bar{y},\tfrac{1}{2}+z; & \tfrac{1}{2}-y,\bar{z},\tfrac{1}{2}+x; & \tfrac{1}{2}-z,\bar{x},\tfrac{1}{2}+y; & \tfrac{1}{4}+y,\tfrac{3}{4}+x,\tfrac{3}{4}-z; & \tfrac{1}{4}+z,\tfrac{3}{4}+y,\tfrac{3}{4}-x; \quad \tfrac{1}{4}+x,\tfrac{3}{4}+z,\tfrac{3}{4}-y
\end{array}\right|$$

$$A=8\cos 2\pi\frac{h+k+l}{4}\Big\{\cos 2\pi\Big(hx+\frac{l}{4}\Big)\cos 2\pi\Big(ky+\frac{h}{4}\Big)\cos 2\pi\Big(lz+\frac{k}{4}\Big)+\cos 2\pi\Big(hy+\frac{l}{4}\Big)\cos 2\pi\Big(kz+\frac{h}{4}\Big)\cos 2\pi\Big(lx+\frac{k}{4}\Big)+$$
$$\cos 2\pi\Big(hz+\frac{l}{4}\Big)\cos 2\pi\Big(kx+\frac{h}{4}\Big)\cos 2\pi\Big(ly+\frac{k}{4}\Big)+\cos 2\pi\frac{h+k+l}{4}\Big[\cos 2\pi\Big(kx+\frac{l}{4}\Big)\cos 2\pi\Big(hy+\frac{k}{4}\Big)\cos 2\pi\Big(lz+\frac{h}{4}\Big)+$$
$$\cos 2\pi\Big(ky+\frac{l}{4}\Big)\cos 2\pi\Big(hz+\frac{k}{4}\Big)\cos 2\pi\Big(lx+\frac{h}{4}\Big)+\cos 2\pi\Big(kz+\frac{l}{4}\Big)\cos 2\pi\Big(hx+\frac{k}{4}\Big)\cos 2\pi\Big(ly+\frac{h}{4}\Big)\Big]\Big\}$$

$$B=-8\cos 2\pi\frac{h+k+l}{4}\Big\{\sin 2\pi\Big(hx+\frac{l}{4}\Big)\sin 2\pi\Big(ky+\frac{h}{4}\Big)\sin 2\pi\Big(lz+\frac{k}{4}\Big)+\sin 2\pi\Big(hy+\frac{l}{4}\Big)\sin 2\pi\Big(kz+\frac{h}{4}\Big)\sin 2\pi\Big(lx+\frac{k}{4}\Big)+$$
$$\sin 2\pi\Big(hz+\frac{l}{4}\Big)\sin 2\pi\Big(kx+\frac{h}{4}\Big)\sin 2\pi\Big(ly+\frac{k}{4}\Big)-\cos 2\pi\frac{h+k+l}{4}\Big[\sin 2\pi\Big(kx+\frac{l}{4}\Big)\sin 2\pi\Big(hy+\frac{k}{4}\Big)\sin 2\pi\Big(lz+\frac{h}{4}\Big)+$$
$$\sin 2\pi\Big(ky+\frac{l}{4}\Big)\sin 2\pi\Big(hz+\frac{k}{4}\Big)\sin 2\pi\Big(lx+\frac{h}{4}\Big)+\sin 2\pi\Big(kz+\frac{l}{4}\Big)\sin 2\pi\Big(hx+\frac{k}{4}\Big)\sin 2\pi\Big(ly+\frac{h}{4}\Big)\Big]\Big\}$$

$$|F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$
$$\alpha(hkl)=\alpha(klh)=\alpha(lhk)$$

(1) $\begin{cases} h,\ k,\ l \text{ all even} \\ h+k+l=4n \end{cases}$

$$A=8\{\cos 2\pi hx[\cos 2\pi ky\cos 2\pi lz+\cos 2\pi ly\cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz\cos 2\pi lx+\cos 2\pi lz\cos 2\pi kx]+$$
$$\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly+\cos 2\pi lx\cos 2\pi ky]\}$$
$$B=-8\{\sin 2\pi hx[\sin 2\pi ky\sin 2\pi lz-\sin 2\pi ly\sin 2\pi kz]+$$
$$\sin 2\pi hy[\sin 2\pi kz\sin 2\pi lx-\sin 2\pi lz\sin 2\pi kx]+$$
$$\sin 2\pi hz[\sin 2\pi kx\sin 2\pi ly-\sin 2\pi lx\sin 2\pi ky]\}=0 \text{ if } h=0 \text{ (etc.) or } h=\pm k \text{ (etc.)}$$
$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$$
$$=-\alpha(khl)$$

(2) $\begin{cases} h \text{ even};\quad k,\ l \text{ odd} \\ h+k+l=4n \end{cases}$

$$A=-8\{\sin 2\pi hx[\cos 2\pi ky\sin 2\pi lz+\cos 2\pi ly\sin 2\pi kz]+$$
$$\sin 2\pi hy[\cos 2\pi kz\sin 2\pi lx+\cos 2\pi lz\sin 2\pi kx]+$$
$$\sin 2\pi hz[\cos 2\pi kx\sin 2\pi ly+\cos 2\pi lx\sin 2\pi ky]\}=0 \text{ if } h=0 \text{ or } k=-l$$
$$B=8\{\cos 2\pi hx[\sin 2\pi ky\cos 2\pi lz-\sin 2\pi ly\cos 2\pi kz]+$$
$$\cos 2\pi hy[\sin 2\pi kz\cos 2\pi lx-\sin 2\pi lz\cos 2\pi kx]+$$
$$\cos 2\pi hz[\sin 2\pi kx\cos 2\pi ly-\sin 2\pi lx\cos 2\pi ky]\}=0 \text{ if } k=l$$
$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$$
$$=-\alpha(khl)$$

(3) $\begin{cases} k \text{ even};\quad h,\ l \text{ odd} \\ h+k+l=4n \end{cases}$

Change $h\to k\to l\to h$ in formulae (2)

$A=0$ if $k=0$ or $l=-h$; $B=0$ if $l=h$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(hkl)=-\alpha(hk\bar{l})$$
$$=-\alpha(khl)$$

(4) $\begin{cases} l \text{ even}; \quad h, k \text{ odd} \\ h+k+l=4n \end{cases}$ Change $h \to l \to k \to h$ in formulae (2)

$A=0$ if $l=0$ or $h=-k$; $B=0$ if $h=k$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$$
$$=-\alpha(khl)$$

(5) $\begin{cases} h, k, l \text{ even} \\ h+k+l=4n+2 \end{cases}$

$$A=8\{\cos 2\pi hx[\cos 2\pi ky \cos 2\pi lz-\cos 2\pi ly \cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz \cos 2\pi lx-\cos 2\pi lz \cos 2\pi kx]+$$
$$\cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly-\cos 2\pi lx \cos 2\pi ky]\} \quad =0 \text{ if } h=\pm k \text{ (etc.)}$$
$$B=-8\{\sin 2\pi hx[\sin 2\pi ky \sin 2\pi lz+\sin 2\pi ly \sin 2\pi kz]+$$
$$\sin 2\pi hy[\sin 2\pi kz \sin 2\pi lx+\sin 2\pi lz \sin 2\pi kx]+$$
$$\sin 2\pi hz[\sin 2\pi kx \sin 2\pi ly+\sin 2\pi lx \sin 2\pi ky]\} \quad =0 \text{ if } h=0 \text{ (etc.)}$$

$A=B=0$ if $h=k=0$ (etc.)

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$$
$$=\pi-\alpha(khl)$$

(6) $\begin{cases} h \text{ even}; \quad k, l \text{ odd} \\ h+k+l=4n+2 \end{cases}$

$$A=-8\{\sin 2\pi hx[\cos 2\pi ky \sin 2\pi lz-\cos 2\pi ly \sin 2\pi kz]+$$
$$\sin 2\pi hy[\cos 2\pi kz \sin 2\pi lx-\cos 2\pi lz \sin 2\pi kx]+$$
$$\sin 2\pi hz[\cos 2\pi kx \sin 2\pi ly-\cos 2\pi lx \sin 2\pi ky]\} \quad =0 \text{ if } h=0 \text{ or } k=l$$
$$B=8\{\cos 2\pi hx[\sin 2\pi ky \cos 2\pi lz+\sin 2\pi ly \cos 2\pi kz]+$$
$$\cos 2\pi hy[\sin 2\pi kz \cos 2\pi lx+\sin 2\pi lz \cos 2\pi kx]+$$
$$\cos 2\pi hz[\sin 2\pi kx \cos 2\pi ly+\sin 2\pi lx \cos 2\pi ky]\} \quad =0 \text{ if } k=-l$$
$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$$
$$=\pi-\alpha(khl)$$

(7) $\begin{cases} k \text{ even}; \quad h, l \text{ odd} \\ h+k+l=4n+2 \end{cases}$ Change $h \to k \to l \to h$ in formulae (6)

$A=0$ if $k=0$ or $l=h$; $B=0$ if $l=-h$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$$
$$=\pi-\alpha(khl)$$

(8) $\begin{cases} l \text{ even}; \quad k, h \text{ odd} \\ h+k+l=4n+2 \end{cases}$ Change $h \to l \to k \to h$ in formulae (6)

$A=0$ if $l=0$ or $h=k$; $B=0$ if $h=-k$

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$$
$$=\pi-\alpha(khl)$$

$h+k+l=2n+1$ $\quad A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n}|F(hkl)|[\cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ \cos\alpha(hkl)-\sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ \sin\alpha(hkl)]+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n+1}|F(hkl)|[\cos 2\pi hX \sin 2\pi kY \cos 2\pi lZ \sin\alpha(hkl)-\sin 2\pi hX \cos 2\pi kY \sin 2\pi lZ \cos\alpha(hkl)]+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n}|F(hkl)|[\cos 2\pi hX \cos 2\pi kY \sin 2\pi lZ \sin\alpha(hkl)-\sin 2\pi hX \sin 2\pi kY \cos 2\pi lZ \cos\alpha(hkl)]+$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n+1}|F(hkl)|[\sin 2\pi hX \cos 2\pi kY \cos 2\pi lZ \sin\alpha(hkl)-\cos 2\pi hX \sin 2\pi kY \sin 2\pi lZ \cos\alpha(hkl)]\Big\}$$

$P\bar{4}3m$ T_d^1

No. 215

Origin at $\bar{4}3m$.

$$\left|\begin{array}{llllllllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; \\ y,x,z; & y,\bar{x},\bar{z}; & \bar{y},x,\bar{z}; & \bar{y},\bar{x},z; & z,y,x; & z,\bar{y},\bar{x}; & \bar{z},y,\bar{x}; & \bar{z},\bar{y},x; & x,z,y; & x,\bar{z},\bar{y}; & \bar{x},z,\bar{y}; & \bar{x},\bar{z},y \end{array}\right|$$

$$A=4\{\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky+\cos 2\pi kx \cos 2\pi hy]+\cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly+\cos 2\pi lx \cos 2\pi ky]+ \cos 2\pi kz[\cos 2\pi lx \cos 2\pi hy+\cos 2\pi hx \cos 2\pi ly]\}$$

$$B=-4\{\sin 2\pi lz[\sin 2\pi hx \sin 2\pi ky+\sin 2\pi kx \sin 2\pi hy]+\sin 2\pi hz[\sin 2\pi kx \sin 2\pi ly+\sin 2\pi lx \sin 2\pi ky]+ \sin 2\pi kz[\sin 2\pi lx \sin 2\pi hy+\sin 2\pi hx \sin 2\pi ly]\} \quad =0 \text{ if } h=0 \text{ or } k=0 \text{ or } l=0$$

$$|F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$$\alpha(hkl)=\alpha(klh)=\alpha(lhk)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$$

$\rho(XYZ)$ as for No. 195.

$F\bar{4}3m$ T_d^2

No. 216

Origin at $\bar{4}3m$.

$$(0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0)+\left|\begin{array}{llllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & y,x,z; & y,\bar{x},\bar{z}; & \bar{y},x,\bar{z}; & \bar{y},\bar{x},z; \\ y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & z,y,x; & z,\bar{y},\bar{x}; & \bar{z},y,\bar{x}; & \bar{z},\bar{y},x; \\ z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; & x,z,y; & x,\bar{z},\bar{y}; & \bar{x},z,\bar{y}; & \bar{x},\bar{z},y \end{array}\right|$$

$$A=16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\{\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky+\cos 2\pi kx \cos 2\pi hy]+ \cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly+\cos 2\pi lx \cos 2\pi ky]+\cos 2\pi kz[\cos 2\pi lx \cos 2\pi hy+\cos 2\pi hx \cos 2\pi ly]\}$$

$$B=-16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\{\sin 2\pi lz[\sin 2\pi hx \sin 2\pi ky+\sin 2\pi kx \sin 2\pi hy]+ \sin 2\pi hz[\sin 2\pi kx \sin 2\pi ly+\sin 2\pi lx \sin 2\pi ky]+\sin 2\pi kz[\sin 2\pi lx \sin 2\pi hy+\sin 2\pi hx \sin 2\pi ly]\}$$

$B=0$ if $h=0$ (or $k=0$ or $l=0$)

h, k, l all even or all odd; A and B as for No. 215 (above) but with numerical factor 16 instead of 4.

h, k, l mixed even and odd; $A=B=0$

$|F(hkl)|$ and $\alpha(hkl)$ relationships, and $\rho(XYZ)$ as for No. 215.

No. 217 $I\bar{4}3m$ T_d^3

Origin at $\bar{4}3m$.

$$(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) + \left|\begin{array}{llllllllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; \\ y,x,z; & y,\bar{x},\bar{z}; & \bar{y},x,\bar{z}; & \bar{y},\bar{x},z; & z,y,x; & z,\bar{y},\bar{x}; & \bar{z},y,\bar{x}; & \bar{z},\bar{y},x; & x,z,y; & x,\bar{z},\bar{y}; & \bar{x},z,\bar{y}; & \bar{x},\bar{z},y \end{array}\right|$$

$$A = 8\cos^2 2\pi\frac{h+k+l}{4}\{\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky + \cos 2\pi kx\cos 2\pi hy] + \cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly + \cos 2\pi lx\cos 2\pi ky] + \cos 2\pi kz[\cos 2\pi lx\cos 2\pi hy + \cos 2\pi hx\cos 2\pi ly]\}$$

$$B = -8\cos^2 2\pi\frac{h+k+l}{4}\{\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky + \sin 2\pi kx\sin 2\pi hy] + \sin 2\pi hz[\sin 2\pi kx\sin 2\pi ly + \sin 2\pi lx\sin 2\pi ky] + \sin 2\pi kz[\sin 2\pi lx\sin 2\pi hy + \sin 2\pi hx\sin 2\pi ly]\}$$

$B=0$ if $h=0$ (or $k=0$ or $l=0$)

$h+k+l=2n$ A and B as for No. 215 (page 508) but with numerical factor 8 instead of 4.

$h+k+l=2n+1$ $A=B=0$

$|F(hkl)|$ and $\alpha(hkl)$ relationships, and $\rho(XYZ)$ as for No. 215.

No. 218 $P\bar{4}3n$ T_d^4

Origin at 23.

$$\left|\begin{array}{llllllllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & \tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}+z; & \tfrac{1}{2}+y,\tfrac{1}{2}-x,\tfrac{1}{2}-z; & \tfrac{1}{2}-y,\tfrac{1}{2}+x,\tfrac{1}{2}-z; & \tfrac{1}{2}-y,\tfrac{1}{2}-x,\tfrac{1}{2}+z; \\ y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & \tfrac{1}{2}+z,\tfrac{1}{2}+y,\tfrac{1}{2}+x; & \tfrac{1}{2}+z,\tfrac{1}{2}-y,\tfrac{1}{2}-x; & \tfrac{1}{2}-z,\tfrac{1}{2}+y,\tfrac{1}{2}-x; & \tfrac{1}{2}-z,\tfrac{1}{2}-y,\tfrac{1}{2}+x; \\ z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; & \tfrac{1}{2}+x,\tfrac{1}{2}+z,\tfrac{1}{2}+y; & \tfrac{1}{2}+x,\tfrac{1}{2}-z,\tfrac{1}{2}-y; & \tfrac{1}{2}-x,\tfrac{1}{2}+z,\tfrac{1}{2}-y; & \tfrac{1}{2}-x,\tfrac{1}{2}-z,\tfrac{1}{2}+y \end{array}\right|$$

$$A = 4\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz + \cos 2\pi kx\cos 2\pi ly\cos 2\pi hz + \cos 2\pi lx\cos 2\pi hy\cos 2\pi kz + \cos\pi(h+k+l)[\cos 2\pi kx\cos 2\pi hy\cos 2\pi lz + \cos 2\pi lx\cos 2\pi ky\cos 2\pi hz + \cos 2\pi hx\cos 2\pi ly\cos 2\pi kz]\}$$

$$B = -4\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz + \sin 2\pi kx\sin 2\pi ly\sin 2\pi hz + \sin 2\pi lx\sin 2\pi hy\sin 2\pi kz + \cos\pi(h+k+l)[\sin 2\pi kx\sin 2\pi hy\sin 2\pi lz + \sin 2\pi lx\sin 2\pi ky\sin 2\pi hz + \sin 2\pi hx\sin 2\pi ly\sin 2\pi kz]\}$$

$B=0$ if $h=0$ (or $k=0$ or $l=0$) $\alpha(hkl)=\alpha(klh)=\alpha(lhk)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$

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(1) $h+k+l=2n$ A and B as for No. 215 (page 508) $\alpha(hkl)=\alpha(khl)$

(2) $h+k+l=2n+1$

$$A = 4\{\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky - \cos 2\pi kx\cos 2\pi hy] + \cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly - \cos 2\pi lx\cos 2\pi ky] + \cos 2\pi kz[\cos 2\pi lx\cos 2\pi hy - \cos 2\pi hx\cos 2\pi ly]\}$$

$$B = -4\{\sin 2\pi lz[\sin 2\pi hx\sin 2\pi ky - \sin 2\pi kx\sin 2\pi hy] + \sin 2\pi hz[\sin 2\pi kx\sin 2\pi ly - \sin 2\pi lx\sin 2\pi ky] + \sin 2\pi kz[\sin 2\pi lx\sin 2\pi hy - \sin 2\pi hx\sin 2\pi ly]\}$$

$\alpha(hkl)=\pi+\alpha(khl)$

$A=B=0$ if $h=\pm k$ (or $k=\pm l$ or $l=\pm h$)

$|F(hkl)|$ relationships, and $\rho(XYZ)$ as for No. 215.

$F\bar{4}3c$ T_d^5

No. 219

Origin at 23.

$$(0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0)+\left|\begin{array}{llllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & y,x,\tfrac{1}{2}+z; & y,\bar{x},\tfrac{1}{2}-z; & \bar{y},x,\tfrac{1}{2}-z; & \bar{y},\bar{x},\tfrac{1}{2}+z; \\ y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & z,y,\tfrac{1}{2}+x; & z,\bar{y},\tfrac{1}{2}-x; & \bar{z},y,\tfrac{1}{2}-x; & \bar{z},\bar{y},\tfrac{1}{2}+x; \\ z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; & x,z,\tfrac{1}{2}+y; & x,\bar{z},\tfrac{1}{2}-y; & \bar{x},z,\tfrac{1}{2}-y; & \bar{x},\bar{z},\tfrac{1}{2}+y \end{array}\right|$$

$$A=16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+ \cos 2\pi lx\cos 2\pi hy\cos 2\pi kz+\cos \pi l[\cos 2\pi kx\cos 2\pi hy\cos 2\pi lz+ \cos 2\pi lx\cos 2\pi ky\cos 2\pi hz+\cos 2\pi hx\cos 2\pi ly\cos 2\pi kz]\}$$

$$B=-16\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\{\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz+ \sin 2\pi lx\sin 2\pi hy\sin 2\pi kz+\cos \pi l[\sin 2\pi kx\sin 2\pi hy\sin 2\pi lz+ \sin 2\pi lx\sin 2\pi ky\sin 2\pi hz+\sin 2\pi hx\sin 2\pi ly\sin 2\pi kz]\}$$

$B=0$ if $h=0$ (or $k=0$ or $l=0$)

h, k, l all even A, B as for $P\bar{4}3m$ (page 508), but with numerical factor 16 instead of 4. $\alpha(hkl)=\alpha(khl)$

h, k, l all odd A, B as for $P\bar{4}3n$ (2) (page 509), but with numerical factor 16 instead of 4. $\alpha(hkl)=\pi+\alpha(khl)$

h, k, l mixed even and odd: $A=B=0$

$|F(hkl)|$ and $\alpha(hkl)$ relationships, and $\rho(XYZ)$ as for No. 218.

$I\bar{4}3d$ T_d^6

No. 220

Origin on 3 at mid-point of three pairs of non-intersecting 2-axes. $(0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+$

$$\left|\begin{array}{llllllll} x,y,z; & \tfrac{1}{2}+x,\tfrac{1}{2}-y,\bar{z}; & \tfrac{1}{2}-x,\bar{y},\tfrac{1}{2}+z; & \bar{x},\tfrac{1}{2}+y,\tfrac{1}{2}-z; & \tfrac{1}{4}+y,\tfrac{1}{4}+x,\tfrac{1}{4}+z; & \tfrac{3}{4}+y,\tfrac{1}{4}-x,\tfrac{3}{4}-z; & \tfrac{1}{4}-y,\tfrac{3}{4}-x,\tfrac{3}{4}+z; & \tfrac{3}{4}-y,\tfrac{3}{4}+x,\tfrac{1}{4}-z; \\ y,z,x; & \tfrac{1}{2}+y,\tfrac{1}{2}-z,\bar{x}; & \tfrac{1}{2}-y,\bar{z},\tfrac{1}{2}+x; & \bar{y},\tfrac{1}{2}+z,\tfrac{1}{2}-x; & \tfrac{1}{4}+z,\tfrac{1}{4}+y,\tfrac{1}{4}+x; & \tfrac{3}{4}+z,\tfrac{1}{4}-y,\tfrac{3}{4}-x; & \tfrac{1}{4}-z,\tfrac{3}{4}-y,\tfrac{3}{4}+x; & \tfrac{3}{4}-z,\tfrac{3}{4}+y,\tfrac{1}{4}-x; \\ z,x,y; & \tfrac{1}{2}+z,\tfrac{1}{2}-x,\bar{y}; & \tfrac{1}{2}-z,\bar{x},\tfrac{1}{2}+y; & \bar{z},\tfrac{1}{2}+x,\tfrac{1}{2}-y; & \tfrac{1}{4}+x,\tfrac{1}{4}+z,\tfrac{1}{4}+y; & \tfrac{3}{4}+x,\tfrac{1}{4}-z,\tfrac{3}{4}-y; & \tfrac{1}{4}-x,\tfrac{3}{4}-z,\tfrac{3}{4}+y; & \tfrac{3}{4}-x,\tfrac{3}{4}+z,\tfrac{1}{4}-y \end{array}\right|$$

$$A=8\cos 2\pi\frac{h+k+l}{4}\Big\{\cos 2\pi\Big(hx+\frac{l}{4}\Big)\cos 2\pi\Big(ky+\frac{h}{4}\Big)\cos 2\pi\Big(lz+\frac{k}{4}\Big)+\cos 2\pi\Big(kx+\frac{h}{4}\Big)\cos 2\pi\Big(ly+\frac{k}{4}\Big)\cos 2\pi\Big(hz+\frac{l}{4}\Big)+ \cos 2\pi\Big(lx+\frac{k}{4}\Big)\cos 2\pi\Big(hy+\frac{l}{4}\Big)\cos 2\pi\Big(kz+\frac{h}{4}\Big)+\cos 2\pi\frac{h+k+l}{4}\Big[\cos 2\pi\Big(kx+\frac{l}{4}\Big)\cos 2\pi\Big(hy+\frac{k}{4}\Big)\cos 2\pi\Big(lz+\frac{h}{4}\Big)+ \cos 2\pi\Big(lx+\frac{h}{4}\Big)\cos 2\pi\Big(ky+\frac{l}{4}\Big)\cos 2\pi\Big(hz+\frac{k}{4}\Big)+\cos 2\pi\Big(hx+\frac{k}{4}\Big)\cos 2\pi\Big(ly+\frac{h}{4}\Big)\cos 2\pi\Big(kz+\frac{l}{4}\Big)\Big]\Big\}$$

$$B=-8\cos 2\pi\frac{h+k+l}{4}\Big\{\sin 2\pi\Big(hx+\frac{l}{4}\Big)\sin 2\pi\Big(ky+\frac{h}{4}\Big)\sin 2\pi\Big(lz+\frac{k}{4}\Big)+\sin 2\pi\Big(kx+\frac{h}{4}\Big)\sin 2\pi\Big(ly+\frac{k}{4}\Big)\sin 2\pi\Big(hz+\frac{l}{4}\Big)+ \sin 2\pi\Big(lx+\frac{k}{4}\Big)\sin 2\pi\Big(hy+\frac{l}{4}\Big)\sin 2\pi\Big(kz+\frac{h}{4}\Big)+\cos 2\pi\frac{h+k+l}{4}\Big[\sin 2\pi\Big(kx+\frac{l}{4}\Big)\sin 2\pi\Big(hy+\frac{k}{4}\Big)\sin 2\pi\Big(lz+\frac{h}{4}\Big)+ \sin 2\pi\Big(lx+\frac{h}{4}\Big)\sin 2\pi\Big(ky+\frac{l}{4}\Big)\sin 2\pi\Big(hz+\frac{k}{4}\Big)+\sin 2\pi\Big(hx+\frac{k}{4}\Big)\sin 2\pi\Big(ly+\frac{h}{4}\Big)\sin 2\pi\Big(kz+\frac{l}{4}\Big)\Big]\Big\}$$

$\alpha(hkl)=\alpha(klh)=\alpha(lhk)$; $|F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

(1) $\begin{cases} h, k, l \text{ all even} \\ h+k+l=4n \end{cases}$ A, B as for $P\bar{4}3m$ (page 508), but with numerical factor 8 instead of 4.

$B=0$ if $h=0$ or $k=0$ or $l=0$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\alpha(khl)$

(2) $\begin{cases} h \text{ even;} \quad k, l \text{ odd} \\ h+k+l=4n \end{cases}$

$$A=-8\{\sin 2\pi hx[\cos 2\pi ky \sin 2\pi lz+\cos 2\pi ly \sin 2\pi kz]+ \sin 2\pi hy[\cos 2\pi kz \sin 2\pi lx+\cos 2\pi lz \sin 2\pi kx]+ \sin 2\pi hz[\cos 2\pi kx \sin 2\pi ly+\cos 2\pi lx \sin 2\pi ky]\} \quad =0 \text{ if } h=0$$

$$B=8\{\cos 2\pi hx[\sin 2\pi ky \cos 2\pi lz+\sin 2\pi ly \cos 2\pi kz]+ \cos 2\pi hy[\sin 2\pi kz \cos 2\pi lx+\sin 2\pi lz \cos 2\pi kx]+ \cos 2\pi hz[\sin 2\pi kx \cos 2\pi ly+\sin 2\pi lx \cos 2\pi ky]\}$$

$A=B=0$ if $k=-l$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})=\alpha(khl)$

(3) $\begin{cases} k \text{ even;} \quad h, l \text{ odd} \\ h+k+l=4n \end{cases}$ Change $h\to k\to l\to h$ in formulae (2)

$A=0$ if $k=0$; $A=B=0$ if $l=-h$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$=\alpha(khl)$

(4) $\begin{cases} l \text{ even;} \quad h, k \text{ odd} \\ h+k+l=4n \end{cases}$ Change $h\to l\to k\to h$ in formulae (2)

$A=0$ if $l=0$; $A=B=0$ if $h=-k$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$
$=\alpha(khl)$

(5) $\begin{cases} h, k, l \text{ all even} \\ h+k+l=4n+2 \end{cases}$ A, B as for $P\bar{4}3n$ (2) (page 509), but with numerical factor 8 instead of 4.

$B=0$ if $h=0$ (or $k=0$ or $l=0$)

$A=B=0$ if $h=\pm k$ (or $k=\pm l$ or $l=\pm h$)

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\pi+\alpha(khl)$

(6) $\begin{cases} h \text{ even;} \quad k, l \text{ odd} \\ h+k+l=4n+2 \end{cases}$

$$A=-8\{\sin 2\pi hx[\cos 2\pi ky \sin 2\pi lz-\cos 2\pi ly \sin 2\pi kz]+ \sin 2\pi hy[\cos 2\pi kz \sin 2\pi lx-\cos 2\pi lz \sin 2\pi kx]+ \sin 2\pi hz[\cos 2\pi kx \sin 2\pi ly-\cos 2\pi lx \sin 2\pi ky]\} \quad =0 \text{ if } h=0$$

$$B=8\{\cos 2\pi hx[\sin 2\pi ky \cos 2\pi lz-\sin 2\pi ly \cos 2\pi kz]+ \cos 2\pi hy[\sin 2\pi kz \cos 2\pi lx-\sin 2\pi lz \cos 2\pi kx]+ \cos 2\pi hz[\sin 2\pi kx \cos 2\pi ly-\sin 2\pi lx \cos 2\pi ky]\}$$

$A=B=0$ if $k=l$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})=\pi+\alpha(khl)$

(7) $\begin{cases} k \text{ even;} \quad h, l \text{ odd} \\ h+k+l=4n+2 \end{cases}$ Change $h\to k\to l\to h$ in formulae (6)

$A=0$ if $k=0$; $A=B=0$ if $l=h$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=\pi-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})$
$=\pi+\alpha(khl)$

(8) $\begin{cases} l \text{ even;} \quad h, k \text{ odd} \\ h+k+l=4n+2 \end{cases}$ Change $h\to l\to k\to h$ in formulae (6)

$A=0$ if $l=0$; $A=B=0$ if $h=k$ $\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=\pi-\alpha(h\bar{k}l)=\pi-\alpha(hk\bar{l})$
$=\pi+\alpha(khl)$

$h+k+l=2n+1$ $A=B=0$

$\rho(XYZ)$ as for No. 198.

$Pm3m$ O_h^1

No. 221

Origin at centre at $m3m$.

$$\pm\left|\begin{array}{llllllllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; \\ y,x,z; & y,\bar{x},\bar{z}; & \bar{y},x,\bar{z}; & \bar{y},\bar{x},z; & z,y,x; & z,\bar{y},\bar{x}; & \bar{z},y,\bar{x}; & \bar{z},\bar{y},x; & x,z,y; & x,\bar{z},\bar{y}; & \bar{x},z,\bar{y}; & \bar{x},\bar{z},y \end{array}\right|$$

$$A=8\{\cos 2\pi hx[\cos 2\pi ky \cos 2\pi lz+\cos 2\pi ly \cos 2\pi kz]+\cos 2\pi hy[\cos 2\pi kz \cos 2\pi lx+\cos 2\pi lz \cos 2\pi kx]+ \cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly+\cos 2\pi lx \cos 2\pi ky]\}$$

$B=0$ $\qquad F(hkl)=F(klh)=F(lhk)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty F(hkl)\cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ$$

$Pn3n$ O_h^2

No. 222

Origin at 43 (at $\bar{\frac{1}{4}},\bar{\frac{1}{4}},\bar{\frac{1}{4}}$ from centre at $\bar{3}$).

$$\left|\begin{array}{llllllll} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & \frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z; & \frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z; & \frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z; & \frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z; \\ y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & \frac{1}{2}-y,\frac{1}{2}-z,\frac{1}{2}-x; & \frac{1}{2}-y,\frac{1}{2}+z,\frac{1}{2}+x; & \frac{1}{2}+y,\frac{1}{2}-z,\frac{1}{2}+x; & \frac{1}{2}+y,\frac{1}{2}+z,\frac{1}{2}-x; \\ z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; & \frac{1}{2}-z,\frac{1}{2}-x,\frac{1}{2}-y; & \frac{1}{2}-z,\frac{1}{2}+x,\frac{1}{2}+y; & \frac{1}{2}+z,\frac{1}{2}-x,\frac{1}{2}+y; & \frac{1}{2}+z,\frac{1}{2}+x,\frac{1}{2}-y; \\ \bar{y},\bar{x},\bar{z}; & \bar{y},x,z; & y,\bar{x},z; & y,x,\bar{z}; & \frac{1}{2}+y,\frac{1}{2}+x,\frac{1}{2}+z; & \frac{1}{2}+y,\frac{1}{2}-x,\frac{1}{2}-z; & \frac{1}{2}-y,\frac{1}{2}+x,\frac{1}{2}-z; & \frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}+z; \\ \bar{z},\bar{y},\bar{x}; & \bar{z},y,x; & z,\bar{y},x; & z,y,\bar{x}; & \frac{1}{2}+z,\frac{1}{2}+y,\frac{1}{2}+x; & \frac{1}{2}+z,\frac{1}{2}-y,\frac{1}{2}-x; & \frac{1}{2}-z,\frac{1}{2}+y,\frac{1}{2}-x; & \frac{1}{2}-z,\frac{1}{2}-y,\frac{1}{2}+x; \\ \bar{x},\bar{z},\bar{y}; & \bar{x},z,y; & x,\bar{z},y; & x,z,\bar{y}; & \frac{1}{2}+x,\frac{1}{2}+z,\frac{1}{2}+y; & \frac{1}{2}+x,\frac{1}{2}-z,\frac{1}{2}-y; & \frac{1}{2}-x,\frac{1}{2}+z,\frac{1}{2}-y; & \frac{1}{2}-x,\frac{1}{2}-z,\frac{1}{2}+y \end{array}\right|$$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\{\cos 2\pi hx[\cos 2\pi ky \cos 2\pi lz+\cos 2\pi ly \cos 2\pi kz]+ \cos 2\pi hy[\cos 2\pi kz \cos 2\pi lx+\cos 2\pi lz \cos 2\pi kx]+ \cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly+\cos 2\pi lx \cos 2\pi ky]\}$$

$$B=-8\sin^2 2\pi\frac{h+k+l}{4}\{\sin 2\pi hx[\sin 2\pi ky \sin 2\pi lz-\sin 2\pi ly \sin 2\pi kz]+ \sin 2\pi hy[\sin 2\pi kz \sin 2\pi lx-\sin 2\pi lz \sin 2\pi kx]+ \sin 2\pi hz[\sin 2\pi kx \sin 2\pi ly-\sin 2\pi lx \sin 2\pi ky]\}$$

$\alpha(hkl)=\alpha(klh)=\alpha(lhk)$; $\qquad |F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$

$h+k+l=2n$ $\quad A=8\,\{\cos 2\pi hx[\cos 2\pi ky \cos 2\pi lz+\cos 2\pi ly \cos 2\pi kz]+$

$\cos 2\pi hy[\cos 2\pi kz \cos 2\pi lx+\cos 2\pi lz \cos 2\pi kx]+$

$\cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly+\cos 2\pi lx \cos 2\pi ky]\}$

$B=0$ $\quad \alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=m\pi=\alpha(khl)$

$h+k+l=2n+1$ $\quad A=0$

$B=-8\{\sin 2\pi hx[\sin 2\pi ky \sin 2\pi lz-\sin 2\pi ly \sin 2\pi kz]+$

$\sin 2\pi hy[\sin 2\pi kz \sin 2\pi lx-\sin 2\pi lz \sin 2\pi kx]+$

$\sin 2\pi hz[\sin 2\pi kx \sin 2\pi ly-\sin 2\pi lx \sin 2\pi ky]\}$

$A=B=0$ if $h=0$ (etc.) or $h=\pm k$ (etc.)

$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=m\pi+\frac{\pi}{2}=\pi+\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|\cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ \cos m\pi-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|\sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ \cos m\pi\right\}$$

where m=0 or 1 according as A (or if $A=0$, then B) is positive or negative.

$Pn3n$ O_h^2

No. 222

Origin at centre at $\bar{3}$.

	x,y,z;	$x,\frac{1}{2}-y,\frac{1}{2}-z$;	$\frac{1}{2}-x,y,\frac{1}{2}-z$;	$\frac{1}{2}-x,\frac{1}{2}-y,z$;	$y,x,\frac{1}{2}-z$;	$y,\frac{1}{2}-x,z$;	$\frac{1}{2}-y,x,z$;	$\frac{1}{2}-y,\frac{1}{2}-x,\frac{1}{2}-z$;
$\pm$	y,z,x;	$y,\frac{1}{2}-z,\frac{1}{2}-x$;	$\frac{1}{2}-y,z,\frac{1}{2}-x$;	$\frac{1}{2}-y,\frac{1}{2}-z,x$;	$z,y,\frac{1}{2}-x$;	$z,\frac{1}{2}-y,x$;	$\frac{1}{2}-z,y,x$;	$\frac{1}{2}-z,\frac{1}{2}-y,\frac{1}{2}-x$;
	z,x,y;	$z,\frac{1}{2}-x,\frac{1}{2}-y$;	$\frac{1}{2}-z,x,\frac{1}{2}-y$;	$\frac{1}{2}-z,\frac{1}{2}-x,y$;	$x,z,\frac{1}{2}-y$;	$x,\frac{1}{2}-z,y$;	$\frac{1}{2}-x,z,y$;	$\frac{1}{2}-x,\frac{1}{2}-z,\frac{1}{2}-y$

$$A=8\left\{\cos 2\pi\left(lz+\frac{h+k}{4}\right)\left[\cos 2\pi\left(hx-\frac{k+l}{4}\right)\cos 2\pi\left(ky-\frac{h-l}{4}\right)+\cos 2\pi\left(hy+\frac{k+l}{4}\right)\cos 2\pi\left(kx+\frac{h+l}{4}\right)\right]+\right.$$
$$\cos 2\pi\left(lx+\frac{h+k}{4}\right)\left[\cos 2\pi\left(hy-\frac{k+l}{4}\right)\cos 2\pi\left(kz-\frac{h-l}{4}\right)+\cos 2\pi\left(hz+\frac{k+l}{4}\right)\cos 2\pi\left(ky+\frac{h+l}{4}\right)\right]+$$
$$\left.\cos 2\pi\left(ly+\frac{h+k}{4}\right)\left[\cos 2\pi\left(hz-\frac{k+l}{4}\right)\cos 2\pi\left(kx-\frac{h-l}{4}\right)+\cos 2\pi\left(hx+\frac{k+l}{4}\right)\cos 2\pi\left(kz+\frac{h+l}{4}\right)\right]\right\}$$

$B=0$ $\quad F(hkl)=F(klh)=F(lhk)$

---

(1) $h=2n$, $k=2n$, $l=2n$ $\quad A=8\{\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky+\cos 2\pi hy \cos 2\pi kx]+$

$\cos 2\pi lx[\cos 2\pi hy \cos 2\pi kz+\cos 2\pi hz \cos 2\pi ky]+$

$\cos 2\pi ly[\cos 2\pi hz \cos 2\pi kx+\cos 2\pi hx \cos 2\pi kz]\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

(2) $h=2n+1$, $k=2n+1$, $l=2n$ $\quad A=-8\{\cos 2\pi lz[\sin 2\pi hx \sin 2\pi ky+\sin 2\pi hy \sin 2\pi kx]+$

$\cos 2\pi lx[\sin 2\pi hy \sin 2\pi kz+\sin 2\pi hz \sin 2\pi ky]+$

$\cos 2\pi ly[\sin 2\pi hz \sin 2\pi kx+\sin 2\pi hx \sin 2\pi kz]\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

(3) h even; k, l odd Change $h\to k\to l\to h$ in formulae (2) $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$

(4) k even; h, l odd Change $h\to l\to k\to h$ in formulae (2) $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$

(5) $\begin{cases} h = 2n+1 \\ k = 2n+1 \\ l = 2n+1 \end{cases}$ $A=8\{\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky - \cos 2\pi kx \cos 2\pi hy] + \cos 2\pi lx[\cos 2\pi hy \cos 2\pi kz - \cos 2\pi ky \cos 2\pi hz] + \cos 2\pi ly[\cos 2\pi hz \cos 2\pi kx - \cos 2\pi kz \cos 2\pi hx]\}$

$A=B=0$ if $h=\pm k$ (or $k=\pm l$ or $l=\pm h$) $\quad F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

(6) $\begin{cases} h = 2n \\ k = 2n \\ l = 2n+1 \end{cases}$ $A=-8\{\cos 2\pi lz[\sin 2\pi hx \sin 2\pi ky - \sin 2\pi kx \sin 2\pi hy] + \cos 2\pi lx[\sin 2\pi hy \sin 2\pi kz - \sin 2\pi ky \sin 2\pi hz] + \cos 2\pi ly[\sin 2\pi hz \sin 2\pi kx - \sin 2\pi kz \sin 2\pi hx]\}$ $\quad =-F(khl)$

$A=B=0$ if $h=0$ or $k=0$ or $h=\pm k$ $\quad F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

(7) h odd; k, l even Change $h\to k\to l\to h$ in formulae (6) $\quad =-F(khl)$

$A=B=0$ if $k=0$ or $l=0$ or $k=\pm l$ $\quad F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

(8) k odd; h, l even Change $h\to l\to k\to h$ in formulae (6) $\quad =-F(khl)$

$A=B=0$ if $l=0$ or $h=0$ or $l=\pm h$

$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n} F(hkl)\cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ - \sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\,k+l=2n+1} F(hkl)\sin 2\pi hX \sin 2\pi kY \cos 2\pi lZ - \sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n} F(hkl)\cos 2\pi hX \sin 2\pi kY \sin 2\pi lZ - \sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\,k+l=2n+1} F(hkl)\sin 2\pi hX \cos 2\pi kY \sin 2\pi lZ\Big\}$$

$Pm3n$ $\quad$ No. 223

O_h^3

Origin at centre at $m3$.

$$\pm\left|\begin{matrix} x,y,z; & x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \bar{x},\bar{y},z; & \tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}+z; & \tfrac{1}{2}+y,\tfrac{1}{2}-x,\tfrac{1}{2}-z; & \tfrac{1}{2}-y,\tfrac{1}{2}+x,\tfrac{1}{2}-z; & \tfrac{1}{2}-y,\tfrac{1}{2}-x,\tfrac{1}{2}+z; \\ y,z,x; & y,\bar{z},\bar{x}; & \bar{y},z,\bar{x}; & \bar{y},\bar{z},x; & \tfrac{1}{2}+z,\tfrac{1}{2}+y,\tfrac{1}{2}+x; & \tfrac{1}{2}+z,\tfrac{1}{2}-y,\tfrac{1}{2}-x; & \tfrac{1}{2}-z,\tfrac{1}{2}+y,\tfrac{1}{2}-x; & \tfrac{1}{2}-z,\tfrac{1}{2}-y,\tfrac{1}{2}+x; \\ z,x,y; & z,\bar{x},\bar{y}; & \bar{z},x,\bar{y}; & \bar{z},\bar{x},y; & \tfrac{1}{2}+x,\tfrac{1}{2}+z,\tfrac{1}{2}+y; & \tfrac{1}{2}+x,\tfrac{1}{2}-z,\tfrac{1}{2}-y; & \tfrac{1}{2}-x,\tfrac{1}{2}+z,\tfrac{1}{2}-y; & \tfrac{1}{2}-x,\tfrac{1}{2}-z,\tfrac{1}{2}+y \end{matrix}\right|$$

$A=8\{\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz + \cos 2\pi kx \cos 2\pi ly \cos 2\pi hz + \cos 2\pi lx \cos 2\pi hy \cos 2\pi kz + \cos \pi(h+k+l)[\cos 2\pi kx \cos 2\pi hy \cos 2\pi lz + \cos 2\pi lx \cos 2\pi ky \cos 2\pi hz + \cos 2\pi hx \cos 2\pi ly \cos 2\pi kz]\}$

$B=0$ $\quad F(hkl)=F(klh)=F(lhk)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=(hk\bar{l})$

(1) $h+k+l=2n$ $\quad A=8\{\cos 2\pi hx[\cos 2\pi ky \cos 2\pi lz + \cos 2\pi ly \cos 2\pi kz] + \cos 2\pi hy[\cos 2\pi kz \cos 2\pi lx + \cos 2\pi lz \cos 2\pi kx] + \cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly + \cos 2\pi lx \cos 2\pi ky]\}$

$F(hkl)=F(khl)$

(2) $h+k+l=2n+1$ $\quad A=8\{\cos 2\pi hx[\cos 2\pi ky \cos 2\pi lz - \cos 2\pi ly \cos 2\pi kz] + \cos 2\pi hy[\cos 2\pi kz \cos 2\pi lx - \cos 2\pi lz \cos 2\pi kx] + \cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly - \cos 2\pi lx \cos 2\pi ky]\}$

$F(hkl)=-F(khl)$

$A=B=0$ if $h=\pm k$ (etc.)

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty F(hkl)\cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ$$

$Pn3m$ O_h^4

Origin at $\bar{4}3m$ (at $\bar{\tfrac{1}{4}},\bar{\tfrac{1}{4}},\bar{\tfrac{1}{4}}$ from centre at $\bar{3}m$).

x,y,z;	$x,\bar{y},\bar{z}$;	$\bar{x},y,\bar{z}$;	$\bar{x},\bar{y},z$;	$\tfrac{1}{2}-x,\tfrac{1}{2}-y,\tfrac{1}{2}-z$;	$\tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{2}+z$;	$\tfrac{1}{2}+x,\tfrac{1}{2}-y,\tfrac{1}{2}+z$;	$\tfrac{1}{2}+x,\tfrac{1}{2}+y,\tfrac{1}{2}-z$;
y,z,x;	$y,\bar{z},\bar{x}$;	$\bar{y},z,\bar{x}$;	$\bar{y},\bar{z},x$;	$\tfrac{1}{2}-y,\tfrac{1}{2}-z,\tfrac{1}{2}-x$;	$\tfrac{1}{2}-y,\tfrac{1}{2}+z,\tfrac{1}{2}+x$;	$\tfrac{1}{2}+y,\tfrac{1}{2}-z,\tfrac{1}{2}+x$;	$\tfrac{1}{2}+y,\tfrac{1}{2}+z,\tfrac{1}{2}-x$;
z,x,y;	$z,\bar{x},\bar{y}$;	$\bar{z},x,\bar{y}$;	$\bar{z},\bar{x},y$;	$\tfrac{1}{2}-z,\tfrac{1}{2}-x,\tfrac{1}{2}-y$;	$\tfrac{1}{2}-z,\tfrac{1}{2}+x,\tfrac{1}{2}+y$;	$\tfrac{1}{2}+z,\tfrac{1}{2}-x,\tfrac{1}{2}+y$;	$\tfrac{1}{2}+z,\tfrac{1}{2}+x,\tfrac{1}{2}-y$;
y,x,z;	$y,\bar{x},\bar{z}$;	$\bar{y},x,\bar{z}$;	$\bar{y},\bar{x},z$;	$\tfrac{1}{2}-y,\tfrac{1}{2}-x,\tfrac{1}{2}-z$;	$\tfrac{1}{2}-y,\tfrac{1}{2}+x,\tfrac{1}{2}+z$;	$\tfrac{1}{2}+y,\tfrac{1}{2}-x,\tfrac{1}{2}+z$;	$\tfrac{1}{2}+y,\tfrac{1}{2}+x,\tfrac{1}{2}-z$;
z,y,x;	$z,\bar{y},\bar{x}$;	$\bar{z},y,\bar{x}$;	$\bar{z},\bar{y},x$;	$\tfrac{1}{2}-z,\tfrac{1}{2}-y,\tfrac{1}{2}-x$;	$\tfrac{1}{2}-z,\tfrac{1}{2}+y,\tfrac{1}{2}+x$;	$\tfrac{1}{2}+z,\tfrac{1}{2}-y,\tfrac{1}{2}+x$;	$\tfrac{1}{2}+z,\tfrac{1}{2}+y,\tfrac{1}{2}-x$;
x,z,y;	$x,\bar{z},\bar{y}$;	$\bar{x},z,\bar{y}$;	$\bar{x},\bar{z},y$;	$\tfrac{1}{2}-x,\tfrac{1}{2}-z,\tfrac{1}{2}-y$;	$\tfrac{1}{2}-x,\tfrac{1}{2}+z,\tfrac{1}{2}+y$;	$\tfrac{1}{2}+x,\tfrac{1}{2}-z,\tfrac{1}{2}+y$;	$\tfrac{1}{2}+x,\tfrac{1}{2}+z,\tfrac{1}{2}-y$

$$A=8\cos^2 2\pi\frac{h+k+l}{4}\{\cos 2\pi hx[\cos 2\pi ky\cos 2\pi lz+\cos 2\pi ly\cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz\cos 2\pi lx+\cos 2\pi lz\cos 2\pi kx]+\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly+\cos 2\pi lx\cos 2\pi ky]\}$$

$$B=-8\sin^2 2\pi\frac{h+k+l}{4}\{\sin 2\pi hx[\sin 2\pi ky\sin 2\pi lz+\sin 2\pi ly\sin 2\pi kz]+$$
$$\sin 2\pi hy[\sin 2\pi kz\sin 2\pi lx+\sin 2\pi lz\sin 2\pi kx]+\sin 2\pi hz[\sin 2\pi kx\sin 2\pi ly+\sin 2\pi lx\sin 2\pi ky]\}$$

$$|F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}\bar{k}\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$$\alpha(hkl)=\alpha(klh)=\alpha(lhk)=\alpha(khl);$$

$h+k+l=2n$

$$A=8\{\cos 2\pi hx[\cos 2\pi ky\cos 2\pi lz+\cos 2\pi ly\cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz\cos 2\pi lx+\cos 2\pi lz\cos 2\pi kx]+$$
$$\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly+\cos 2\pi lx\cos 2\pi ky]\}$$

$B=0$ $\qquad \alpha(hkl)=\alpha(\bar{h}\bar{k}\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=\mathrm{m}\pi$

$h+k+l=2n+1$

$A=0$

$$B=-8\{\sin 2\pi hx[\sin 2\pi ky\sin 2\pi lz+\sin 2\pi ly\sin 2\pi kz]+$$
$$\sin 2\pi hy[\sin 2\pi kz\sin 2\pi lx+\sin 2\pi lz\sin 2\pi kx]+$$
$$\sin 2\pi hz[\sin 2\pi kx\sin 2\pi ly+\sin 2\pi lx\sin 2\pi ky]\}$$

$A=B=0$ if $h=0$ (or $k=0$ or $l=0$)

$$\alpha(hkl)=-\alpha(\bar{h}\bar{k}\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=\mathrm{m}\pi+\frac{\pi}{2}$$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n}|F(hkl)|\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ\cos \mathrm{m}\pi-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=2n+1}|F(hkl)|\sin 2\pi hX\sin 2\pi kY\sin 2\pi lZ\cos \mathrm{m}\pi\right\}$$

where m=0 or 1 according as A (or B) is positive or negative.

$Pn3m$ O_h^4

No. 224

Origin at centre at $\bar{3}m$.

$$\pm\left|\begin{array}{llllllll} x,y,z; & x,\tfrac{1}{2}-y,\tfrac{1}{2}-z; & \tfrac{1}{2}-x,y,\tfrac{1}{2}-z; & \tfrac{1}{2}-x,\tfrac{1}{2}-y,z; & y,x,z; & y,\tfrac{1}{2}-x,\tfrac{1}{2}-z; & \tfrac{1}{2}-y,x,\tfrac{1}{2}-z; & \tfrac{1}{2}-y,\tfrac{1}{2}-x,z; \\ y,z,x; & y,\tfrac{1}{2}-z,\tfrac{1}{2}-x; & \tfrac{1}{2}-y,z,\tfrac{1}{2}-x; & \tfrac{1}{2}-y,\tfrac{1}{2}-z,x; & z,y,x; & z,\tfrac{1}{2}-y,\tfrac{1}{2}-x; & \tfrac{1}{2}-z,y,\tfrac{1}{2}-x; & \tfrac{1}{2}-z,\tfrac{1}{2}-y,x; \\ z,x,y; & z,\tfrac{1}{2}-x,\tfrac{1}{2}-y; & \tfrac{1}{2}-z,x,\tfrac{1}{2}-y; & \tfrac{1}{2}-z,\tfrac{1}{2}-x,y; & x,z,y; & x,\tfrac{1}{2}-z,\tfrac{1}{2}-y; & \tfrac{1}{2}-x,z,\tfrac{1}{2}-y; & \tfrac{1}{2}-x,\tfrac{1}{2}-z,y \end{array}\right|$$

$$A=8\left\{\cos 2\pi\left(lz+\frac{k-h}{4}\right)\left[\cos 2\pi\left(hx+\frac{l-k}{4}\right)\cos 2\pi\left(ky+\frac{h-l}{4}\right)+\cos 2\pi\left(hy+\frac{l-k}{4}\right)\cos 2\pi\left(kx+\frac{h-l}{4}\right)\right]+\right.$$
$$\cos 2\pi\left(lx+\frac{k-h}{4}\right)\left[\cos 2\pi\left(hy+\frac{l-k}{4}\right)\cos 2\pi\left(kz+\frac{h-l}{4}\right)+\cos 2\pi\left(hz+\frac{l-k}{4}\right)\cos 2\pi\left(ky+\frac{h-l}{4}\right)\right]+$$
$$\left.\cos 2\pi\left(ly+\frac{k-h}{4}\right)\left[\cos 2\pi\left(hz+\frac{l-k}{4}\right)\cos 2\pi\left(kx+\frac{h-l}{4}\right)+\cos 2\pi\left(hx+\frac{l-k}{4}\right)\cos 2\pi\left(kz+\frac{h-l}{4}\right)\right]\right\}$$

$B=0$

$F(hkl)=F(klh)=F(lhk)=F(khl)$

(1) $\begin{cases} h+k=2n \\ k+l=2n \end{cases}$

$$A=8\{\cos 2\pi lz[\cos 2\pi hx\cos 2\pi ky+\cos 2\pi hy\cos 2\pi kx]+$$
$$\cos 2\pi lx[\cos 2\pi hy\cos 2\pi kz+\cos 2\pi hz\cos 2\pi ky]+$$
$$\cos 2\pi ly[\cos 2\pi hz\cos 2\pi kx+\cos 2\pi hx\cos 2\pi kz]\}$$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

(2) $\begin{cases} h+k=2n \\ k+l=2n+1 \end{cases}$

$$A=-8\{\cos 2\pi lz[\sin 2\pi hx\sin 2\pi ky+\sin 2\pi hy\sin 2\pi kx]+$$
$$\cos 2\pi lx[\sin 2\pi hy\sin 2\pi kz+\sin 2\pi hz\sin 2\pi ky]+$$
$$\cos 2\pi ly[\sin 2\pi hz\sin 2\pi kx+\sin 2\pi hx\sin 2\pi kz]\}$$

$A=B=0$ if $h=0$ or $k=0$ $\qquad F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

(3) $\begin{cases} h+k=2n+1 \\ k+l=2n \end{cases}$ Change $h\to k\to l\to h$ in formulae (2)

$A=B=0$ if $k=0$ or $l=0$ $\qquad F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

(4) $\begin{cases} h+k=2n+1 \\ k+l=2n+1 \end{cases}$ Change $h\to l\to k\to h$ in formulae (2)

$A=B=0$ if $l=0$ or $h=0$ $\qquad F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ k+l=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n,\ k+l=2n+1}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ k+l=2n}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k=2n+1,\ k+l=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ\right\}$$

No. 225

$Fm3m$ O_h^5

Origin at centre at $m3m$. $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)\ \pm$

	$x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ y,z,x;\ y,\bar{z},\bar{x};\ \bar{y},z,\bar{x};\ \bar{y},\bar{z},x;\ z,x,y;\ z,\bar{x},\bar{y};\ \bar{z},x,\bar{y};\ \bar{z},\bar{x},y;$
	$y,x,z;\ y,\bar{x},\bar{z};\ \bar{y},x,\bar{z};\ \bar{y},\bar{x},z;\ z,y,x;\ z,\bar{y},\bar{x};\ \bar{z},y,\bar{x};\ \bar{z},\bar{y},x;\ x,z,y;\ x,\bar{z},\bar{y};\ \bar{x},z,\bar{y};\ \bar{x},\bar{z},y$

$$A=32\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\{\cos 2\pi hx[\cos 2\pi ky\cos 2\pi lz+\cos 2\pi ly\cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz\cos 2\pi lx+\cos 2\pi lz\cos 2\pi kx]+\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly+\cos 2\pi lx\cos 2\pi ky]\}$$

$B=0$ $\qquad F(hkl)=F(klh)=F(lhk)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

h, k, l all even or all odd. A as for No. 221 (page 512), but multiplied by 4.

h, k, l mixed even and odd. $A=B=0$

$\rho(XYZ)$ as for No. 221.

No. 226

$Fm3c$ O_h^6

Origin at centre at $m3$.

$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)\ \pm$	$x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ y,x,\frac{1}{2}+z;\ y,\bar{x},\frac{1}{2}-z;\ \bar{y},x,\frac{1}{2}-z;\ \bar{y},\bar{x},\frac{1}{2}+z;$
	$y,z,x;\ y,\bar{z},\bar{x};\ \bar{y},z,\bar{x};\ \bar{y},\bar{z},x;\ z,y,\frac{1}{2}+x;\ z,\bar{y},\frac{1}{2}-x;\ \bar{z},y,\frac{1}{2}-x;\ \bar{z},\bar{y},\frac{1}{2}+x;$
	$z,x,y;\ z,\bar{x},\bar{y};\ \bar{z},x,\bar{y};\ \bar{z},\bar{x},y;\ x,z,\frac{1}{2}+y;\ x,\bar{z},\frac{1}{2}-y;\ \bar{x},z,\frac{1}{2}-y;\ \bar{x},\bar{z},\frac{1}{2}+y$

$$A=32\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\{\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+$$
$$\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz+\cos \pi l[\cos 2\pi kx\cos 2\pi hy\cos 2\pi lz+$$
$$\cos 2\pi lx\cos 2\pi ky\cos 2\pi hz+\cos 2\pi hx\cos 2\pi ly\cos 2\pi kz]\}$$

$B=0$ $\qquad F(hkl)=F(klh)=F(lhk)=F(\bar{h}\bar{k}l)=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

h, k, l all even. A as for No. 223 (1) (page 148), but multiplied by 4. $F(hkl)=F(khl)$

h, k, l all odd. A as for No. 223 (2) (page 148), but multiplied by 4. $F(hkl)=-F(khl)$

h, k, l mixed even and odd. $A=B=0$

$\rho(XYZ)$ as for No. 223.

$Fd3m$ O_h^7

No. 227

Origin at $\bar{4}3m$ (at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from centre at $\bar{3}m$). $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)$ +

x,y,z;	$x,\bar{y},\bar{z}$;	$\bar{x},y,\bar{z}$;	$\bar{x},\bar{y},z$;	$\frac{1}{4}-x,\frac{1}{4}-y,\frac{1}{4}-z$;	$\frac{1}{4}-x,\frac{1}{4}+y,\frac{1}{4}+z$;	$\frac{1}{4}+x,\frac{1}{4}-y,\frac{1}{4}+z$;	$\frac{1}{4}+x,\frac{1}{4}+y,\frac{1}{4}-z$;
y,z,x;	$y,\bar{z},\bar{x}$;	$\bar{y},z,\bar{x}$;	$\bar{y},\bar{z},x$;	$\frac{1}{4}-y,\frac{1}{4}-z,\frac{1}{4}-x$;	$\frac{1}{4}-y,\frac{1}{4}+z,\frac{1}{4}+x$;	$\frac{1}{4}+y,\frac{1}{4}-z,\frac{1}{4}+x$;	$\frac{1}{4}+y,\frac{1}{4}+z,\frac{1}{4}-x$;
z,x,y;	$z,\bar{x},\bar{y}$;	$\bar{z},x,\bar{y}$;	$\bar{z},\bar{x},y$;	$\frac{1}{4}-z,\frac{1}{4}-x,\frac{1}{4}-y$;	$\frac{1}{4}-z,\frac{1}{4}+x,\frac{1}{4}+y$;	$\frac{1}{4}+z,\frac{1}{4}-x,\frac{1}{4}+y$;	$\frac{1}{4}+z,\frac{1}{4}+x,\frac{1}{4}-y$;
y,x,z;	$y,\bar{x},\bar{z}$;	$\bar{y},x,\bar{z}$;	$\bar{y},\bar{x},z$;	$\frac{1}{4}-y,\frac{1}{4}-x,\frac{1}{4}-z$;	$\frac{1}{4}-y,\frac{1}{4}+x,\frac{1}{4}+z$;	$\frac{1}{4}+y,\frac{1}{4}-x,\frac{1}{4}+z$;	$\frac{1}{4}+y,\frac{1}{4}+x,\frac{1}{4}-z$;
z,y,x;	$z,\bar{y},\bar{x}$;	$\bar{z},y,\bar{x}$;	$\bar{z},\bar{y},x$;	$\frac{1}{4}-z,\frac{1}{4}-y,\frac{1}{4}-x$;	$\frac{1}{4}-z,\frac{1}{4}+y,\frac{1}{4}+x$;	$\frac{1}{4}+z,\frac{1}{4}-y,\frac{1}{4}+x$;	$\frac{1}{4}+z,\frac{1}{4}+y,\frac{1}{4}-x$;
x,z,y;	$x,\bar{z},\bar{y}$;	$\bar{x},z,\bar{y}$;	$\bar{x},\bar{z},y$;	$\frac{1}{4}-x,\frac{1}{4}-z,\frac{1}{4}-y$;	$\frac{1}{4}-x,\frac{1}{4}+z,\frac{1}{4}+y$;	$\frac{1}{4}+x,\frac{1}{4}-z,\frac{1}{4}+y$;	$\frac{1}{4}+x,\frac{1}{4}+z,\frac{1}{4}-y$

$A=G.\cos 2\pi\frac{h+k+l}{8}$; $B=G.\sin 2\pi\frac{h+k+l}{8}$; where

$$G=32\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\Big\{\cos 2\pi\frac{h+k+l}{8}[\cos 2\pi hx(\cos 2\pi ky\cos 2\pi lz+\cos 2\pi ly\cos 2\pi kz)+$$
$$\cos 2\pi hy(\cos 2\pi kz\cos 2\pi lx+\cos 2\pi lz\cos 2\pi kx)+\cos 2\pi hz(\cos 2\pi kx\cos 2\pi ly+\cos 2\pi lx\cos 2\pi ky)]-$$
$$\sin 2\pi\frac{h+k+l}{8}[\sin 2\pi hx(\sin 2\pi ky\sin 2\pi lz+\sin 2\pi ly\sin 2\pi kz)+$$
$$\sin 2\pi hy(\sin 2\pi kz\sin 2\pi lx+\sin 2\pi lz\sin 2\pi kx)+\sin 2\pi hz(\sin 2\pi kx\sin 2\pi ly+\sin 2\pi lx\sin 2\pi ky)]\Big\}$$

$$|F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$
$$\alpha(hkl)=\alpha(klh)=\alpha(lhk)=\alpha(khl);$$

$\begin{cases} h,k,l \text{ all even} \\ h+k+l=4n \end{cases}$

$$A=32\{\cos 2\pi hx[\cos 2\pi ky\cos 2\pi lz+\cos 2\pi ly\cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz\cos 2\pi lx+\cos 2\pi lz\cos 2\pi kx]+$$
$$\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly+\cos 2\pi lx\cos 2\pi ky]\}$$

$B=0$ $\qquad \alpha(hkl)=\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=m\pi$

$\begin{cases} h,k,l \text{ all odd} \\ h+k+l=4n+1 \end{cases}$

$$A=16\{\cos 2\pi hx[\cos 2\pi ky\cos 2\pi lz+\cos 2\pi ly\cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz\cos 2\pi lx+\cos 2\pi lz\cos 2\pi kx]+$$
$$\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly+\cos 2\pi lx\cos 2\pi ky]-$$
$$\sin 2\pi hx[\sin 2\pi ky\sin 2\pi lz+\sin 2\pi ly\sin 2\pi kz]-$$
$$\sin 2\pi hy[\sin 2\pi kz\sin 2\pi lx+\sin 2\pi lz\sin 2\pi kx]-$$
$$\sin 2\pi hz[\sin 2\pi kx\sin 2\pi ly+\sin 2\pi lx\sin 2\pi ky]\}$$

$B=A$ $\qquad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=m\pi+\frac{\pi}{4}$

$\begin{cases} h,k,l \text{ all even} \\ h+k+l=4n+2 \end{cases}$

$A=0$

$$B=-32\{\sin 2\pi hx[\sin 2\pi ky\sin 2\pi lz+\sin 2\pi ly\sin 2\pi kz]+$$
$$\sin 2\pi hy[\sin 2\pi kz\sin 2\pi lx+\sin 2\pi lz\sin 2\pi kx]+$$
$$\sin 2\pi hz[\sin 2\pi kx\sin 2\pi ly+\sin 2\pi lx\sin 2\pi ky]\}$$

$A=B=0$ if $h=0$ (etc.) $\qquad \alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=m\pi+\frac{\pi}{2}$

$\begin{cases} h, k, l \text{ all odd} \\ h+k+l=4n+3 \end{cases}$ $A=16\{\cos 2\pi hx[\cos 2\pi ky \cos 2\pi lz+\cos 2\pi ly \cos 2\pi kz]+$

$\cos 2\pi hy[\cos 2\pi kz \cos 2\pi lx+\cos 2\pi lz \cos 2\pi kx]+$

$\cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly+\cos 2\pi lx \cos 2\pi ky]+$

$\sin 2\pi hx[\sin 2\pi ky \sin 2\pi lz+\sin 2\pi ly \sin 2\pi kz]+$

$\sin 2\pi hy[\sin 2\pi kz \sin 2\pi lx+\sin 2\pi lz \sin 2\pi kx]+$

$\sin 2\pi hz[\sin 2\pi kx \sin 2\pi ly+\sin 2\pi lx \sin 2\pi ky]\}$

$B=-A$ $\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=m\pi-\frac{\pi}{4}$

h, k, l mixed even and odd $A=B=0$

$\rho(XYZ)$ as for No. 203 ($Fd3$, origin at 23, page 495).

No. 227

$Fd3m$
O_h^7

Origin at centre at $\bar{3}m$. $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)\ \pm$

$x,y,z;$	$x,\frac{1}{4}-y,\frac{1}{4}-z;$	$\frac{1}{4}-x,y,\frac{1}{4}-z;$	$\frac{1}{4}-x,\frac{1}{4}-y,z;$	$y,x,z;$	$y,\frac{1}{4}-x,\frac{1}{4}-z;$	$\frac{1}{4}-y,x,\frac{1}{4}-z;$	$\frac{1}{4}-y,\frac{1}{4}-x,z;$
$y,z,x;$	$y,\frac{1}{4}-z,\frac{1}{4}-x;$	$\frac{1}{4}-y,z,\frac{1}{4}-x;$	$\frac{1}{4}-y,\frac{1}{4}-z,x;$	$z,y,x;$	$z,\frac{1}{4}-y,\frac{1}{4}-x;$	$\frac{1}{4}-z,y,\frac{1}{4}-x;$	$\frac{1}{4}-z,\frac{1}{4}-y,x;$
$z,x,y;$	$z,\frac{1}{4}-x,\frac{1}{4}-y;$	$\frac{1}{4}-z,x,\frac{1}{4}-y;$	$\frac{1}{4}-z,\frac{1}{4}-x,y;$	$x,z,y;$	$x,\frac{1}{4}-z,\frac{1}{4}-y;$	$\frac{1}{4}-x,z,\frac{1}{4}-y;$	$\frac{1}{4}-x,\frac{1}{4}-z,y$

$A=8\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}.G$, where

$$G=\cos 2\pi(hx+ky+lz)+\cos 2\pi\left(hx+ky-lz-\frac{h+k}{4}\right)+\cos 2\pi\left(hx-ky+lz-\frac{l+h}{4}\right)+\cos 2\pi\left(-hx+ky+lz-\frac{k+l}{4}\right)+$$
$$\cos 2\pi(hy+kz+lx)+\cos 2\pi\left(hy+kz-lx-\frac{h+k}{4}\right)+\cos 2\pi\left(hy-kz+lx-\frac{l+h}{4}\right)+\cos 2\pi\left(-hy+kz+lx-\frac{k+l}{4}\right)+$$
$$\cos 2\pi(hz+kx+ly)+\cos 2\pi\left(hz+kx-ly-\frac{h+k}{4}\right)+\cos 2\pi\left(hz-kx+ly-\frac{l+h}{4}\right)+\cos 2\pi\left(-hz+kx+ly-\frac{k+l}{4}\right)+$$
$$\cos 2\pi(hy+kx+lz)+\cos 2\pi\left(hy+kx-lz-\frac{h+k}{4}\right)+\cos 2\pi\left(hy-kx+lz-\frac{l+h}{4}\right)+\cos 2\pi\left(-hy+kx+lz-\frac{k+l}{4}\right)+$$
$$\cos 2\pi(hz+ky+lx)+\cos 2\pi\left(hz+ky-lx-\frac{h+k}{4}\right)+\cos 2\pi\left(hz-ky+lx-\frac{l+h}{4}\right)+\cos 2\pi\left(-hz+ky+lx-\frac{k+l}{4}\right)+$$
$$\cos 2\pi(hx+kz+ly)+\cos 2\pi\left(hx+kz-ly-\frac{h+k}{4}\right)+\cos 2\pi\left(hx-kz+ly-\frac{l+h}{4}\right)+\cos 2\pi\left(-hx+kz+ly-\frac{k+l}{4}\right)$$

$B=0$ $F(hkl)=F(klh)=F(lhk)=F(khl)$

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(1) $\begin{cases} h+k=4n \\ k+l=4n \\ l+h=4n \end{cases}$ $A=32\{\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky+\cos 2\pi hy \cos 2\pi kx]+$

$\cos 2\pi lx[\cos 2\pi hy \cos 2\pi kz+\cos 2\pi hz \cos 2\pi ky]+$

$\cos 2\pi ly[\cos 2\pi hz \cos 2\pi kx+\cos 2\pi hx \cos 2\pi kz]\}$

$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

(2) $\begin{cases} h+k=4n \\ k+l=4n+2 \\ l+h=4n+2 \end{cases}$ $A=-32\{\cos 2\pi lz[\sin 2\pi hx \sin 2\pi ky+\sin 2\pi hy \sin 2\pi kx]+$
$\cos 2\pi lx[\sin 2\pi hy \sin 2\pi kz+\sin 2\pi hz \sin 2\pi ky]+$
$\cos 2\pi ly[\sin 2\pi hz \sin 2\pi kx+\sin 2\pi hx \sin 2\pi kz]\}$

$A=B=0$ if $h=0$ or $k=0$ $\qquad F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

(3) $\begin{cases} h+k=4n+2 \\ k+l=4n \\ l+h=4n+2 \end{cases}$ Change $h\to k\to l\to h$ in formulae (2)

$A=B=0$ if $k=0$ or $l=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

(4) $\begin{cases} h+k=4n+2 \\ k+l=4n+2 \\ l+h=4n \end{cases}$ Change $h\to l\to k\to h$ in formulae (2)

$A=B=0$ if $l=0$ or $h=0$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

(5) $\begin{cases} h+k=4n+2 \\ k+l=4n+2 \\ l+h=4n+2 \end{cases}$ $A=-32\{\cos 2\pi lz \cos \pi(h-k)(x+y) \cos \pi(h+k)(x-y)+$
$\sin 2\pi lz \sin \pi(h+k)(x+y) \cos \pi(h-k)(x-y)+$
$\cos 2\pi lx \cos \pi(h-k)(y+z) \cos \pi(h+k)(y-z)+$
$\sin 2\pi lx \sin \pi(h+k)(y+z) \cos \pi(h-k)(y-z)+$
$\cos 2\pi ly \cos \pi(h-k)(z+x) \cos \pi(h+k)(z-x)+$
$\sin 2\pi ly \sin \pi(h+k)(z+x) \cos \pi(h-k)(z-x)\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$

(6) $\begin{cases} h+k=4n \\ k+l=4n \\ l+h=4n+2 \end{cases}$ $A=32\{\cos 2\pi lz \cos \pi(h+k)(x+y) \cos \pi(h-k)(x-y)+$
$\sin 2\pi lz \sin \pi(h-k)(x+y) \cos \pi(h+k)(x-y)+$
$\cos 2\pi lx \cos \pi(h+k)(y+z) \cos \pi(h-k)(y-z)+$
$\sin 2\pi lx \sin \pi(h-k)(y+z) \cos \pi(h+k)(y-z)+$
$\cos 2\pi ly \cos \pi(h+k)(z+x) \cos \pi(h-k)(z-x)+$
$\sin 2\pi ly \sin \pi(h-k)(z+x) \cos \pi(h+k)(z-x)\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$

(7) $\begin{cases} h+k=4n+2 \\ k+l=4n \\ l+h=4n \end{cases}$ Change $h\to k\to l\to h$ in formulae (6)

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$

(8) $\begin{cases} h+k=4n \\ k+l=4n+2 \\ l+h=4n \end{cases}$ Change $h\to l\to k\to h$ in formulae (6)

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$

h, k, l mixed even and odd $\qquad A=B=0$

$\rho(XYZ)$ as for No. 70 (*Fddd*, origin at $\bar{1}$, page 413).

$Fd3c$ O_h^8

Origin at 23 (at $\bar{\tfrac{3}{8}},\bar{\tfrac{3}{8}},\bar{\tfrac{3}{8}}$ from centre at $\bar{3}$). $(0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0)+$

$x,y,z;$	$x,\bar{y},\bar{z};$	$\bar{x},y,\bar{z};$	$\bar{x},\bar{y},z;$	$\tfrac{1}{4}-x,\tfrac{1}{4}-y,\tfrac{3}{4}-z;$	$\tfrac{1}{4}-x,\tfrac{1}{4}+y,\tfrac{3}{4}+z;$	$\tfrac{1}{4}+x,\tfrac{1}{4}-y,\tfrac{3}{4}+z;$	$\tfrac{1}{4}+x,\tfrac{1}{4}+y,\tfrac{3}{4}-z;$
$y,z,x;$	$y,\bar{z},\bar{x};$	$\bar{y},z,\bar{x};$	$\bar{y},\bar{z},x;$	$\tfrac{1}{4}-y,\tfrac{1}{4}-z,\tfrac{3}{4}-x;$	$\tfrac{1}{4}-y,\tfrac{1}{4}+z,\tfrac{3}{4}+x;$	$\tfrac{1}{4}+y,\tfrac{1}{4}-z,\tfrac{3}{4}+x;$	$\tfrac{1}{4}+y,\tfrac{1}{4}+z,\tfrac{3}{4}-x;$
$z,x,y;$	$z,\bar{x},\bar{y};$	$\bar{z},x,\bar{y};$	$\bar{z},\bar{x},y;$	$\tfrac{1}{4}-z,\tfrac{1}{4}-x,\tfrac{3}{4}-y;$	$\tfrac{1}{4}-z,\tfrac{1}{4}+x,\tfrac{3}{4}+y;$	$\tfrac{1}{4}+z,\tfrac{1}{4}-x,\tfrac{3}{4}+y;$	$\tfrac{1}{4}+z,\tfrac{1}{4}+x,\tfrac{3}{4}-y;$
$y,x,\tfrac{1}{2}+z;$	$y,\bar{x},\tfrac{1}{2}-z;$	$\bar{y},x,\tfrac{1}{2}-z;$	$\bar{y},\bar{x},\tfrac{1}{2}+z;$	$\tfrac{1}{4}-y,\tfrac{1}{4}-x,\tfrac{1}{4}-z;$	$\tfrac{1}{4}-y,\tfrac{1}{4}+x,\tfrac{1}{4}+z;$	$\tfrac{1}{4}+y,\tfrac{1}{4}-x,\tfrac{1}{4}+z;$	$\tfrac{1}{4}+y,\tfrac{1}{4}+x,\tfrac{1}{4}-z;$
$z,y,\tfrac{1}{2}+x;$	$z,\bar{y},\tfrac{1}{2}-x;$	$\bar{z},y,\tfrac{1}{2}-x;$	$\bar{z},\bar{y},\tfrac{1}{2}+x;$	$\tfrac{1}{4}-z,\tfrac{1}{4}-y,\tfrac{1}{4}-x;$	$\tfrac{1}{4}-z,\tfrac{1}{4}+y,\tfrac{1}{4}+x;$	$\tfrac{1}{4}+z,\tfrac{1}{4}-y,\tfrac{1}{4}+x;$	$\tfrac{1}{4}+z,\tfrac{1}{4}+y,\tfrac{1}{4}-x;$
$x,z,\tfrac{1}{2}+y;$	$x,\bar{z},\tfrac{1}{2}-y;$	$\bar{x},z,\tfrac{1}{2}-y;$	$\bar{x},\bar{z},\tfrac{1}{2}+y;$	$\tfrac{1}{4}-x,\tfrac{1}{4}-z,\tfrac{1}{4}-y;$	$\tfrac{1}{4}-x,\tfrac{1}{4}+z,\tfrac{1}{4}+y;$	$\tfrac{1}{4}+x,\tfrac{1}{4}-z,\tfrac{1}{4}+y;$	$\tfrac{1}{4}+x,\tfrac{1}{4}+z,\tfrac{1}{4}-y$

$A=32\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\cos 2\pi\frac{h+k+l}{8}.G$; $B=-32\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}\sin 2\pi\frac{h+k+l}{8}.G$, where

$$G=\cos 2\pi\frac{h+k+l}{8}[\cos 2\pi hx\cos 2\pi ky\cos 2\pi lz+\cos 2\pi kx\cos 2\pi ly\cos 2\pi hz+\cos 2\pi lx\cos 2\pi hy\cos 2\pi kz+$$
$$\cos\pi l(\cos 2\pi kx\cos 2\pi hy\cos 2\pi lz+\cos 2\pi lx\cos 2\pi ky\cos 2\pi hz+\cos 2\pi hx\cos 2\pi ly\cos 2\pi kz)]+$$
$$\sin 2\pi\frac{h+k+l}{8}[\sin 2\pi hx\sin 2\pi ky\sin 2\pi lz+\sin 2\pi kx\sin 2\pi ly\sin 2\pi hz+\sin 2\pi lx\sin 2\pi hy\sin 2\pi kz+$$
$$\cos\pi l(\sin 2\pi kx\sin 2\pi hy\sin 2\pi lz+\sin 2\pi lx\sin 2\pi ky\sin 2\pi hz+\sin 2\pi hx\sin 2\pi ly\sin 2\pi kz)]$$

$$|F(hkl)|=|F(klh)|=|F(lhk)|=|F(\bar{h}k\bar{l})|=|F(\bar{h}kl)|=|F(h\bar{k}l)|=|F(hk\bar{l})|=|F(khl)|$$

$\begin{cases}h,k,l\text{ all even}\\ h+k+l=4n\end{cases}$

$$A=32\{\cos 2\pi hx[\cos 2\pi ky\cos 2\pi lz+\cos 2\pi ly\cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz\cos 2\pi lx+\cos 2\pi lz\cos 2\pi kx]+$$
$$\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly+\cos 2\pi lx\cos 2\pi ky]\}$$

$B=0$

$$\alpha(hkl)=\alpha(\bar{h}k\bar{l})=\alpha(\bar{h}kl)=\alpha(h\bar{k}l)=\alpha(hk\bar{l})=m\pi=\alpha(khl)$$

$\begin{cases}h,k,l\text{ all odd}\\ h+k+l=4n+1\end{cases}$

$$A=16\{\cos 2\pi hx[\cos 2\pi ky\cos 2\pi lz-\cos 2\pi ly\cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz\cos 2\pi lx-\cos 2\pi lz\cos 2\pi kx]+$$
$$\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly-\cos 2\pi lx\cos 2\pi ky]+$$
$$\sin 2\pi hx[\sin 2\pi ky\sin 2\pi lz-\sin 2\pi ly\sin 2\pi kz]+$$
$$\sin 2\pi hy[\sin 2\pi kz\sin 2\pi lx-\sin 2\pi lz\sin 2\pi kx]+$$
$$\sin 2\pi hz[\sin 2\pi kx\sin 2\pi ly-\sin 2\pi lx\sin 2\pi ky]\}$$

$B=-A$

$A=B=0$ if $h=\pm k$ (etc.)

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=m\pi-\frac{\pi}{4}=\alpha(khl)$$

$\begin{cases}h,k,l\text{ all even}\\ h+k+l=4n+2\end{cases}$

$A=0$

$$B=-32\{\sin 2\pi hx[\sin 2\pi ky\sin 2\pi lz+\sin 2\pi ly\sin 2\pi kz]+$$
$$\sin 2\pi hy[\sin 2\pi kz\sin 2\pi lx+\sin 2\pi lz\sin 2\pi kx]+$$
$$\sin 2\pi hz[\sin 2\pi kx\sin 2\pi ly+\sin 2\pi lx\sin 2\pi ky]\}$$

$A=B=0$ if $h=0$ (etc.)

$$\alpha(hkl)=-\alpha(\bar{h}k\bar{l})=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=m\pi+\frac{\pi}{2}=\pi+\alpha(khl)$$

$\begin{cases} h, k, l \text{ all odd} \\ h+k+l=4n+3 \end{cases}$

$$A=16\{\cos 2\pi hx[\cos 2\pi ky \cos 2\pi lz - \cos 2\pi ly \cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz \cos 2\pi lx - \cos 2\pi lz \cos 2\pi kx]+$$
$$\cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly - \cos 2\pi lx \cos 2\pi ky]-$$
$$\sin 2\pi hx[\sin 2\pi ky \sin 2\pi lz - \sin 2\pi ly \sin 2\pi kz]-$$
$$\sin 2\pi hy[\sin 2\pi kz \sin 2\pi lx - \sin 2\pi lz \sin 2\pi kx]-$$
$$\sin 2\pi hz[\sin 2\pi kx \sin 2\pi ly - \sin 2\pi lx \sin 2\pi ky]\}$$

$B=A$

$A=B=0$ if $h=\pm k$ (etc.) $\qquad \alpha(hkl)=-\alpha(\bar{h}kl)=-\alpha(h\bar{k}l)=-\alpha(hk\bar{l})=-\alpha(hkl)=\mathrm{m}\pi+\frac{\pi}{4}$

h, k, l mixed even and odd $\qquad A=B=0 \qquad =\pi+\alpha(khl)$

$$\rho(XYZ)=\frac{8}{V_c}\Big\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n}|F(hkl)|\cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ \cos \mathrm{m}\pi+$$
$$\frac{1}{\sqrt{2}}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n+1}|F(hkl)|[\cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ+\sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ]\cos \mathrm{m}\pi-$$
$$\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n+2}|F(hkl)|\sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ \cos \mathrm{m}\pi+$$
$$\frac{1}{\sqrt{2}}\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h+k+l=4n+3}|F(hkl)|[\cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ-\sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ]\cos \mathrm{m}\pi\Big\}$$

where m=0 or 1 according as A (or if $A=0$ then B) is positive or negative.

$Fd3c$
O_h^8

No. 228

Origin at centre at $\bar{3}$. $(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)\ \pm$

x,y,z;	$x,\frac{1}{4}-y,\frac{1}{4}-z$;	$\frac{1}{4}-x,y,\frac{1}{4}-z$;	$\frac{1}{4}-x,\frac{1}{4}-y,z$;	$y,x,\frac{1}{2}+z$;	$y,\frac{1}{4}-x,\frac{3}{4}-z$;	$\frac{1}{4}-y,x,\frac{3}{4}-z$;
y,z,x;	$y,\frac{1}{4}-z,\frac{1}{4}-x$;	$\frac{1}{4}-y,z,\frac{1}{4}-x$;	$\frac{1}{4}-y,\frac{1}{4}-z,x$;	$z,y,\frac{1}{2}+x$;	$z,\frac{1}{4}-y,\frac{3}{4}-x$;	$\frac{1}{4}-z,y,\frac{3}{4}-x$;
z,x,y;	$z,\frac{1}{4}-x,\frac{1}{4}-y$;	$\frac{1}{4}-z,x,\frac{1}{4}-y$;	$\frac{1}{4}-z,\frac{1}{4}-x,y$,	$x,z,\frac{1}{2}+y$;	$x,\frac{1}{4}-z,\frac{3}{4}-y$;	$\frac{1}{4}-x,z,\frac{3}{4}-y$;

$A=8\cos^2 2\pi\frac{h+k}{4}\cos^2 2\pi\frac{k+l}{4}.G$, where

$$G=\cos 2\pi(hx+ky+lz)+\cos 2\pi\left(hx+ky-lz-\frac{h+k}{4}\right)+\cos 2\pi\left(hx-ky+lz-\frac{l+h}{4}\right)+\cos 2\pi\left(-hx+ky+lz-\frac{k+l}{4}\right)+$$
$$\cos 2\pi(hy+kz+lx)+\cos 2\pi\left(hy+kz-lx-\frac{h+k}{4}\right)+\cos 2\pi\left(hy-kz+lx-\frac{l+h}{4}\right)+\cos 2\pi\left(-hy+kz+lx-\frac{k+l}{4}\right)+$$
$$\cos 2\pi(hz+kx+ly)+\cos 2\pi\left(hz+kx-ly-\frac{h+k}{4}\right)+\cos 2\pi\left(hz-kx+ly-\frac{l+h}{4}\right)+\cos 2\pi\left(-hz+kx+ly-\frac{k+l}{4}\right)+$$
$$\cos \pi l\Big[\cos 2\pi(hy+kx+lz)+\cos 2\pi\left(hy+kx-lz-\frac{h+k}{4}\right)+\cos 2\pi\left(hy-kx+lz-\frac{l+h}{4}\right)+$$
$$\cos 2\pi\left(-hy+kx+lz-\frac{k+l}{4}\right)+\cos 2\pi(hz+ky+lx)+\cos 2\pi\left(hz+ky-lx-\frac{h+k}{4}\right)+$$
$$\cos 2\pi\left(hz-ky+lx-\frac{l+h}{4}\right)+\cos 2\pi\left(-hz+ky+lx-\frac{k+l}{4}\right)+\cos 2\pi(hx+kz+ly)+$$
$$\cos 2\pi\left(hx+kz-ly-\frac{h+k}{4}\right)+\cos 2\pi\left(hx-kz+ly-\frac{l+h}{4}\right)+\cos 2\pi\left(-hx+kz+ly-\frac{k+l}{4}\right)\Big]$$

$B=0 \qquad F(hkl)=F(klh)=F(lhk)$

---

(1) $\begin{cases} h+k=4n \\ k+l=4n \\ l+h=4n \end{cases}$ $A=32\{\cos 2\pi lz[\cos 2\pi hx \cos 2\pi ky+\cos 2\pi hy \cos 2\pi kx]+$
$\cos 2\pi lx[\cos 2\pi hy \cos 2\pi kz+\cos 2\pi hz \cos 2\pi ky]+$
$\cos 2\pi ly[\cos 2\pi hz \cos 2\pi kx+\cos 2\pi hx \cos 2\pi kz]\}$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

(2) $\begin{cases} h+k=4n \\ k+l=4n+2 \\ l+h=4n+2 \end{cases}$ $A=-32\{\cos 2\pi lz[\sin 2\pi hx \sin 2\pi ky+\sin 2\pi hy \sin 2\pi kx]+$
$\cos 2\pi lx[\sin 2\pi hy \sin 2\pi kz+\sin 2\pi hz \sin 2\pi ky]+$
$\cos 2\pi ly[\sin 2\pi hz \sin 2\pi kx+\sin 2\pi hx \sin 2\pi kz]\}$

$A=B=0$ if $h=0$ or $k=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

(3) $\begin{cases} h+k=4n+2 \\ k+l=4n \\ l+h=4n+2 \end{cases}$ Change $h\to k\to l\to h$ in formulae (2)

$A=B=0$ if $k=0$ or $l=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$

(4) $\begin{cases} h+k=4n+2 \\ k+l=4n+2 \\ l+h=4n \end{cases}$ Change $h\to l\to k\to h$ in formulae (2)

$A=B=0$ if $l=0$ or $h=0$ $\quad F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=F(khl)$

(5) $\begin{cases} h+k=4n+2 \\ k+l=4n+2 \\ l+h=4n+2 \end{cases}$ $A=-32\{\sin 2\pi lz \sin \pi(h-k)(x-y) \cos \pi(h+k)(x+y)-$
$\cos 2\pi lz \sin \pi(h-k)(x+y) \sin \pi(h+k)(x-y)+$
$\sin 2\pi lx \sin \pi(h-k)(y-z) \cos \pi(h+k)(y+z)-$
$\cos 2\pi lx \sin \pi(h-k)(y+z) \sin \pi(h+k)(y-z)+$
$\sin 2\pi ly \sin \pi(h-k)(z-x) \cos \pi(h+k)(z+x)-$
$\cos 2\pi ly \sin \pi(h-k)(z+x) \sin \pi(h+k)(z-x)\}$

$A=B=0$ if $h=k$ or $k=l$ or $l=h$. $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$

(6) $\begin{cases} h+k=4n \\ k+l=4n \\ l+h=4n+2 \end{cases}$ $A=32\{\sin 2\pi lz \sin \pi(h+k)(x-y) \cos \pi(h-k)(x+y)-$
$\cos 2\pi lz \sin \pi(h+k)(x+y) \sin \pi(h-k)(x-y)+$
$\sin 2\pi lx \sin \pi(h+k)(y-z) \cos \pi(h-k)(y+z)-$
$\cos 2\pi lx \sin \pi(h+k)(y+z) \sin \pi(h-k)(y-z)+$
$\sin 2\pi ly \sin \pi(h+k)(z-x) \cos \pi(h-k)(z+x)-$
$\cos 2\pi ly \sin \pi(h+k)(z+x) \sin \pi(h-k)(z-x)\}$

$A=B=0$ if $h=l$ or $h=-k$ or $k=-l$. $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

(7) $\begin{cases} h+k=4n \\ k+l=4n+2 \\ l+h=4n \end{cases}$ Change $h\to l\to k\to h$ in formulae (6)

$A=B=0$ if $k=l$ or $l=-h$ or $h=-k$. $F(hkl)=F(\bar{h}\bar{k}\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=-F(khl)$

(8) $\begin{cases} h+k=4n+2 \\ k+l=4n \\ l+h=4n \end{cases}$ Change $h\to k\to l\to h$ in formulae (6)

$A=B=0$ if $h=k$ or $k=-l$ or $l=-h$. $F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})=-F(khl)$

h, k, l mixed even and odd $\quad A=B=0$

$\rho(XYZ)$ as for No. 70 (*Fddd*, origin at $\bar{1}$, page 413).

$Im3m$ O_h^9

No. 229

Origin at centre at $m3m$.

$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})\ \pm$	$x,y,z;\ x,\bar{y},\bar{z};\ \bar{x},y,\bar{z};\ \bar{x},\bar{y},z;\ y,z,x;\ y,\bar{z},\bar{x};\ \bar{y},z,\bar{x};\ \bar{y},\bar{z},x;\ z,x,y;\ z,\bar{x},\bar{y};\ \bar{z},x,\bar{y};\ \bar{z},\bar{x},y;$ $y,x,z;\ y,\bar{x},\bar{z};\ \bar{y},x,\bar{z};\ \bar{y},\bar{x},z;\ z,y,x;\ z,\bar{y},\bar{x};\ \bar{z},y,\bar{x};\ \bar{z},\bar{y},x;\ x,z,y;\ x,\bar{z},\bar{y};\ \bar{x},z,\bar{y};\ \bar{x},\bar{z},y$

$$A=16\cos^2 2\pi\frac{h+k+l}{4}\{\cos 2\pi hx[\cos 2\pi ky\cos 2\pi lz+\cos 2\pi ly\cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz\cos 2\pi lx+\cos 2\pi lz\cos 2\pi kx]+\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly+\cos 2\pi lx\cos 2\pi ky]\}$$

$B=0$ $\qquad F(hkl)=F(klh)=F(lhk)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

$h+k+l=2n$ $\quad$ A as for No. 221 (page 512), but with numerical factor 16 instead of 8.

$h+k+l=2n+1$ $\quad$ $A=B=0$

$$\rho(XYZ)=\frac{8}{V_c}\sum_0^\infty\sum_0^\infty\sum_0^\infty F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ$$

$Ia3d$ O_h^{10}

No. 230

Origin at centre at $\bar{3}$.

$(0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2})\ \pm$	$x,y,z;\ y,z,x;\ z,x,y;\ \frac{1}{4}+y,\frac{1}{4}+x,\frac{1}{4}+z;\ \frac{1}{4}+z,\frac{1}{4}+y,\frac{1}{4}+x;\ \frac{1}{4}+x,\frac{1}{4}+z,\frac{1}{4}+y;$ $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z};\ \frac{1}{2}+y,\frac{1}{2}-z,\bar{x};\ \frac{1}{2}+z,\frac{1}{2}-x,\bar{y};\ \frac{3}{4}+y,\frac{1}{4}-x,\frac{3}{4}-z;\ \frac{3}{4}+z,\frac{1}{4}-y,\frac{3}{4}-x;\ \frac{3}{4}+x,\frac{1}{4}-z,\frac{3}{4}-y;$ $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z;\ \bar{y},\frac{1}{2}+z,\frac{1}{2}-x;\ \bar{z},\frac{1}{2}+x,\frac{1}{2}-y;\ \frac{3}{4}-y,\frac{3}{4}+x,\frac{1}{4}-z;\ \frac{3}{4}-z,\frac{3}{4}+y,\frac{1}{4}-x;\ \frac{3}{4}-x,\frac{3}{4}+z,\frac{1}{4}-y;$ $\frac{1}{2}-x,\bar{y},\frac{1}{2}+z;\ \frac{1}{2}-y,\bar{z},\frac{1}{2}+x;\ \frac{1}{2}-z,\bar{x},\frac{1}{2}+y;\ \frac{1}{4}-y,\frac{3}{4}-x,\frac{3}{4}+z;\ \frac{1}{4}-z,\frac{3}{4}-y,\frac{3}{4}+x;\ \frac{1}{4}-x,\frac{3}{4}-z,\frac{3}{4}+y$

$$A=16\cos 2\pi\frac{h+k+l}{4}\Big\{\cos 2\pi\left(hx+\frac{l}{4}\right)\cos 2\pi\left(ky+\frac{h}{4}\right)\cos 2\pi\left(lz+\frac{k}{4}\right)+$$
$$\cos 2\pi\left(kx+\frac{h}{4}\right)\cos 2\pi\left(ly+\frac{k}{4}\right)\cos 2\pi\left(hz+\frac{l}{4}\right)+\cos 2\pi\left(lx+\frac{k}{4}\right)\cos 2\pi\left(hy+\frac{l}{4}\right)\cos 2\pi\left(kz+\frac{h}{4}\right)+$$
$$\cos 2\pi\frac{h+k+l}{4}\Big[\cos 2\pi\left(kx+\frac{l}{4}\right)\cos 2\pi\left(hy+\frac{k}{4}\right)\cos 2\pi\left(lz+\frac{h}{4}\right)+$$
$$\cos 2\pi\left(lx+\frac{h}{4}\right)\cos 2\pi\left(ky+\frac{l}{4}\right)\cos 2\pi\left(hz+\frac{k}{4}\right)+\cos 2\pi\left(hx+\frac{k}{4}\right)\cos 2\pi\left(ly+\frac{h}{4}\right)\cos 2\pi\left(kz+\frac{l}{4}\right)\Big]\Big\}$$

$B=0$ $\qquad F(hkl)=F(klh)=F(lhk)$

(1) $\begin{cases} h,k,l \text{ all even} \\ h+k+l=4n \end{cases}$

$$A=16\{\cos 2\pi hx[\cos 2\pi ky\cos 2\pi lz+\cos 2\pi ly\cos 2\pi kz]+$$
$$\cos 2\pi hy[\cos 2\pi kz\cos 2\pi lx+\cos 2\pi lz\cos 2\pi kx]+$$
$$\cos 2\pi hz[\cos 2\pi kx\cos 2\pi ly+\cos 2\pi lx\cos 2\pi ky]\}$$

$F(hkl)=F(\bar{h}\bar{k}\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})=F(khl)$

(2)	$\begin{cases} h \text{ even}; \quad k, l \text{ odd} \\ h+k+l=4n \end{cases}$	$A=-16\{\sin 2\pi hx[\cos 2\pi ky \sin 2\pi lz+\cos 2\pi ly \sin 2\pi kz]+$ $\sin 2\pi hy[\cos 2\pi kz \sin 2\pi lx+\cos 2\pi lz \sin 2\pi kx]+$ $\sin 2\pi hz[\cos 2\pi kx \sin 2\pi ly+\cos 2\pi lx \sin 2\pi ky]\}$	
		$A=B=0$ if $h=0$ or $k=-l$	$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$ $=F(khl)$
(3)	$\begin{cases} k \text{ even}; \quad h, l \text{ odd} \\ h+k+l=4n \end{cases}$	Change $h\to k\to l\to h$ in formulae (2)	
		$A=B=0$ if $k=0$ or $l=-h$	$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$ $=F(khl)$
(4)	$\begin{cases} l \text{ even}; \quad h, k \text{ odd} \\ h+k+l=4n \end{cases}$	Change $h\to l\to k\to h$ in formulae (2)	
		$A=B=0$ if $l=0$ or $h=-k$	$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$ $=F(khl)$
(5)	$\begin{cases} h, k, l \text{ even} \\ h+k+l=4n+2 \end{cases}$	$A=16\{\cos 2\pi hx[\cos 2\pi ky \cos 2\pi lz-\cos 2\pi ly \cos 2\pi kz]+$ $\cos 2\pi hy[\cos 2\pi kz \cos 2\pi lx-\cos 2\pi lz \cos 2\pi kx]+$ $\cos 2\pi hz[\cos 2\pi kx \cos 2\pi ly-\cos 2\pi lx \cos 2\pi ky]\}$	
		$A=B=0$ if $h=\pm k$ (or $k=\pm l$, or $l=\pm h$)	$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=F(h\bar{k}l)=F(hk\bar{l})$ $=-F(khl)$
(6)	$\begin{cases} h \text{ even}; \quad k, l \text{ odd} \\ h+k+l=4n+2 \end{cases}$	$A=-16\{\sin 2\pi hx[\cos 2\pi ky \sin 2\pi lz-\cos 2\pi ly \sin 2\pi kz]+$ $\sin 2\pi hy[\cos 2\pi kz \sin 2\pi lx-\cos 2\pi lz \sin 2\pi kx]+$ $\sin 2\pi hz[\cos 2\pi kx \sin 2\pi ly-\cos 2\pi lx \sin 2\pi ky]\}$	
		$A=B=0$ if $h=0$ or $k=l$	$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=F(h\bar{k}l)=-F(hk\bar{l})$ $=-F(khl)$
(7)	$\begin{cases} k \text{ even}; \quad l, h \text{ odd} \\ h+k+l=4n+2 \end{cases}$	Change $h\to k\to l\to h$ in formulae (6)	
		$A=B=0$ if $k=0$ or $l=h$	$F(hkl)=F(\bar{h}k\bar{l})=-F(\bar{h}kl)=-F(h\bar{k}l)=F(hk\bar{l})$ $=-F(khl)$
(8)	$\begin{cases} l \text{ even}; \quad h, k \text{ odd} \\ h+k+l=4n+2 \end{cases}$	Change $h\to l\to k\to h$ in formulae (6)	
		$A=B=0$ if $l=0$ or $h=k$	$F(hkl)=F(\bar{h}k\bar{l})=F(\bar{h}kl)=-F(h\bar{k}l)=-F(hk\bar{l})$ $=-F(khl)$
$h+k+l=2n+1$		$A=B=0$	

$$\rho(XYZ)=\frac{8}{V_c}\left\{\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n}F(hkl)\cos 2\pi hX\cos 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n,\,k=2n+1}F(hkl)\sin 2\pi hX\cos 2\pi kY\sin 2\pi lZ-\right.$$
$$\left.\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n}F(hkl)\sin 2\pi hX\sin 2\pi kY\cos 2\pi lZ-\sum_0^\infty\sum_0^\infty\sum_0^\infty{}^{h=2n+1,\,k=2n+1}F(hkl)\cos 2\pi hX\sin 2\pi kY\sin 2\pi lZ\right\}$$

4.8. Patterson and Patterson-Harker Functions

The function[1-2]

$$P(UVW)=\frac{1}{V_c}\sum_{-\infty}^{\infty}h\sum_{-\infty}^{\infty}k\sum_{-\infty}^{\infty}l\,|F(hkl)|^2\cos 2\pi(hU+kV+lW)$$

which is used to determine the vector relationships (distances, directions) between the main scattering centres (atoms, groups of atoms) in the unit cell, is independent of phase angles and phase relationships and therefore a few simplified expressions serve for all space groups. The simplification consists only in making use of the symmetry relationships between the absolute $|F|$ values (that is, between the observed intensity values) for different values of h, k, l.

It will be seen that, as in the case of the electron density formulae in section 4.7, only the general term ($h\neq k\neq l\neq 0$) is given for each expression. Where h, k and/or l have zero values, the numerical factor in the expression may be reduced. If the factor in the general term is 8, it will be reduced to 4 for one zero index, to 2 for two zero indices (and to 1 for $|F(000)|$, if it is desired to include this term).

It is only in the tetragonal system that the absolute $|F|$ relationships vary for the two Laue groups.

Triclinic

$$P(UVW)=\frac{2}{V_c}\sum_{0}^{\infty}\sum_{0}^{\infty}\sum_{0}^{\infty}\{|F(hkl)|^2\cos 2\pi(hU+kV+lW)+|F(\bar{h}kl)|^2\cos 2\pi(-hU+kV+lW)+$$
$$|F(h\bar{k}l)|^2\cos 2\pi(hU-kV+lW)+|F(hk\bar{l})|^2\cos 2\pi(hU+kV-lW)\}$$

Monoclinic

$$P(UVW)=\frac{4}{V_c}\sum_{0}^{\infty}\sum_{0}^{\infty}\sum_{0}^{\infty}\{|F(hkl)|^2\cos 2\pi(hU+kV)+|F(\bar{h}kl)|^2\cos 2\pi(hU-kV)\}\cos 2\pi lW \quad c \text{ axis unique}$$

$$P(UVW)=\frac{4}{V_c}\sum_{0}^{\infty}\sum_{0}^{\infty}\sum_{0}^{\infty}\{|F(hkl)|^2\cos 2\pi(hU+lW)+|F(\bar{h}kl)|^2\cos 2\pi(hU-lW)\}\cos 2\pi kV \quad b \text{ axis unique}$$

Orthorhombic

$$P(UVW)=\frac{8}{V_c}\sum_{0}^{\infty}\sum_{0}^{\infty}\sum_{0}^{\infty}|F(hkl)|^2\cos 2\pi hU\cos 2\pi kV\cos 2\pi lW$$

Tetragonal

$$P(UVW)=\frac{4}{V_c}\sum_{0}^{\infty}\sum_{0}^{\infty}\sum_{0}^{\infty}\{|F(hkl)|^2\cos 2\pi(hU+kV)+|F(\bar{h}kl)|^2\cos 2\pi(hU-kV)\}\cos 2\pi lW \quad 4,\ \bar{4},\ 4/m$$

$$P(UVW)=\frac{8}{V_c}\sum_{0}^{\infty}\sum_{0}^{\infty}\sum_{0}^{\infty}|F(hkl)|^2\cos 2\pi hU\cos 2\pi kV\cos 2\pi lW \quad 422,\ 4mm,\ \bar{4}2m,\ 4/mmm$$

Trigonal

$$P(UVW)=\frac{2}{V_c}\sum_{0}^{\infty}\sum_{0}^{\infty}\sum_{0}^{\infty}\{|F(hkl)|^2\cos 2\pi(hU+kV+lW)+|F(\bar{h}kl)|^2\cos 2\pi(-hU+kV+lW)+$$
$$|F(h\bar{k}l)|^2\cos 2\pi(hU-kV+lW)+|F(hk\bar{l})|^2\cos 2\pi(hU+kV-lW)\}$$

$3,\ \bar{3},\ 32,\ 3m,\ \bar{3}m$

Hexagonal

$$P(UVW)=\frac{4}{V_c}\sum_{0}^{\infty}\sum_{0}^{\infty}\sum_{0}^{\infty}\{|F(hkl)|^2\cos 2\pi(hU+kV)+|F(\bar{h}kl)|^2\cos 2\pi(hU-kV)\}\cos 2\pi lW \quad 6,\ \bar{6},\ 6/m,\ 622,\ 6mm,\ \bar{6}m2,\ 6/mmm$$

Cubic

$$P(UVW)=\frac{8}{V_c}\sum_{0}^{\infty}\sum_{0}^{\infty}\sum_{0}^{\infty}|F(hkl)|^2\cos 2\pi hU\cos 2\pi kV\cos 2\pi lW \quad 23,\ m3,\ 432,\ \bar{4}3m,\ m3m$$

(1) Patterson, A. L. 1934, *Phys. Rev.*, **46**, 372; 1935, *Zeit. f. Kristallog.*, **90**, 517.
(2) James, R. W. 1948, *The Optical Principles of the Diffraction of X-rays*, p. 373 (G. Bell & Sons, London).

Methods of simplifying these expressions still further which avoid the labour of a full three-dimensional analysis have been described by D. Harker (*J. Chem. Phys.*, **4**, 381 (1936)). These involve the use of the following particular cases of $P(UVW)$ for the symmetry elements named.

Symmetry Element	*Form of* $P(UVW)$
(*a*) Axes parallel to *c*-axis	
(i) $2, 4, 4_2, \bar{4}, 3, \bar{3}, 6, 6_3, \bar{6}$	$P(U, V, 0)$
(ii) $2_1, 4_1, 4_3, 6_1, 6_5$	$P(U, V, \frac{1}{2})$
(iii) $3_1, 3_2, 6_2, 6_4$	$P(U, V, \frac{1}{3})$
(*b*) Planes perpendicular to *c*-axis	
(i) Reflection plane	$P(0, 0, W)$
(ii) Glide $a/2$	$P(\frac{1}{2}, 0, W)$
(iii) Glide $b/2$	$P(0, \frac{1}{2}, W)$
(iv) Glide $(a/2+b/2)$	$P(\frac{1}{2}, \frac{1}{2}, W)$
(v) Glide $(a/4+b/4)$	$P(\frac{1}{4}, \frac{1}{4}, W)$
(vi) Glide $(3a/4+b/4)$	$P(\frac{3}{4}, \frac{1}{4}, W)$

4.9. Transformation of Co-ordinates

Transformation of the co-ordinates of equivalent positions are necessary:

1. If there is a change of origin, relative to the symmetry elements, but without change of the unit-cell size and orientation.
2. If there is a change of unit-cell size or shape or orientation relative to the symmetry elements.

Change of Origin Only

In practice the origin is always taken in a special position, if one exists, and any change of origin simply involves a translation, without reorientation, of the symmetry elements relative to the axes of co-ordinates of the unit cell, which is assumed to be otherwise unchanged. The space-group symbol is not altered, and the only transformation necessary is that which involves the co-ordinates of equivalent positions, and hence the form of the structure factor and electron density formulae (see section 4.7).

Such transformations commonly involve a change to or from a centre of symmetry as origin. In section 4.3 the co-ordinates of equivalent positions are given, in certain space groups, both for an origin at a centre of symmetry and for some other origin which may, from the point of view of space-group derivation, have been simpler.

If the co-ordinates of the new origin are x_1, y_1, z_1 relative to the old origin, then the new co-ordinates are obtained first by subtracting x_1 from each former x co-ordinate (y_1 from y, z_1 from z) so that

$$x \text{ becomes } x-x_1,\ \bar{x} \text{ becomes } -x-x_1,\ \tfrac{1}{2}+x \text{ becomes } \tfrac{1}{2}+x-x_1,\ \tfrac{1}{2}-x \text{ becomes } \tfrac{1}{2}-x-x_1, \text{ etc.,}$$

and similarly for y and z.

The old (x, y, z) has now become $(x-x_1, y-y_1, z-z_1)$ which is to be the *new* (x_0, y_0, z_0).

In terms of the new x_0, y_0, z_0

$$\begin{aligned} -x-x_1 &\text{ is } -(x-x_1)-2x_1, && \text{that is, } \bar{x}_0-2x_1 \\ \tfrac{1}{2}+x-x_1 &\text{ is } \tfrac{1}{2}+(x-x_1), && \text{that is, } \tfrac{1}{2}+x_0 \\ \tfrac{1}{2}-x-x_1 &\text{ is } \tfrac{1}{2}-(x-x_1)-2x_1, && \text{that is, } \tfrac{1}{2}-x_0-2x_1 \end{aligned}$$

and so on.

As an example we may take the space group *Pban*, No. 50, first referred (p. 137) to a point of symmetry 222 as origin, for which the co-ordinates of equivalent positions are

$$\begin{array}{llll} x,y,z; & \bar{x},\bar{y},z; & \tfrac{1}{2}-x,\tfrac{1}{2}-y,\bar{z}; & \tfrac{1}{2}+x,\tfrac{1}{2}+y,\bar{z}; \\ x,\bar{y},\bar{z}; & \bar{x},y,\bar{z}; & \tfrac{1}{2}-x,\tfrac{1}{2}+y,z; & \tfrac{1}{2}+x,\tfrac{1}{2}-y,z. \end{array}$$

If the origin is transferred to the point $(-\frac{1}{4},-\frac{1}{4},0)$ these co-ordinates become

$$x+\tfrac{1}{4},y+\tfrac{1}{4},z;\quad -x+\tfrac{1}{4},-y+\tfrac{1}{4},z;\quad \tfrac{3}{4}-x,\tfrac{3}{4}-y,\bar{z};\quad \tfrac{3}{4}+x,\tfrac{3}{4}+y,\bar{z};$$
$$x+\tfrac{1}{4},-y+\tfrac{1}{4},\bar{z};\quad -x+\tfrac{1}{4},y+\tfrac{1}{4},\bar{z};\quad \tfrac{3}{4}-x,\tfrac{3}{4}+y,z;\quad \tfrac{3}{4}+x,\tfrac{3}{4}-y,z.$$

Substituting $x_0=x+\frac{1}{4}$, $y_0=y+\frac{1}{4}$, $z_0=z$ we obtain for the new co-ordinates (dropping 1 when it occurs)

$$x_0,y_0,z_0;\quad \tfrac{1}{2}-x_0,\tfrac{1}{2}-y_0,z_0;\quad \bar{x}_0,\bar{y}_0,\bar{z}_0;\quad \tfrac{1}{2}+x_0,\tfrac{1}{2}+y_0,\bar{z}_0;$$
$$x_0,\tfrac{1}{2}-y_0,\bar{z}_0;\quad \tfrac{1}{2}-x_0,y_0,\bar{z}_0;\quad \bar{x}_0,\tfrac{1}{2}+y_0,z_0;\quad \tfrac{1}{2}+x_0,\bar{y}_0,z_0.$$

Without the subscript, these are the co-ordinates referred to a centre of symmetry as origin, given on p. 138. It is important to realise that such a change of co-ordinates involves not only a change of form (though not of value) of $|F(hkl)|$ but also of the value of the phase angle α, for all reflections.

Change of Unit-cell Size, Shape or Orientation relative to the Symmetry Elements, without Change of Origin

This corresponds to a transformation of the axial vectors **a**, **b**, **c**, and the corresponding change of co-ordinates are shown in matrix form in section 2.5. If

$$\begin{aligned}\mathbf{a}_2&=s_{11}\mathbf{a}_1+s_{12}\mathbf{b}_1+s_{13}\mathbf{c}_1 &&\text{and}\quad \mathbf{a}_1=t_{11}\mathbf{a}_2+t_{12}\mathbf{b}_2+t_{13}\mathbf{c}_2\\ \mathbf{b}_2&=s_{21}\mathbf{a}_1+s_{22}\mathbf{b}_1+s_{23}\mathbf{c}_1 &&\phantom{\text{and}}\quad \mathbf{b}_1=t_{21}\mathbf{a}_2+t_{22}\mathbf{b}_2+t_{23}\mathbf{c}_2\\ \mathbf{c}_2&=s_{31}\mathbf{a}_1+s_{32}\mathbf{b}_1+s_{33}\mathbf{c}_1 &&\phantom{\text{and}}\quad \mathbf{c}_1=t_{31}\mathbf{a}_2+t_{32}\mathbf{b}_2+t_{33}\mathbf{c}_2\end{aligned}$$

then

$$\begin{aligned}x_2&=t_{11}x_1+t_{21}y_1+t_{31}z_1 &&\text{and}\quad x_1=s_{11}x_2+s_{21}y_2+s_{31}z_2\\ y_2&=t_{12}x_1+t_{22}y_1+t_{32}z_1 &&\phantom{\text{and}}\quad y_1=s_{12}x_2+s_{22}y_2+s_{32}z_2\\ z_2&=t_{13}x_1+t_{23}y_1+t_{33}z_1 &&\phantom{\text{and}}\quad z_1=s_{13}x_2+s_{23}y_2+s_{33}z_2\end{aligned}$$

A change of crystal setting (section 6.2) can be dealt with quite simply by means of this type of transformation matrix. Thus if the standard setting in space group No. 60, *Pbcn*, is transformed so that the space-group symbol becomes *Pnab*, Table 6.2.1 indicates that this corresponds to a change of axial vectors from $\mathbf{a}_1$, $\mathbf{b}_1$, $\mathbf{c}_1$ to $\mathbf{a}_2$, $\mathbf{b}_2$, $\mathbf{c}_2$ such that $\mathbf{a}_2=-\mathbf{c}_1$, $\mathbf{b}_2=\mathbf{b}_1$, $\mathbf{c}_2=\mathbf{a}_1$; hence $\mathbf{a}_1=\mathbf{c}_2$, $\mathbf{b}_1=\mathbf{b}_2$, $\mathbf{c}_1=-\mathbf{a}_2$ and the transformation matrices are

$$\text{I}\qquad \begin{array}{c|ccc|} & & 1 & \\ \hline 2 & 0 & 0 & \bar{1}\\ & 0 & 1 & 0\\ & 1 & 0 & 0\\ \hline \end{array}\qquad\qquad \text{II}\qquad \begin{array}{c|ccc|} & & 2 & \\ \hline 1 & 0 & 0 & 1\\ & 0 & 1 & 0\\ & \bar{1} & 0 & 0\\ \hline \end{array}$$

so that

$$x_1=z_2,\quad y_1=y_2,\ z_1=-x_2$$
$$x_2=-z_1,\ y_2=y_1,\ z_2=x_1$$

The co-ordinates of equivalent positions in this space group *Pbcn* are

$$x,y,z;\quad \tfrac{1}{2}-x,\tfrac{1}{2}+y,z;\quad x,\bar{y},\tfrac{1}{2}+z;\quad \tfrac{1}{2}-x,\tfrac{1}{2}-y,\tfrac{1}{2}+z;$$
$$\bar{x},\bar{y},\bar{z};\quad \tfrac{1}{2}+x,\tfrac{1}{2}-y,\bar{z};\quad \bar{x},y,\tfrac{1}{2}-z;\quad \tfrac{1}{2}+x,\tfrac{1}{2}+y,\tfrac{1}{2}-z.$$

These same co-ordinates, referred to the new axes $\mathbf{a}_2$, $\mathbf{b}_2$, $\mathbf{c}_2$ (which are $\bar{\mathbf{c}}_1$, $\mathbf{b}_1$, $\mathbf{a}_1$) become (matrix II)

$$\bar{z},y,x;\quad \bar{z},\tfrac{1}{2}+y,\tfrac{1}{2}-x;\quad \tfrac{1}{2}-z,\bar{y},x;\quad \tfrac{1}{2}-z,\tfrac{1}{2}-y,\tfrac{1}{2}-x;$$
$$z,\bar{y},\bar{x};\quad z,\tfrac{1}{2}-y,\tfrac{1}{2}+x;\quad \tfrac{1}{2}+z,y,\bar{x};\quad \tfrac{1}{2}+z,\tfrac{1}{2}+y,\tfrac{1}{2}+x,$$

and now replacing $\bar{z}$ by x_2, y by y_2, x by z_2 everywhere, we have

$$x_2,y_2,z_2;\quad x_2,\tfrac{1}{2}+y_2,\tfrac{1}{2}-z_2;\quad \tfrac{1}{2}+x_2,\bar{y}_2,z_2;\quad \tfrac{1}{2}+x_2,\tfrac{1}{2}-y_2,\tfrac{1}{2}-z_2;$$
$$\bar{x}_2,\bar{y}_2,\bar{z}_2;\quad \bar{x}_2,\tfrac{1}{2}-y_2,\tfrac{1}{2}+z_2;\quad \tfrac{1}{2}-x_2,y_2,\bar{z}_2;\quad \tfrac{1}{2}-x_2,\tfrac{1}{2}+y_2,\tfrac{1}{2}+z_2.$$

Without the subscripts, these are the new co-ordinates of equivalent positions for the space group in its new setting *Pnab*.

It is, of course, an equally simple matter to derive the co-ordinates directly for any given space-group symbol, if the assumption is made that the origin is to be at a given symmetry position. It is best to draw a diagram as a check.

Example. Transformation of co-ordinates from the rhombohedral to the hexagonal axes (rhombohedral lattice).

If calcite is referred to a rhombohedral unit cell having $a=6{\cdot}361A$, $\alpha=46°\ 7'$, $Z=2$, the atoms have the following co-ordinates:

$$\begin{array}{lllllll}
\text{Ca} & \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}; & \tfrac{\bar{1}}{4},\tfrac{\bar{1}}{4},\tfrac{\bar{1}}{4}. & & & & \\
\text{C} & 0,0,0; & \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}. & & & & \\
\text{O} & x,\bar{x},0; & 0,x,\bar{x}; & \bar{x},0,x; & \tfrac{1}{2}-x,\tfrac{1}{2}+x,\tfrac{1}{2}; & \tfrac{1}{2},\tfrac{1}{2}-x,\tfrac{1}{2}+x; & \tfrac{1}{2}+x,\tfrac{1}{2},\tfrac{1}{2}-x.
\end{array}$$

It is required to find the atomic positions referred to the corresponding hexagonal unit cell of three times the volume. The transformation matrices (section 2.5) are

$$\begin{array}{c|ccc|}
 & & \mathbf{R}_{\text{hex}} & \\
\hline
\mathbf{R}_{\text{obv}} & \tfrac{2}{3} & \tfrac{1}{3} & \tfrac{1}{3} \\
 & \tfrac{\bar{1}}{3} & \tfrac{1}{3} & \tfrac{1}{3} \\
 & \tfrac{\bar{1}}{3} & \tfrac{\bar{2}}{3} & \tfrac{1}{3} \\
\hline
\end{array}
\quad \text{and} \quad
\begin{array}{c|ccc|}
 & & \mathbf{R}_{\text{obv}} & \\
\hline
\mathbf{R}_{\text{hex}} & 1 & \bar{1} & 0 \\
 & 0 & 1 & \bar{1} \\
 & 1 & 1 & 1 \\
\hline
\end{array}$$

Hence

$$x=\tfrac{1}{3}(2x-y-z)$$
$$y=\tfrac{1}{3}(x+y-2z)$$
$$z=\tfrac{1}{3}(x+y+z)$$

The hexagonal co-ordinates corresponding to *all* corners of the rhombohedral unit cell

$$0,0,0;\quad 1,0,0;\quad 0,1,0;\quad 0,0,1;\quad 1,1,1;\quad 0,1,1;\quad 1,0,1;\quad 1,1,0$$

are

$$0,0,0;\quad \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3};\quad \tfrac{\bar{1}}{3},\tfrac{1}{3},\tfrac{1}{3};\quad \tfrac{\bar{1}}{3},\tfrac{\bar{2}}{3},\tfrac{1}{3};\quad 0,0,1;\quad \tfrac{\bar{2}}{3},\tfrac{\bar{1}}{3},\tfrac{2}{3};\quad \tfrac{1}{3},\tfrac{\bar{1}}{3},\tfrac{2}{3};\quad \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3}.$$

Of these only three, 0,0,0; $\tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3}$; $\tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3}$, lie within the hexagonal unit cell and correspond to the co-ordinates of Bravais-lattice points, the hexagonal unit cell being non-primitive. The atomic positions are now transformed by the same equations

$$x(\text{Ca})=\tfrac{1}{3}(2\,.\,\tfrac{1}{4}-\tfrac{1}{4}-\tfrac{1}{4})=0$$
$$y(\text{Ca})=\tfrac{1}{3}(\tfrac{1}{4}+\tfrac{1}{4}-2\,.\,\tfrac{1}{4})=0$$
$$z(\text{Ca})=\tfrac{1}{3}(\tfrac{1}{4}+\tfrac{1}{4}+\tfrac{1}{4})=\tfrac{1}{4}, \text{ etc.}$$

$$x(\text{O}) = \tfrac{1}{3}(2x+x)=x$$
$$y(\text{O}) = \tfrac{1}{3}(x-x)=0$$
$$z(\text{O}) = \tfrac{1}{3}(x-x)=0$$

Adding the positions obtained by inclusion of the extra Bravais-lattice points, we have

$$\begin{array}{lll}
\text{Ca} & (0,0,0;\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3};\ \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3}) + |0,0,\tfrac{1}{4};\ 0,0,\tfrac{\bar{1}}{4}.| & \\
\text{C} & (0,0,0;\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3};\ \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3}) + |0,0,0;\ 0,0,\tfrac{1}{2}.| & \\
\text{O} & (0,0,0;\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3};\ \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3}) + |x,0,0;\ 0,x,0;\ \bar{x},\bar{x},0;\ \bar{x},0,\tfrac{1}{2};\ 0,\bar{x},\tfrac{1}{2};\ x,x,\tfrac{1}{2}.| &
\end{array}$$

NOTE. x, y, z are hexagonal co-ordinates corresponding to x, y, z rhombohedral (obverse) co-ordinates.

5.1. Reduced Cells

This section, which replaces a previous one on the Delaunay reduction, has been contributed by A. D. Mighell, A. Santoro, and J. D. H. Donnay, National Bureau of Standards, Washington, D.C., U.S.A.

5.1.1. General

A crystal lattice can be specified in terms of an infinite number of cells, either primitive or centered. In order to avoid confusion in the description of crystals, one of these cells should be selected as standard.

It has been shown (Section 2.2) that, when the lattice possesses symmetry other than a center, it is convenient to select cell vectors along symmetry directions of the lattice. The selection of the cell in the triclinic system is thus arbitrary. Furthermore, in all systems other than cubic, the choice of a unique cell cannot be made on the basis of symmetry considerations alone. Rules are required whose nature and complexity depend on the symmetry of the lattice (for a listing of such rules see, for examples, the footnote of Table 2.2.1 and J. D. H. Donnay, G. Donnay, E. G. Cox, O. Kennard and M. V. King: Crystal Data, 2nd Edition, Monograph 5, American Crystallographic Association. Washington: Williams and Heintz, 1963).

Cells can also be defined independently of the symmetry of the lattice. These cells have several important applications in crystallography and are needed to describe triclinic lattices. Two such cells have been introduced in the past fifty years: the reduced cell, which stems from Bravais' Principal Triangle and Tetrahedron (A. Johnsen, *Kristallstruktur*, Fortschritte Mineralog., **5**, 17 (see p. 36), 1916; P. Niggli, *Krystallographische und Strukturtheoretische Grundbegriffe*, **7**, Part 1, Handbuch der Experimental Physik, Akademische Verlagsgesellschaft, **108**, 1928; M. J. Buerger, Z. Krist., **109**, 42, 1957; **113**, 52, 1960) and the Delaunay cell (B. Delaunay, *Z. Krist.*, **84**, 109, 1933). As pointed out by Buerger (1957) there are several reasons for prefering the reduced cell. We will consider it here mainly because it is unambiguously defined while the Delaunay cell is not unique in all cases (B. Delaunay, 1933; A. L. Patterson and W. E. Love, *Acta Cryst.*, **10**, 111, 1957).

5.1.2. Reduced Cells

We will represent a primitive cell of lattice parameters a,b,c,α,β,γ, by the matrix

$$\mathbf{S}=\begin{pmatrix}\mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c}\\ \mathbf{b}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{b}\end{pmatrix} \tag{1}$$

In addition we will require that the triplet **a,b,c** be right-handed and that the cell be given in its normal representation, *i.e.* with all interaxial angles either acute (Type I cell) or nonacute (Type II cell). (See, for example, L. V. Azaroff and M. J. Buerger, The Powder Method, New York: McGraw-Hill, 1958). If one or more of the unsymmetrical scalar products in (1) is zero, the cell is of Type II. The cell represented by matrix (1) is reduced if, and only if, it satisfies the conditions (Niggli, 1928) given in Table 5.1.2.1. As shown by Buerger (1957, 1960) the main conditions define a cell based on the shortest three non coplanar translations of the lattice. The cell, therefore, is necessarily primitive. Conditions (3a), (3b), (5a), and (5b) in Table 5.1.2.1 make it possible to label the cell edges uniquely when two of them are equal. The other special conditions define the unique reduced cell in a lattice where there is more than one symmetrically independent cell based on the shortest three translations. Buerger's procedure (1957), later extended by Davis (R. J. Davis, *Mineralog. Mag.*, **32**, 817, 1961), transforms an arbitrary primitive cell into a cell that satisfies the main conditions in Table 5.1.2.1. We will now briefly describe the main steps in this procedure.

Let us call the vectors that define the original primitive cell $\mathbf{a}_0$, $\mathbf{b}_0$, $\mathbf{c}_0$. Each of these vectors can be transformed by the addition or subtraction of either of the other two. For example $\mathbf{c}_0$ can be changed into $\mathbf{c}'=\mathbf{c}_0+m\mathbf{b}_0$ or $\mathbf{c}''=\mathbf{c}_0+m\mathbf{a}_0$, with m a positive or negative integer. $\mathbf{a}_0$ and $\mathbf{b}_0$ can be changed in a

TABLE 5.1.2.1 **Conditions for Reduced Cell**

A Positive reduced form, Type I cell, all angles $<90°$.

Main conditions:

$$\mathbf{a}\cdot\mathbf{a} \leqslant \mathbf{b}\cdot\mathbf{b} \leqslant \mathbf{c}\cdot\mathbf{c};\ \mathbf{b}\cdot\mathbf{c} \leqslant \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b};\ \mathbf{a}\cdot\mathbf{c} \leqslant \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a};\ \mathbf{a}\cdot\mathbf{b} \leqslant \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \qquad (2)$$

Special conditions:

(a)	if $\mathbf{a}\cdot\mathbf{a}=\mathbf{b}\cdot\mathbf{b}$	then	$\mathbf{b}\cdot\mathbf{c} \leqslant \mathbf{a}\cdot\mathbf{c}$	
(b)	if $\mathbf{b}\cdot\mathbf{b}=\mathbf{c}\cdot\mathbf{c}$	then	$\mathbf{a}\cdot\mathbf{c} \leqslant \mathbf{a}\cdot\mathbf{b}$	
(c)	if $\mathbf{b}\cdot\mathbf{c}=\tfrac{1}{2}\mathbf{b}\cdot\mathbf{b}$	then	$\mathbf{a}\cdot\mathbf{b} \leqslant 2\mathbf{a}\cdot\mathbf{c}$	(3)
(d)	if $\mathbf{a}\cdot\mathbf{c}=\tfrac{1}{2}\mathbf{a}\cdot\mathbf{a}$	then	$\mathbf{a}\cdot\mathbf{b} \leqslant 2\mathbf{b}\cdot\mathbf{c}$	
(e)	if $\mathbf{a}\cdot\mathbf{b}=\tfrac{1}{2}\mathbf{a}\cdot\mathbf{a}$	then	$\mathbf{a}\cdot\mathbf{c} \leqslant 2\mathbf{b}\cdot\mathbf{c}$	

B Negative reduced form, Type II cell, all angles $\geqslant 90°$.

Main conditions:

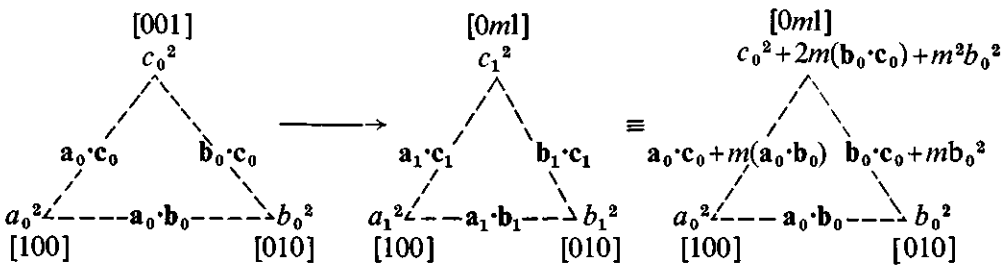
(a) $\mathbf{a}\cdot\mathbf{a} \leqslant \mathbf{b}\cdot\mathbf{b} \leqslant \mathbf{c}\cdot\mathbf{c};\ |\mathbf{b}\cdot\mathbf{c}| \leqslant \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b};\ |\mathbf{a}\cdot\mathbf{c}| \leqslant \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a};\ |\mathbf{a}\cdot\mathbf{b} \leqslant \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a}$ (4)

(b) $(|\mathbf{b}\cdot\mathbf{c}|+|\mathbf{a}\cdot\mathbf{c}|+|\mathbf{a}\cdot\mathbf{b}|) \leqslant \tfrac{1}{2}(\mathbf{a}\cdot\mathbf{a}+\mathbf{b}\cdot\mathbf{b})$

Special conditions:

(a)	if $\mathbf{a}\cdot\mathbf{a}=\mathbf{b}\cdot\mathbf{b}$	then	$\lvert\mathbf{b}\cdot\mathbf{c}\rvert \leqslant \lvert\mathbf{a}\cdot\mathbf{c}\rvert$	
(b)	if $\mathbf{b}\cdot\mathbf{b}=\mathbf{c}\cdot\mathbf{c}$	then	$\lvert\mathbf{a}\cdot\mathbf{c}\rvert \leqslant \lvert\mathbf{a}\cdot\mathbf{b}\rvert$	
(c)	if $\mathbf{b}\cdot\mathbf{c}=\tfrac{1}{2}\mathbf{b}\cdot\mathbf{b}$	then	$\mathbf{a}\cdot\mathbf{b}=0$	(5)
(d)	if $\mathbf{a}\cdot\mathbf{c}=\tfrac{1}{2}\mathbf{a}\cdot\mathbf{a}$	then	$\mathbf{a}\cdot\mathbf{b}=0$	
(e)	if $\mathbf{a}\cdot\mathbf{b}=\tfrac{1}{2}\mathbf{a}\cdot\mathbf{a}$	then	$\mathbf{a}\cdot\mathbf{c}=0$	
(f)	if $(\lvert\mathbf{b}\cdot\mathbf{c}\rvert+\lvert\mathbf{a}\cdot\mathbf{c}\rvert+\lvert\mathbf{a}\cdot\mathbf{b}\rvert)=\tfrac{1}{2}(\mathbf{a}\cdot\mathbf{a}+\mathbf{b}\cdot\mathbf{b})$	then	$\mathbf{a}\cdot\mathbf{a} \leqslant 2\lvert\mathbf{a}\cdot\mathbf{c}\rvert+\lvert\mathbf{a}\cdot\mathbf{b}\rvert$	

similar manner, as the same type of transformation may be applied in six different ways. A convenient way of representing a change of one of the axial vectors is as follows (Davis, 1961):



In the above scheme $\mathbf{c}_0$ has been changed into $\mathbf{c}_1=\mathbf{c}_0+m\mathbf{b}_0$. The zone symbol [0*ml*] gives the new axis $\mathbf{c}_1$ in terms of the old axes so that the matrix 100/010/0*ml* gives the transformation of indices from the old to the new axes. The strategy of the Buerger method consists in applying the possible six transformations repeatedly until the unsymmetrical scalars are brought as near zero as possible, that is, until conditions (2) or (4a) are satisfied (before checking these conditions, the three cell edges must be so labelled as to obey $a \leqslant b \leqslant c$.). When the results of this procedure is a cell of type II, condition (4b) has to be checked; if it is violated, then the longest axis has to be discarded in favor of the body diagonal [111] (Buerger, 1960). The final transformation involved then consists in changing the vector $\mathbf{c}_{n-1}$ into a vector $\mathbf{c}_n=\mathbf{a}_{n-1}+\mathbf{b}_{n-1}+\mathbf{c}_{n-1}$. At this point we have a cell based on the shortest three translations $\mathbf{a}_n$,$\mathbf{b}_n$, and $\mathbf{c}_n$ This cell, expressed in normal representation, satisfies conditions (2) or (4a,b). This does not guarantee that the reduced cell has been obtained, for conditions (3), or conditions (5), must also be satisfied. If one or more of these conditions is violated, then the cell obtained with the Buerger algorithm has to be transformed into the reduced cell. The transformations to be applied in the various cases have been derived (A. Santoro and A. Mighell, *Acta Cryst.*, in press). In Table 5.1.2.2, the cells, given in normal representation, are expressed by the matrices **S** and **S**′. Any given cell **S** is based on the shortest three noncoplanar translations of the lattice and it is unreduced if the scalars are related as indicated in column 3. In this case the transformation will give a cell **S**′ that satisfies the special condition violated by **S**. In certain cases more than one transformation is required to obtain the reduced cell. Matrix **S**′, therefore, has to be checked against the special conditions appropriate for the cell type

TABLE 5.1.2.2

Transformations for determining the reduced cell* from an unreduced cell* based on the shortest three translations of the lattice

Type of Cell S	Matrix of Cell S	Relations between scalars	Transformation Matrix S to S′	Matrix of Cell S′	Type of Cell S′
I or II	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{b} \end{pmatrix}$	$\lvert\mathbf{a}\cdot\mathbf{c}\rvert < \lvert\mathbf{b}\cdot\mathbf{c}\rvert$	$0\bar{1}0/\bar{1}00/00\bar{1}$	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{a}\cdot\mathbf{c} & \mathbf{b}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{b} \end{pmatrix}$	I or II
I or II	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{b} \\ \mathbf{b}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{b} \end{pmatrix}$	$\lvert\mathbf{a}\cdot\mathbf{b}\rvert < \lvert\mathbf{a}\cdot\mathbf{c}\rvert$	$\bar{1}00/00\bar{1}/0\bar{1}0$	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{b} \\ \mathbf{b}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \end{pmatrix}$	I or II
I	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \frac{\mathbf{b}\cdot\mathbf{b}}{2} & \mathbf{a}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{b} \end{pmatrix}$	$2\mathbf{a}\cdot\mathbf{c} < \mathbf{a}\cdot\mathbf{b}$	$\bar{1}00/0\bar{1}0/0\bar{1}1$	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \frac{\mathbf{b}\cdot\mathbf{b}}{2} & (\mathbf{a}\cdot\mathbf{b}-\mathbf{a}\cdot\mathbf{c}) & \mathbf{a}\cdot\mathbf{b} \end{pmatrix}$	I
I	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{c} & \frac{\mathbf{a}\cdot\mathbf{a}}{2} & \mathbf{a}\cdot\mathbf{b} \end{pmatrix}$	$2\mathbf{b}\cdot\mathbf{c} < \mathbf{a}\cdot\mathbf{b}$	$\bar{1}00/0\bar{1}0/\bar{1}01$	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{a}\cdot\mathbf{b}-\mathbf{a}\cdot\mathbf{c} & \frac{\mathbf{a}\cdot\mathbf{a}}{2} & \mathbf{a}\cdot\mathbf{b} \end{pmatrix}$	I
I	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{c} & \frac{\mathbf{a}\cdot\mathbf{a}}{2} \end{pmatrix}$	$2\mathbf{b}\cdot\mathbf{c} < \mathbf{a}\cdot\mathbf{c}$	$\bar{1}00/\bar{1}10/00\bar{1}$	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{a}\cdot\mathbf{c}-\mathbf{b}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{c} & \frac{\mathbf{a}\cdot\mathbf{a}}{2} \end{pmatrix}$	I
II	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \frac{\mathbf{b}\cdot\mathbf{b}}{2} & \mathbf{a}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{b} \end{pmatrix}$	$\mathbf{a}\cdot\mathbf{b} \neq 0$	$100/0\bar{1}0/0\bar{1}\bar{1}$	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \frac{\mathbf{b}\cdot\mathbf{b}}{2} & (\lvert\mathbf{a}\cdot\mathbf{c}\rvert+\lvert\mathbf{a}\cdot\mathbf{b}\rvert) & \lvert\mathbf{a}\cdot\mathbf{b}\rvert \end{pmatrix}$	I
II	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{c} & \frac{\mathbf{a}\cdot\mathbf{a}}{2} & \mathbf{a}\cdot\mathbf{b} \end{pmatrix}$	$\mathbf{a}\cdot\mathbf{b} \neq 0$	$\bar{1}00/010/\bar{1}0\bar{1}$	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \lvert\mathbf{b}\cdot\mathbf{c}\rvert+\lvert\mathbf{a}\cdot\mathbf{b}\rvert & \frac{\mathbf{a}\cdot\mathbf{a}}{2} & \lvert\mathbf{a}\cdot\mathbf{b}\rvert \end{pmatrix}$	I
II	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{c}-\frac{\mathbf{a}\cdot\mathbf{a}}{2} & \end{pmatrix}$	$\mathbf{a}\cdot\mathbf{c} \neq 0$	$\bar{1}00/\bar{1}\bar{1}0/001$	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \lvert\mathbf{b}\cdot\mathbf{c}\rvert+\lvert\mathbf{a}\cdot\mathbf{c}\rvert & \lvert\mathbf{a}\cdot\mathbf{c}\rvert & \frac{\mathbf{a}\cdot\mathbf{a}}{2} \end{pmatrix}$	I
II	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ X & \mathbf{a}\cdot\mathbf{c} & \mathbf{a}\cdot\mathbf{b} \end{pmatrix}$	$2\lvert\mathbf{a}\cdot\mathbf{c}\rvert+2\lvert\mathbf{a}\cdot\mathbf{b}\rvert < \mathbf{a}\cdot\mathbf{a}$	$100/010/111$	$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ Y & Z & \mathbf{a}\cdot\mathbf{b} \end{pmatrix}$	II
where	$X=(\mathbf{a}\cdot\mathbf{a}+\mathbf{b}\cdot\mathbf{b}-2\lvert\mathbf{a}\cdot\mathbf{c}\rvert-2\lvert\mathbf{a}\cdot\mathbf{b}\rvert)/2$		$Y=\lvert\mathbf{a}\cdot\mathbf{b}\rvert+\lvert\mathbf{b}\cdot\mathbf{c}\rvert-\mathbf{b}\cdot\mathbf{b}$	$Z=\lvert\mathbf{a}\cdot\mathbf{b}\rvert+\lvert\mathbf{a}\cdot\mathbf{c}\rvert-\mathbf{a}\cdot\mathbf{a}$	

* All cells given in normal representation.

the cell type and, if necessary, transformed again. The matrices given in column 4 represent the transformation of indices from cell S to cell S′.

The reduction procedure previously described consists of a series of transformations of axes applied in sequence. For each transformation a matrix relating the two cells can easily be determined. The matrix relative to the total transformation is then derived by multiplying, in the proper order, the matrices relative to individual transformations. (For a treatment of transformations in sequence, see for example M. J. Buerger, X-Ray Crystallography, New York: John Wiley and Sons, 1949).

5.1.3. Reduced cells and Bravais lattices

The Bravais lattice can be determined, via the reduced cell, from any primitive cell, if the relationship between a reduced cell and the corresponding Bravais lattices is established. The reduced cells for all the Bravais lattices have been derived by Niggli (1928) and tables of Niggli's matrices together with the index-transformation matrices have been given by Buerger (1957) and by Azaroff and Buerger (1958). In Table 5.1.3.1 the matrices representing the various reduced cells are presented in a self-explanatory form suitable for identification purposes. The matrices given in the second column represent the transformation from the reduced to the conventional cell as defined in the footnote of the table. The dimensions of this cell are given in the third column in terms of those of the reduced cell.

In the last column some of the relationships between cell dimensions are given. These relations are typical for each reduced form and explain why the same Bravais lattice may have more than one reduced cell. The nomenclature used in column 4 is the one given by Niggli (1928). The footnote of the Table explains the conventions used. It also gives the additional transformation matrices to go from the conventional cell of Table 5.1.3.1 to the cell used for space-group description (Section 4.3) or to the determinative setting used by Donnay *et al.* (1963) in the classification of crystalline substances. If any primitive reciprocal cell is derived from accurate powder or single crystal diffraction patterns, then the corresponding direct cell, which is also primitive, can be reduced according to the procedure described above. The Bravais lattice can then be determined from Table 5.1.3.1.* This application of reduced cells is useful when crystals are grown and studied under unusual conditions in which it is difficult or impossible to determine the lattice symmetry by conventional means. Such conditions are encountered, for example, in high pressure and in high or low temperature studies.

* Note that the lattice symmetry determined in this way is purely metric and may be the same as or higher than the true symmetry of the crystal lattice.

TABLE 5.1.3.1

No	Second Row of Matrix $\underline{b}\cdot\underline{c}$	$\underline{a}\cdot\underline{c}$	$\underline{a}\cdot\underline{b}$	Transformation from reduced cell to conventional cell*	Dimensions of conventional cell	Bravais Lattice	Relations between cell dimensions
$\underline{a}=\underline{b}=\underline{c}$							
Positive reduced form							
1	$\frac{\underline{a}\cdot\underline{a}}{2}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$1\bar{1}1/11\bar{1}/\bar{1}11$	$a_1=a\sqrt{2}$	cubic F	
2	$\underline{b}\cdot\underline{c}$	$\underline{b}\cdot\underline{c}$	$\underline{b}\cdot\underline{c}$	$1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$	$a_1=[2(\underline{a}\cdot\underline{a}-\underline{b}\cdot\underline{c})]^{\frac{1}{2}}$ $c_1=[3(\underline{a}\cdot\underline{a}+2\underline{b}\cdot\underline{c})]^{\frac{1}{2}}$	rhombohedral (hR) (intermediate pos.)	$(3/2)^{\frac{1}{2}}<c_1/a_1<\sqrt{6}$
Negative reduced form							
3	0	0	0	100/010/001	$a_1=a$	cubic P	
4	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$	$a_1=[2(\underline{a}\cdot\underline{a}+\lvert\underline{b}\cdot\underline{c}\rvert)]^{\frac{1}{2}}$ $c_1=[3(\underline{a}\cdot\underline{a}-2\lvert\underline{b}\cdot\underline{c}\rvert)]^{\frac{1}{2}}$	rhombohedral (hR) (intermediate neg.)	$(3/8)^{\frac{1}{2}}<c_1/a_1<(3/2)^{\frac{1}{2}}$
5	$-\frac{\underline{a}\cdot\underline{a}}{3}$	$-\frac{\underline{a}\cdot\underline{a}}{3}$	$-\frac{\underline{a}\cdot\underline{a}}{3}$	101/110/011	$a_1=2a/\sqrt{3}$	cubic I	
6	$\frac{-\underline{a}\cdot\underline{a}+\lvert\underline{a}\cdot\underline{b}\rvert}{2}$	$\frac{-\underline{a}\cdot\underline{a}+\lvert\underline{a}\cdot\underline{b}\rvert}{2}$	$-\lvert\underline{a}\cdot\underline{b}\rvert$	011/101/110	$a_1=[\underline{a}\cdot\underline{a}+\lvert\underline{a}\cdot\underline{b}\rvert]^{\frac{1}{2}}$ $c_1=[2(\underline{a}\cdot\underline{a}-\lvert\underline{a}\cdot\underline{b}\rvert)]^{\frac{1}{2}}$	tetragonal I (intermediate)	$(2/3)^{\frac{1}{2}}<c_1/a_1<1$
7	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$\frac{-\underline{a}\cdot\underline{a}+\lvert\underline{b}\cdot\underline{c}\rvert}{2}$	$\frac{-\underline{a}\cdot\underline{a}+\lvert\underline{b}\cdot\underline{c}\rvert}{2}$	101/110/011	$a_1=[\underline{a}\cdot\underline{a}+\lvert\underline{b}\cdot\underline{c}\rvert]^{\frac{1}{2}}$ $c_1=[2(\underline{a}\cdot\underline{a}-\lvert\underline{b}\cdot\underline{c}\rvert)]^{\frac{1}{2}}$	tetragonal I (intermediate)	$1<c_1/a_1<\sqrt{2}$
8	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$-\lvert\underline{a}\cdot\underline{c}\rvert$	$-(\lvert\underline{a}\cdot\underline{a}\rvert-\lvert\underline{b}\cdot\underline{c}\rvert-\lvert\underline{a}\cdot\underline{c}\rvert)$	$\bar{1}\bar{1}0/\bar{1}0\bar{1}/0\bar{1}\bar{1}$	$a_1=[2(\lvert\underline{b}\cdot\underline{c}\rvert+\lvert\underline{a}\cdot\underline{c}\rvert)]^{\frac{1}{2}}$ $b_1=[2(\underline{a}\cdot\underline{a}-\lvert\underline{a}\cdot\underline{c}\rvert)]^{\frac{1}{2}}$ $c_1=[a(\underline{a}\cdot\underline{a}-\lvert\underline{b}\cdot\underline{c}\rvert)]^{\frac{1}{2}}$	orthorhombic I	$b_1^2+c_1^2<3a_1^2$ $a_1^2+c_1^2<3b_1^2$ $a_1<b_1<c_1$
$\underline{a}=\underline{b}$							
Positive reduced form							
9	$\frac{\underline{a}\cdot\underline{a}}{2}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$100/\bar{1}10/\bar{1}\bar{1}3$	$a_1=a$ $c_1=[3(3c^2-a^2)]^{\frac{1}{2}}$	rhombohedral (hR) (positive)	$c_1/a_1>\sqrt{6}$
10	$\underline{b}\cdot\underline{c}$	$\underline{b}\cdot\underline{c}$	$\underline{a}\cdot\underline{b}$	$110/1\bar{1}0/00\bar{1}$	$a_1=[2(\underline{a}\cdot\underline{a}+\underline{a}\cdot\underline{b})]^{\frac{1}{2}}$ $b_1=[2(\underline{a}\cdot\underline{a}-\underline{a}\cdot\underline{b})]^{\frac{1}{2}}$ $c_1=c$ $\cos\beta_1=-2\underline{b}\cdot\underline{c}/a_1c_1$	monoclinic C	$(1/3)^{\frac{1}{2}}<b_1/a_1<1$
Negative reduced form							
11	0	0	0	100/010/001	$a_1=a$ $c_1=c$	tetragonal P (positive)	$c_1/a_1>1$
12	0	0	$-\frac{\underline{a}\cdot\underline{a}}{2}$	100/010/001	$a_1=a$ $c_1=c$	hexagonal P (positive)	$c_1/a_1>1$
13	0	0	$-\lvert\underline{a}\cdot\underline{b}\rvert$	$110/\bar{1}10/001$	$a_1=[2(\underline{a}\cdot\underline{a}-\lvert\underline{a}\cdot\underline{b}\rvert)]^{\frac{1}{2}}$ $b_1=[2(\underline{a}\cdot\underline{a}+\lvert\underline{a}\cdot\underline{b}\rvert)]^{\frac{1}{2}}$ $c_1=c$	orthorhombic C	$(1/3)^{\frac{1}{2}}<b_1/a_1<\sqrt{3}$
14	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$-\lvert\underline{a}\cdot\underline{b}\rvert$	$110/\bar{1}10/001$	$a_1=[2(\underline{a}\cdot\underline{a}-\lvert\underline{a}\cdot\underline{b}\rvert)]^{\frac{1}{2}}$ $b_1=[2(\underline{a}\cdot\underline{a}+\lvert\underline{a}\cdot\underline{b}\rvert)]^{\frac{1}{2}}$ $c_1=c$ $\cos\beta_1=-2\lvert\underline{b}\cdot\underline{c}\rvert/[2(\underline{a}\cdot\underline{a}-\lvert\underline{a}\cdot\underline{b}\rvert)]^{\frac{1}{2}}c$	monoclinic C	$1<b_1/a_1<\sqrt{3}$
15	$-\frac{\underline{a}\cdot\underline{a}}{2}$	$-\frac{\underline{a}\cdot\underline{a}}{2}$	0	100/010/112	$a_1=a$ $c_1=[2(c^2-a^2)]^{\frac{1}{2}}$	tetragonal I (positive)	$c_1/a_1>\sqrt{2}$
16	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$-(\underline{a}\cdot\underline{a}-2\lvert\underline{b}\cdot\underline{c}\rvert)$	$\bar{1}\bar{1}0/1\bar{1}0/112$	$a_1=2(\lvert\underline{b}\cdot\underline{c}\rvert)^{\frac{1}{2}}$ $b_1=2(\underline{a}\cdot\underline{a}-\lvert\underline{b}\cdot\underline{c}\rvert)^{\frac{1}{2}}$ $c_1=2(\underline{c}\cdot\underline{c}-\lvert\underline{b}\cdot\underline{c}\rvert)^{\frac{1}{2}}$	orthorhombic F	$b_1/a_1<\sqrt{3}$
17	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$-\lvert\underline{a}\cdot\underline{c}\rvert$	$-(\underline{a}\cdot\underline{a}-\lvert\underline{b}\cdot\underline{c}\rvert-\lvert\underline{a}\cdot\underline{c}\rvert)$	$\bar{1}0\bar{1}/\bar{1}\bar{1}0/011$	$a_1=(\underline{a}\cdot\underline{a}+\underline{c}\cdot\underline{c}-2\lvert\underline{a}\cdot\underline{c}\rvert)^{\frac{1}{2}}$ $b_1=[2(\lvert\underline{b}\cdot\underline{c}\rvert+\lvert\underline{a}\cdot\underline{c}\rvert)]^{\frac{1}{2}}$ $c_1=(\underline{a}\cdot\underline{a}+\underline{c}\cdot\underline{c}-2\lvert\underline{b}\cdot\underline{c}\rvert)^{\frac{1}{2}}$ $\cos\beta_1=(a^2-c^2)/a_1c_1$	monoclinic I	$a_1<c_1$
$\underline{b}=\underline{c}$							
Positive reduced form							
18	$\frac{\underline{a}\cdot\underline{a}}{2}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$0\bar{1}1/1\bar{1}\bar{1}/100$	$a_1=[2b^2-\frac{a^2}{2}]^{\frac{1}{2}}$ $c_1=a$	tetragonal I (negative)	$c_1/a_1<(2/3)^{\frac{1}{2}}$
19	$\underline{b}\cdot\underline{c}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$\bar{1}00/0\bar{1}1/\bar{1}11$	$a_1=a$ $b_1=[2(b^2-\underline{b}\cdot\underline{c})]^{\frac{1}{2}}$ $c_1=[2b^2-a^2+\underline{b}\cdot\underline{c}]^{\frac{1}{2}}$	orthorhombic I	$b_1^2+c_1^2>3a_1^2$ $a_1^2+c_1^2<3b_1^2$ $a_1<b_1<c_1$
20	$\underline{b}\cdot\underline{c}$	$\underline{a}\cdot\underline{c}$	$\underline{a}\cdot\underline{c}$	$011/01\bar{1}/\bar{1}00$	$a_1=[2(\underline{b}\cdot\underline{b}+\underline{b}\cdot\underline{c})]^{\frac{1}{2}}$ $b_1=[2(\underline{b}\cdot\underline{b}-\underline{b}\cdot\underline{c})]^{\frac{1}{2}}$ $c_1=a$ $\cos\beta_1=-2\underline{a}\cdot\underline{c}/a_1c_1$	monoclinic C	$(1/3)^{\frac{1}{2}}<b_1/a_1<1$ $c_1<b_1<a_1$
Negative reduced form							
21	0	0	0	010/001/100	$a_1=b$ $c_1=a$	tetragonal P (negative)	$c_1/a_1<1$
22	$-\frac{\underline{b}\cdot\underline{b}}{2}$	0	0	010/001/100	$a_1=b$ $c_1=a$	hexagonal P (negative)	$c_1/a_1<1$
23	$-\lvert\underline{b}\cdot\underline{c}\rvert$	0	0	$011/0\bar{1}1/100$	$a_1=[2(\underline{b}\cdot\underline{b}-\lvert\underline{b}\cdot\underline{c}\rvert)]^{\frac{1}{2}}$ $b_1=[2(\underline{b}\cdot\underline{b}+\lvert\underline{b}\cdot\underline{c}\rvert)]^{\frac{1}{2}}$ $c_1=a$	orthorhombic C	$b_1/a_1<\sqrt{3}$ $c_1<a_1<b_1$
24	$-\frac{\underline{b}\cdot\underline{b}-\underline{a}\cdot\underline{a}/3}{2}$	$-\frac{\underline{a}\cdot\underline{a}}{3}$	$-\frac{\underline{a}\cdot\underline{a}}{3}$	$121/0\bar{1}1/100$	$a_1=[3b^2-(a^2/3)]^{\frac{1}{2}}$ $c_1=a$	rhombohedral (hR) (negative)	$c_1/a_1<(3/8)^{\frac{1}{2}}$
25	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$-\lvert\underline{a}\cdot\underline{c}\rvert$	$-\lvert\underline{a}\cdot\underline{c}\rvert$	$011/0\bar{1}1/100$	$a_1=[2(\underline{b}\cdot\underline{b}-\lvert\underline{b}\cdot\underline{c}\rvert)]^{\frac{1}{2}}$ $b_1=[2(\underline{b}\cdot\underline{b}+\lvert\underline{b}\cdot\underline{c}\rvert)]^{\frac{1}{2}}$ $c_1=a$ $\cos\beta_1=-2\lvert\underline{a}\cdot\underline{c}\rvert/a_1c_1$	monoclinic C	$a_1/b_1<1$ $c_1<a_1<b_1$

TABLE 5.1.3.1 (continued)

No.	Second Row of Matrix $\underline{b}\cdot\underline{c}$	$\underline{a}\cdot\underline{c}$	$\underline{a}\cdot\underline{b}$	Transformation from reduced cell to conventional cell*	Dimensions of conventional cell	Bravais Lattice	Relations between cell dimensions
No two cell edges equal							
Positive reduced form							
26	$\frac{\underline{a}\cdot\underline{a}}{4}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$100/\bar{1}20/\bar{1}02$	$a_1=a$ $b_1=(4b^2-a^2)^{\frac{1}{2}}$ $c_1=(4c^2-a^2)^{\frac{1}{2}}$	orthorhombic P	$a_1/b_1<\sqrt{3}$ $a_1<b_1<c_1$
27	$\underline{b}\cdot\underline{c}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$0\bar{1}1/\bar{1}00/1\bar{1}\bar{1}$	$a_1=(\underline{b}\cdot\underline{b}+\underline{c}\cdot\underline{c}-2\underline{b}\cdot\underline{c})^{\frac{1}{2}}$ $b_1=a$ $c_1=(-\underline{a}\cdot\underline{a}+\underline{b}\cdot\underline{b}+\underline{c}\cdot\underline{c}+2\underline{b}\cdot\underline{c})^{\frac{1}{2}}$ $\cos\beta_1=(b^2-c^2)/a_1c_1$	monoclinic I	$a_1, c_1>b_1$
28	$\frac{\underline{a}\cdot\underline{b}}{2}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$\underline{a}\cdot\underline{b}$	$\bar{1}00/\bar{1}02/010$	$a_1=a$ $b_1=(4c^2-a^2)^{\frac{1}{2}}$ $c_1=b$ $\cos\beta_1=-\underline{a}\cdot\underline{b}/a_1c_1$	monoclinic C	$a_1/b_1<\sqrt{3}$ $a_1<c_1<b_1$
29	$\frac{\underline{a}\cdot\underline{c}}{2}$	$\underline{a}\cdot\underline{c}$	$\frac{\underline{a}\cdot\underline{a}}{2}$	$100/1\bar{1}0/00\bar{1}$	$a_1=a$ $b_1=(4b^2-a^2)^{\frac{1}{2}}$ $c_1=c$ $\cos\beta_1=-\underline{a}\cdot\underline{c}/a_1c_1$	monoclinic C	$a_1/b_1<\sqrt{3}$ $a_1<b_1$ $a_1<c_1$
30	$\frac{\underline{b}\cdot\underline{b}}{2}$	$\frac{\underline{a}\cdot\underline{b}}{2}$	$\underline{a}\cdot\underline{b}$	$010/01\bar{1}/\bar{1}00$	$a_1=a$ $b_1=(4c^2-b^2)^{\frac{1}{2}}$ $c_1=b$ $\cos\beta_1=-\underline{a}\cdot\underline{b}/a_1c_1$	monoclinic C	$c_1<a_1<b_1$
31	$\underline{b}\cdot\underline{c}$	$\underline{a}\cdot\underline{c}$	$\underline{a}\cdot\underline{b}$	$100/010/001$	$a_1=a$, $\cos\alpha_1=\underline{b}\cdot\underline{c}/b_1c_1$ $b_1=b$, $\cos\beta_1=\underline{a}\cdot\underline{c}/a_1c_1$ $c_1=c$, $\cos\gamma_1=\underline{a}\cdot\underline{b}/a_1b_1$	triclinic P	$a_1<b_1<c_1$
Negative reduced form							
32	0	0	0	$100/010/001$	$a_1=a$ $b_1=b$ $c_1=c$	orthorhombic P	$a_1<b_1<c_1$
33	0	$-\lvert\underline{a}\cdot\underline{c}\rvert$	0	$100/010/001$	$a_1=a$, $b_1=b$, $c_1=c$, $\cos\beta_1=-\lvert\underline{a}\cdot\underline{c}\rvert/a_1c_1$	monoclinic P	$a_1<b_1<c_1$
34	0	0	$-\lvert\underline{a}\cdot\underline{b}\rvert$	$\bar{1}00/00\bar{1}/0\bar{1}0$	$a_1=a$, $b_1=c$, $c_1=b$, $\cos\beta_1=-\lvert\underline{a}\cdot\underline{b}\rvert/a_1c_1$	monoclinic P	$a_1<c_1<b_1$
35	$-\lvert\underline{b}\cdot\underline{c}\rvert$	0	0	$0\bar{1}0/\bar{1}00/00\bar{1}$	$a_1=b$, $b_1=a$, $c_1=c$, $\cos\beta_1=-\lvert\underline{b}\cdot\underline{c}\rvert/a_1c_1$	monoclinic P	$b_1<a_1<c_1$
36	0	$-\frac{\underline{a}\cdot\underline{a}}{2}$	0	$100/\bar{1}0\bar{2}/010$	$a_1=a$ $b_1=(4c^2-a^2)^{\frac{1}{2}}$ $c_1=b$	orthorhombic C	$a_1/b_1<(1/3)^{\frac{1}{2}}$ $a_1<c_1<b_1$
37	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$-\frac{\underline{a}\cdot\underline{a}}{2}$	0	$102/100/010$	$a_1=(4c^2-a^2)^{\frac{1}{2}}$ $b_1=a$ $c_1=b$ $\cos\beta_1=-2\lvert\underline{b}\cdot\underline{c}\rvert/a_1c_1$	monoclinic C	$a_1/b_1>\sqrt{3}$ $b_1<c_1<a_1$
38	0	0	$-\frac{\underline{a}\cdot\underline{a}}{2}$	$\bar{1}00/120/00\bar{1}$	$a_1=a$ $b_1=(4b^2-a^2)^{\frac{1}{2}}$ $c_1=c$	orthorhombic C	$a_1/b_1<(1/3)^{\frac{1}{2}}$ $a_1<b_1$ $a_1<c_1$
39	$-\lvert\underline{b}\cdot\underline{c}\rvert$	0	$-\frac{\underline{a}\cdot\underline{a}}{2}$	$\bar{1}\bar{2}0/\bar{1}00/00\bar{1}$	$a_1=(4b^2-a^2)^{\frac{1}{2}}$ $b_1=a$ $c_1=c$ $\cos\beta_1=-2\lvert\underline{b}\cdot\underline{c}\rvert/a_1c_1$	monoclinic C	$b_1<a_1$ $b_1<c_1$
40	$-\frac{\underline{b}\cdot\underline{b}}{2}$	0	0	$0\bar{1}0/012/\bar{1}00$	$a_1=b$ $b_1=(4c^2-b^2)^{\frac{1}{2}}$ $c_1=a$	orthorhombic C	$a_1/b_1<(1/3)^{\frac{1}{2}}$ $c_1<a_1<b_1$
41	$-\frac{\underline{b}\cdot\underline{b}}{2}$	$-\lvert\underline{a}\cdot\underline{c}\rvert$	0	$0\bar{1}\bar{2}/0\bar{1}0/\bar{1}00$	$a_1=(4c^2-b^2)^{\frac{1}{2}}$ $b_1=b$ $c_1=a$ $\cos\beta_1=-2\lvert\underline{a}\cdot\underline{c}\rvert/a_1c_1$	monoclinic C	$a_1/b_1>\sqrt{3}$ $c_1<b_1<a_1$
42	$-\frac{\underline{b}\cdot\underline{b}}{2}$	$-\frac{\underline{a}\cdot\underline{a}}{2}$	0	$\bar{1}00/0\bar{1}0/112$	$a_1=a$ $b_1=b$ $c_1=(4c^2-a^2-b^2)^{\frac{1}{2}}$	orthorhombic I	$b_1^2+c_1^2>3a_1^2$ $a_1^2+c_1^2>3b_1^2$ $a_1<b_1<c_1$
43	$-\frac{\underline{b}\cdot\underline{b}-\lvert\underline{a}\cdot\underline{b}\rvert}{2}$	$-\frac{\underline{a}\cdot\underline{a}-\lvert\underline{a}\cdot\underline{b}\rvert}{2}$	$-\frac{\lvert\underline{a}\cdot\underline{b}\rvert}{2}$	$\bar{1}00/\bar{1}\bar{1}2/0\bar{1}0$	$a_1=a$ $b_1=(4\underline{c}\cdot\underline{c}-\underline{a}\cdot\underline{a}-\underline{b}\cdot\underline{b}+2\lvert\underline{a}\cdot\underline{b}\rvert)^{\frac{1}{2}}$ $c_1=b$ $\cos\beta_1=-\lvert\underline{a}\cdot\underline{b}\rvert/a_1c_1$	monoclinic I	$a_1<c_1<b_1$
44	$-\lvert\underline{b}\cdot\underline{c}\rvert$	$-\lvert\underline{a}\cdot\underline{c}\rvert$	$-\lvert\underline{a}\cdot\underline{b}\rvert$	$100/010/001$	$a_1=a$, $\cos\alpha_1=-\lvert\underline{b}\cdot\underline{c}\rvert/b_1c_1$ $b_1=b$, $\cos\beta_1=-\lvert\underline{a}\cdot\underline{c}\rvert/a_1c_1$ $c_1=c$, $\cos\gamma_1=-\lvert\underline{a}\cdot\underline{b}\rvert/a_1b_1$	triclinic P	$a_1<b_1<c_1$

*The following conventions have been found convenient for the purpose of this table: (1) In the orthorhombic system, the axes of primitive, body-centered, and face-centered lattices are labelled to obey $a_1<b_1<c_1$. The side-centered lattice is taken as C-centered with $a_1<b_1$. (2) In the monoclinic system, b_1 is taken as the unique axis, and a_1 and c_1 are chosen coincident with the shortest two translations in the net $(010)_0$. The angle β is taken non acute. This choice allows a primitive, a side-centered, and a body-centered lattice. In the primitive and body-centered lattices, a_1 and c_1 obey $a_1<c_1$. The side-centered lattice is taken as C-centered. -- To conform to the conventions used in Table 2.2.1, the monoclinic body-centered cell has to be converted into the C-centered cell by means of the transformation $101/0\bar{1}0/00\bar{1}$. In addition, for the space groups of the point group mm2, the orthorhombic C-centered cell has to be converted into the A-centered cell by means of the transformation $001/100/010$.

For identification purposes, the cell given in column 3 of Table 5.1.3.1 has to be converted into the cell defined in "Crystal Data" (Donnay et al. 1963) by applying one of the following transformations: Triclinic system: Type I cell: $0\bar{1}0/00\bar{1}/100$, Type II cell: $010/001/100$. -- Monoclinic system: P and I lattices: $00\bar{1}/0\bar{1}0/\bar{1}00$; C lattice: $100/010/001$ if $c_1<a_1$, $00\bar{1}/0\bar{1}0/\bar{1}00$ if $c_1>a_1$ (the resulting cell is A centered). -- Orthorhombic system: P,I, and F lattices: $010/001/100$; C lattice: $100/010/001$ if $c_1<a_1<b_1$, $00\bar{1}/0\bar{1}0/\bar{1}00$ if $a_1<c_1<b_1$ (the resulting cell is A centered); $010/001/100$ if $a_1<b_1<c_1$ (the resulting cell is B-centered). -- No transformations are required in the hexagonal, tetragonal, and cubic systems.

In the case of a rhombohedral lattice, note that the hexagonal axes (hR) are used.

5.2. Sub- and Super-groups of the Space Groups

A sub-group of a given space group is a space group of lower symmetry obtained by the removal of certain symmetry elements from the given space group. Correspondingly a super-group of a given space group is a space group of higher symmetry which contains the given space group as one of its sub-groups. Sub- and super-groups are of two kinds:

1. Those in which the unit cell differs from that of the given space group. These can be sub-divided as follows:
   (i) Those belonging to the same point group as the given group.
   (ii) Those belonging to a different point group from that of the given group.
2. Those in which the unit cell is the same as that of the given group.

In this section only sub- and super-groups with the same unit cell as the given space group will be considered, except that, with the square, tetragonal and hexagonal systems of axes, alternative unit cells are permitted. For a discussion of sub- and super-groups with unit cell different from that of the given space group, reference may be made to C. Hermann, *Zeits. Krist.*, **69**, 546, 1929.

Table 5.2.1 gives the sub- and super-operators corresponding to the crystallographic operators of first and second kinds. The repeat distance of translation is assumed to be fixed. These are useful when looking for sub- and super-groups.

In Table 5.2.2 the sub- and super-groups are listed for two dimensions. The sub-groups of a given space group on the left are listed on the same horizontal line to the right. Correspondingly the super-groups of a given space group in the bottom line are those in the left-hand column against which the symbol of the given space group is listed.

TABLE 5.2.1. **Sub- and Super-operators of Symmetry (Three Dimensions)**

Operators	Sub-operators (repeat distance of translation fixed)								
1	–	–	–	–	–	–	–	–	–
$\bar{1}$	1	–	–	–	–	–	–	–	–
2	1	–	–	–	–	–	–	–	–
$\bar{2}$	1	–	–	–	–	–	–	–	–
2_1	1	–	–	–	–	–	–	–	–
3	1	–	–	–	–	–	–	–	–
$\bar{3}$	1	$\bar{1}$	–	–	–	3	–	–	–
3_1	1	–	–	–	–	–	–	–	–
3_2	1	–	–	–	–	–	–	–	–
4	1	–	2	–	–	–	–	–	–
$\bar{4}$	1	–	2	–	–	–	–	–	–
4_1	1	–	–	–	2_1	–	–	–	–
4_2	1	–	2	–	–	–	–	–	–
4_3	1	–	–	–	2_1	–	–	–	–
6	1	–	2	–	–	3	–	–	–
$\bar{6}$	1	–	–	$\bar{2}$	–	3	–	–	–
6_1	1	–	–	–	2_1	–	–	3_1	–
6_2	1	–	2	–	–	–	–	–	3_2
6_3	1	–	–	–	2_1	3	–	–	–
6_4	1	–	2	–	–	–	–	3_1	–
6_5	1	–	–	–	2_1	–	–	–	3_2
↑ Super-operator	1	$\bar{1}$	2	$\bar{2}$	2_1	3	$\bar{3}$	3_1	3_2
	Operators								

TABLE 5.2.2

Sub- and Super-groups of the 17 Two-dimensional Space Groups

Examples: 1. The sub-groups of *p4mm* are *p1*, *p2*, *p1m*, *c1m*, *p2mm*, *c2mm*, *p4*.
2. The super-groups of *c1m* are *c2mm*, *p4mm*, *p4gm*, *p3m1*, *p31m*, *p6mm*.

NOTE. With the square lattice, the alternative unit cell of side $\sqrt{2}a$ is permitted. With the hexagonal lattice, the orthohexagonal cell is permitted. Otherwise only sub- and super-groups with the same unit cells are considered.

Point groups ↓	Space groups ↓																
1	*p1*																
2	*p2*	*p1*															
m	*p1m*	*p1*															
	p1g	*p1*															
	c1m	*c1*															
2mm	*p2mm*	*p1*	*p2*	*p1m*													
	p2mg	*p1*	*p2*	*p1m*	*p1g*												
	p2gg	*p1*	*p2*		*p1g*												
	c2mm	*c1*	*c2*			*c1m*											
4	*p4*	*p1*	*p2*														
4mm	*p4mm*	*p1*	*p2*	*p1m*		*c1m*	*p2mm*			*c2mm*	*p4*						
	p4gm	*p1*	*p2*		*p1g*	*c1m*			*p2gg*	*c2mm*	*p4*						
3	*p3*	*p1*															
3m	*p3m1*	*p1*				*c1m*								*p3*			
	p31m	*p1*				*c1m*								*p3*			
6	*p6*	*p1*	*p2*											*p3*			
6mm	*p6mm*	*p1*	*p2*			*c1m*				*c2mm*				*p3*	*p3m1*	*p31m*	*p6*
↑ Point groups	↑ Super-groups	*p1*	*p2*	*p1m*	*p1g*	*c1m*	*p2mm*	*p2mg*	*p2gg*	*c2mm*	*p4*	*p4mm*	*p4gm*	*p3*	*p3m1*	*p31m*	*p6*	*p6mm*
		Space groups															

Sub-groups

A set of similar tables for the three-dimensional sub- and super-groups would occupy much more space, and the inclusion of such tables in the present volume was not considered to be justified. The space groups of the point group 422 have, however, been taken as an example of such tables for sub- and super-groups with the same lattice as the given space group. In Table 5.2.3 the sub-groups of the 10 given space groups are shown. These sub-groups are grouped according to the parent point groups 1, 2, 222 and 4 which are, of course, the sub-groups of the point group 422.

TABLE 5.2.3

Sub-groups of the Space Groups of Point Group 422

Point group of sub-groups	Space groups $P422$	$P42_12$	$P4_122$	$P4_12_12$	$P4_222$	$P4_22_12$	$P4_322$	$P4_32_12$	$I422$	$I4_122$	Unit-cell relations
1	$P1$	$P1$	$P1$	$P1$	$P1$	$P1$	$P1$	$P1$	$I1$	$I1$	$\frac{c'}{a'}=\frac{c}{a}$
2	$P2$	$P2$	$P2$		$P2$	$P2$	$P2$		$I2$	$I2$	
		$P2_1$	$P2_1$	$P2_1$		$P2_1$	$P2_1$	$P2_1$			
	$C2$	$C2$	$C2$	$C2$	$C2$	$C2$	$C2$	$C2$	$F2$	$F2$	$\frac{c'}{a'}=\frac{c}{\sqrt{2}a}$
222	$C222$	$C222$	$C222_1$	$C222_1$	$C222$	$C222$	$C222_1$	$C222_1$	$F222$	$F222$	
	$P222$	$P2_12_12$	$P222_1$	$P2_12_12_1$	$P222$	$P2_12_12$	$P222_1$	$P2_12_12_1$	$I222$	$I2_12_12_1$	$\frac{c'}{a'}=\frac{c}{a}$
4	$P4$	$P4$	$P4_1$	$P4_1$	$P4_2$	$P4_2$	$P4_3$	$P4_3$	$I4$	$I4_1$	

NOTES
1. Owing to the unit-cell relations, certain symbols of sub-groups are not given in the standard form in the table.
2. The symbols a and c stand for the sides of the unit cell of the original space group, while a' and c' stand for those of the sub-group.

In Table 5.2.4 the super-groups of the 10 given space groups are shown. The super-groups are grouped according to the parent point groups $4/mmm$, 432 and $m3m$ which are, of course, the super-groups of the point group 422.

TABLE 5.2.4

Super-groups of the Space Groups of the Point Group 422

Point group of super-groups	Space groups $P422$	$P42_12$	$P4_122$	$P4_12_12$	$P4_222$	$P4_22_12$	$P4_322$	$P4_32_12$	$I422$	$I4_122$	Unit-cell relations
$4/mmm$	$P4/mmm$	$P4/mbm$			$P4_2/mmc$	$P4_2/mbc$			$I4/mmm$	$I4_1/amd$	$\frac{c'}{a'}=\frac{c}{a}$
	$P4/mcc$	$P4/mnc$			$P4_2/mcm$	$P4_2/mnm$			$I4/mcm$	$I4_1/acd$	
	$P4/nbm$	$P4/nmm$			$P4_2/nbc$	$P4_2/nmc$					
	$P4/nnc$	$P4/ncc$			$P4_2/nnm$	$P4_2/ncm$					
432	$P432$		$P4_132$		$P4_232$		$P4_332$		$I432$	$I4_132$	
$m3m$									$F432$	$F4_132$	$\frac{c'}{a'}=\frac{c}{\sqrt{2}a}$
									$Fm3m$	$Fd3m$	
									$Fm3c$	$Fd3c$	
	$Pm3m$				$Pm3n$				$Im3m$	$Ia3d$	$\frac{c'}{a'}=\frac{c}{a}$
	$Pn3n$				$Pn3m$						

NOTE. The symbols a and c stand for the sides of the unit cell of the original space group, while a' and c' stand for those of the super-group.

5.3. Space-group Determination by Methods outside the Friedel Law

In section 4.4 there is a discussion of the amount of information which can be obtained about the symmetry of a crystal by means of morphological study, physical tests and chemical considerations, combined with X-ray data. This discussion is carried on within the operation of the Friedel Law which states that it is not possible, by ordinary X-ray methods, to detect the presence or absence of centrosymmetry in a crystal. In more recent years, however, two types of X-ray method have been devised which are capable, in certain cases, of giving more information about the symmetry of a crystal. In the first of these, due to Coster, Knol and Prins (1930), use is made of a wave-length near the resonance level of a particular atom in the crystal. If this condition can be satisfied, a difference of intensity between hkl and $\bar{h}\bar{k}\bar{l}$ may be observed for a non-centrosymmetric crystal. The method can therefore be used to detect the absence of a centre of symmetry. It can also be used to determine the *absolute* configuration of a structure which belongs to one of the 11 pairs of enantiomorphous space groups, provided that the structure is fully known in all respects except that of "hand." The actual (hkl) and $(\bar{h}\bar{k}\bar{l})$ intensities can be calculated on the assumption that the structure is based on, say, a left-hand screw; if the observed values are the reverse of those calculated, the screw must be a right-hand one. Although this method is a direct one, the chemical composition of the crystals to which it can be successfully applied is limited by the available wave-lengths (see references on p. 347).

The second method, due to Wilson and others (see references on p. 540), involves a statistical examination of certain groups of intensities, as outlined in the present section. This method may be particularly useful for crystals in which the properties of pyroelectricity and of piezoelectricity are very weakly developed. It is in this latter type of crystal that the determination of non-centrosymmetry is difficult by physical methods, as it is also where the specimen consists of very small crystals or of only a very small amount of material.

In this second method a statistical examination is made of the intensities of reflections for the whole array, or for certain zones, or for certain rows, of reflections in the reciprocal lattice, and then two main kinds of observations can be made.

1. Certain zones or rows may be found to have an average intensity which is a small integral multiple of the average for the whole array. The zones or rows affected in this way indicate the presence, the type and the orientation, within the point group, of all the non-translatory symmetry elements except centrosymmetry. This information, taken along with the Laue symmetry, suffices to determine uniquely all space groups except:

(*a*) individual members of the enantiomorphous pairs,
(*b*) individual members of the pairs ($I222$ and $I2_12_12_1$) and ($I23$, $I2_13$),
(*c*) between $P1$ and $P\bar{1}$, $P3$ and $P\bar{3}$, and $R3$ and $R\bar{3}$.

For example, $P2_1$ may be distinguished from $P2_1/m$ by the fact that, for the latter but not for the former, the average intensity of the $h0l$ reflections is twice that of the hkl reflections.

2. The structure factors of the whole array, or of certain zones, or of certain rows, will have phase angles systematically zero or π if the space group, or the corresponding projection, is centrosymmetric. These arrays, zones or rows may be distinguished experimentally from others for which the structure factors are not systematically real by a difference in the probability distribution of the observed intensities. The acentric distribution is an unambiguous indication of the absence of a centre of symmetry. The centric distribution may be found either with true centrosymmetry or with pseudo-centrosymmetry (Kitajgorodskij, 1951), but in the latter case the distribution will ordinarily differ in type when evaluated for ranges of low and of high $\sin\theta$ (Wilson, 1951*b*). This "distribution method" makes possible, at least in principle, the unique determination of each point group and hence of all space groups except:

(*a*) individual members of the enantiomorphous pairs,
(*b*) individual members of the pairs ($I222$, $I2_12_12_1$) and ($I23$, $I2_13$).

The distribution may be investigated by the ratio test (Wilson, 1949), the $N(z)$ test (Howells, Phillips and Rogers, 1949), and by the variance test (Wilson, 1951*a*).

Statistical methods thus offer the chance of distinguishing between space-group possibilities when the point group is unknown, except that they do not distinguish between the individual members of the enantiomorphous pairs and of the pairs ($I222$, $I2_12_12_1$) and ($I23$, $I2_13$). In section 4.4 it was noticed

that individual members of certain enantiomorphous pairs could be distinguished, provided that the polar axes could be orientated in the same sense for both members of the pair. The method of Coster, Knol and Prins, mentioned earlier in the present section, offers the possibility of distinguishing between the members of all the enantiomorphous pairs. The only method that is at present able to distinguish between the individual members of the pairs ($I222$, $I2_12_12_1$) and ($I23$, $I2_13$) is the method of vector sets (Patterson analysis) as developed by M. J. Buerger (1950) (see Nowacki, 1952).

The statistical tests have differing ranges of applicability. The Wilson ratio test ($\langle|F|\rangle^2/\langle|F|^2\rangle$) and the Rogers $N(z)$ test for centrosymmetry are the most limited and require the following conditions:

(i) that the unit cell should contain a sufficient number of non-equivalent atoms;

(ii) that the positions of these atoms should be reasonably general;

(iii) that heavy atoms, if present, should not occupy true or apparent centres of symmetry, nor should they possess a considerable fraction of the total scattering power.

The variance test for centrosymmetry tolerates considerable departures from these conditions and also permits precise allowance for condition (i) above. The average-multiple test is equally general in its applicability. Atoms lying on the symmetry element are not repeated and do not contribute to the enhanced intensity average. The observed multiple is then somewhat less than the integer. A knowledge of the unit-cell contents, possible molecular symmetry and possible space group may give warning of atoms in special positions. Due allowance can then be made in the use of the average-multiple test, and caution can be exercised in the interpretation of the results of the Wilson or the Rogers tests. Successful determinations have, however, been made with the Rogers $N(z)$ test in spite of considerable departures from the above requirements.

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5.4. Inequalities arising from Symmetry Elements

If it is supposed that the general form of all atomic scattering factor curves is approximately the same, then we can define a "unitary atomic scattering factor" $u=f_r/Z_r$ where Z_r is the number of electrons in an atom of scattering factor f_r.

If the total number of electrons in the unit cell is Z, then let $U(hkl)=F(hkl)/Zu$, where $F(hkl)$ is the observed structure factor in absolute units.

Now it may be shown (see references [1], [2], [3] and [5] below) that inequality relationships hold between the U values for various reflections, according to the crystal symmetry, and that these relationships may sometimes be used for the determination of at least a limited number of phases.

Thus, for example, if the crystal contains a centre of symmetry, then

$$2|U(hkl)|^2 \leqq [1+U(2h,2k,2l)]$$

This may be written

$$U(2h,2k,2l) \geqq 2|U(hkl)|^2-1$$

$U(2h,2k,2l)$ must be positive if $|U(hkl)|^2 \geqq 1/2$;
or if $|U(2h,2k,2l)| \geqq 1/2$ and if $|U(hkl)|^2 > 1/4$, then $U(2h,2k,2l)$ must also be positive.

Table 5.4.1 gives a list of simple inequalities but this list by no means exhausts the possibilities of the method. For an extension of the list to space groups containing large numbers of symmetrically related atoms of a given kind, and to inequalities of the "sum and difference" types, reference should be made to the original papers. A straightforward derivation of the inequalities for a particular space group can be made by the application of group theory [5].

TABLE 5.4.1. **The Inequalities arising from the Various Elements of Symmetry**

NOTE. All symmetry elements pass through the origin.

Symbol of axis	Equivalent symbol	System of co-ordinates	Inequality
1	—	Triclinic	$\lvert U(hkl)\rvert^2 \leq 1$
$\bar{1}$	—	Triclinic	$U(hkl)^2 \leq \frac{1}{2}+\frac{1}{2}U(2h,2k,2l)$
2	—	Monoclinic	$\lvert U(hkl)\rvert^2 \leq \frac{1}{2}+\frac{1}{2}U(2h,0,2l)$
$\bar{2}$	m	Monoclinic	$\lvert U(hkl)\rvert^2 \leq \frac{1}{2}+\frac{1}{2}U(0,2k,0)$
2_1	—	Monoclinic	$\lvert U(hkl)\rvert^2 \leq \frac{1}{2}+\frac{1}{2}(-1)^k U(2h,0,2l)$
3	—	Hexagonal	$\lvert U(hkil)\rvert^2 \leq \frac{1}{3}+\frac{2}{3}\lvert U(h-k,k-i,i-h,0)\rvert \cos\,[2\pi\alpha(h-k,k-i,i-h,0)]$
$\bar{3}$	$3+\bar{1}$	Hexagonal	$U(hkil)^2 \leq \frac{1}{6}+\frac{1}{6}U(2h,2k,2i,2l)+\frac{1}{3}U(h,k,i,2l)+\frac{1}{3}U(h-k,k-i,i-h,0)$
3_1	—	Hexagonal	$\lvert U(hkil)\rvert^2 \leq \frac{1}{3}+\frac{2}{3}\lvert U(h-k,k-i,i-h,0)\rvert \cos\,2\pi[\alpha(h-k,k-i,i-h,0)+l/3]$
4	—	Tetragonal	$\lvert U(hkl)\rvert^2 \leq \frac{1}{4}+\frac{1}{4}U(2h,2k,0)+\frac{1}{2}U(h-k,h+k,0)$
$\bar{4}$	—	Tetragonal	$\lvert U(hkl)\rvert^2 \leq \frac{1}{4}+\frac{1}{4}U(2h,2k,0)+\frac{1}{2}U(h-k,h+k,2l) \cos\,[2\pi\alpha(h-k,h+k,2l)]$
4_1	—	Tetragonal	$\lvert U(hkl)\rvert^2 \leq \frac{1}{4}+\frac{1}{4}(-1)^l U(2h,2k,0)+\frac{1}{2}U(h-k,h+k,0) \cos\,(2\pi l/4)$
4_2	—	Tetragonal	$\lvert U(hkl)\rvert^2 < \frac{1}{4}+\frac{1}{4}U(2h,2k,0)+\frac{1}{2}(-1)^l U(h-k,h+k,0)$
6	—	Hexagonal	$\lvert U(hkil)\rvert^2 \leq \frac{1}{6}+\frac{1}{6}U(2h,2k,2i,0)+\frac{1}{3}U(h-k,k-i,i-h,0)+\frac{1}{3}U(h,k,i,0)$
$\bar{6}$	$3/m$	Hexagonal	$\lvert U(hkil)\rvert^2 \leq \frac{1}{6}+\frac{1}{6}U(0,0,0,2l)+\frac{1}{3}U(h-k,k-i,i-h,0) \cos\,[2\pi\alpha(h-k,k-i,i-h,0)]+\frac{1}{3}U(h-k,k-i,i-h,2l) \cos\,[2\pi\alpha(h-k,k-i,i-h,2l)]$
6_1	—	Hexagonal	$\lvert U(hkil)\rvert^2 \leq \frac{1}{6}+\frac{1}{6}(-1)^l U(2h,2k,2i,0)+\frac{1}{3}U(h-k,k-i,i-h,0) \cos\,(2\pi l/3)+\frac{1}{3}U(h,k,i,0) \cos\,(2\pi l/6)$
6_2	—	Hexagonal	$\lvert U(hkil)\rvert^2 \leq \frac{1}{6}+\frac{1}{6}U(2h,2k,2i,0)+\frac{1}{3}U(h-k,k-i,i-h,0) \cos\,(2\pi l/3)+\frac{1}{3}U(h,k,i,0) \cos\,(2\pi l/3)$
6_3	—	Hexagonal	$\lvert U(hkil)\rvert^2 \leq \frac{1}{6}+\frac{1}{6}(-1)^l U(2h,2k,2i,0)+\frac{1}{3}U(h-k,k-i,i-h,0)+\frac{1}{3}(-1)^l U(h,k,i,0)$
—	a	Monoclinic	$\lvert U(hkl)\rvert^2 \leq \frac{1}{2}+\frac{1}{2}(-1)^h U(0,2k,0)$

In Table 5.4.1 the symmetry element has been assumed to pass through the origin; since altering the origin may change the phase, although it does not change the intensity of reflection, it is clear that the inequalities may be altered by a change of origin. The necessary correction may be applied by multiplying values of $U(hkl)$ in the inequality by $\exp 2\pi i(hx+ky+lz)$ where x, y, z is the position of the new origin. Values of $U(hkl)^2$ are unaltered. Thus $2\lvert U(hkl)\rvert^2 \leq [1+U(2h,0,2l)]$ becomes $2\lvert U(hkl)\rvert^2 \leq [1+(-1)^{h+l}U(2h,0,2l)]$ if the origin is transferred from the 2-fold axis to the point $\frac{1}{4},0,\frac{1}{4}$.

A basic assumption in the derivation of the inequalities is that the Fourier series representing the electron density is a positive function [6]. A more extensive system of inequalities can be derived on the basis of this assumption without regard to symmetry. These general relations can then be simplified and put into more usable form by the application of symmetry operations [6, 7].

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6. INDEX OF SYMBOLS OF SPACE GROUPS

6.1. Index of Symbols of Two-dimensional Space Groups

In the present work both the symbols and the diagrams for the two-dimensional space groups have been brought into accordance with those used for the three-dimensional groups. A full description of the symbols is given in section 4.1. Names have been assigned to the "systems" into which the two-dimensional point and space groups can be divided, in accordance with the procedure in three dimensions.

In Table 6.1.1 the names of the systems and the numbers and symbols of the 17 two-dimensional space groups are given, with alternative symbols where other orientations are likely to be useful. In the last two columns of the table are given for reference the symbols used by Patterson (1935), which were modified from those used by Niggli (1924), and the symbols used by Buerger (1942).

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TABLE 6.1.1. **Index of Symbols of Two-dimensional Space Groups**

System	No. of group	Standard symbols short	Standard symbols full	Symbols for other setting	Symbols for other unit cells	Niggli-Patterson symbols	Buerger symbols
Oblique	1	*p*1	*p*1	—	*c*1	C_1^{I}	*P*1
	2	*p*2	*p*211	—	*c*2	C_2^{I}	*P*2
Rectangular	3	*pm*	*p*1*m*1	*p*11*m*	—	C_s^{I}	*Pl*
	4	*pg*	*p*1*g*1	*p*11*g*	—	C_s^{II}	*Pb*
	5	*cm*	*c*1*m*1	*c*11*m*	—	C_s^{III}	*Cl*
	6	*pmm*	*p*2*mm*	*p*2*mm*	—	C_{2v}^{I}	*Pll*
	7	*pmg*	*p*2*mg*	*p*2*gm*	—	C_{2v}^{III}	*Pbl*
	8	*pgg*	*p*2*gg*	*p*2*gg*	—	C_{2v}^{II}	*Pba*
	9	*cm̀m*	*c*2*mm*	*c*2*mm*	—	C_{2v}^{IV}	*Cll*
Square	10	*p*4	*p*4	—	*c*4	C_4^{I}	*P*4 (*C*4)
	11	*p*4*m*	*p*4*mm*	—	*c*4*mm*	C_{4v}^{I}	*P*4*ll* (*C*4*ll*)
	12	*p*4*g*	*p*4*gm*	—	*c*4*mg*	C_{4v}^{II}	*P*4*bl* (*C*4*lb*)
Hexagonal	13	*p*3	*p*3	—	—	C_3^{I}	*C*3 (*H*3)
	14	*p*3*m*1	*p*3*m*1	—	—	C_{3v}^{I}	*C*3*l*1 (*H*31*l*)
	15	*p*31*m*	*p*31*m*	—	—	C_{3v}^{II}	*C*31*l* (*H*3*l*1)
	16	*p*6	*p*6	—	—	C_6^{I}	*C*6 (*H*6)
	17	*p*6*m*	*p*6*mm*	—	—	C_{6v}^{I}	*C*6*ll* (*H*6*ll*)

6.2. Index of Three-dimensional Space-group Symbols for Various Settings

In the symbolism used in these tables it is possible for a particular space group to be indicated by more than one symbol. For purposes of tabulation, therefore, a standard symbol has to be chosen. In the systems of higher symmetry the conventional choice of axes reduces the choice of standard symbol (but see p. 544). In the systems of lower symmetry, however, there is considerable freedom of choice. It should be emphasised that we are not concerned here with any conventions as to the choice of interaxial angles and relative axial unit lengths which have been put forward for the systems of lower symmetry. We are concerned only with the choice of a standard space-group symbol for purposes of tabulation.

In general the choice of standard symbol can be resolved into two parts: first there is the choice of standard setting of the unit cell within the conventions appropriate to the system; secondly, given the standard setting, there may be the choice of symbol, as more than one kind of symmetry element exists in certain directions in all space groups which have a non-primitive lattice. The first part of this choice is discussed in section 2.3, and the application of this is given below under various systems. In the second part of the choice the following rule is used in the monoclinic and orthorhombic systems:

Where more than one kind of symmetry element exists in a given direction, the choice of the corresponding symbol in the space-group symbol is made in order of descending priority:

m, a, b, c, n, d; and rotation axes before screw axes.

There is only one exception to this: in space group No. 73 the standard symbol is *Ibca*, whereas, according to the rule, it should have been taken as *Ibaa*. This exception is made because the symbol *Ibca*, which is the same for all six settings, displays the symmetry of the space group better than the symbol *Ibaa*.

The application of a point group to a centred lattice will produce more than one set of symmetry elements in certain directions. In the monoclinic and orthorhombic space groups where such interleaving symmetry elements are present their symbols are printed below those chosen for the standard symbol in Table 6.2.1.

In Table 6.2.1 the first column gives the number of the space group, as this is the most convenient method of finding the corresponding data in sections 4.3 and 4.7. The Schoenflies symbols, although less used now, are given next for convenience of reference (F. C. Phillips, *An Introduction to Crystallography*, London, 1946, p. 289). In other columns are given the short, full and alternative symbols where these exist, and lastly, symbols for settings other than that chosen as standard.

TRICLINIC SYSTEM

In the triclinic system a primitive unit cell can always be selected, but in some cases it may be advantageous to select a larger unit cell, with lattice A, B, C, I or F.

MONOCLINIC SYSTEM

In the monoclinic system there are two conventional ways of orientating the unique axis (preface to Vol. I and section 2.2). With the unique axis as either the z- or the y-axis, there are two ways of setting the other two axes, and hence four possibilities in all. The full symbol shows the orientation of the unique axis, but it cannot always show which of the two ways of setting the other two axes has been chosen. The unprimed symbols (**a b c**, etc.) at the head of the columns show the permutations starting from the standard orientation in the 1st setting, and the primed symbols (**a′ b′ c′**, etc.) those starting from the standard orientation in the 2nd setting.

In the lattice which cannot conventionally be represented as primitive the choice has been made so that the standard lattice symbols are B (z-axis unique) and C (y-axis unique). The choice of A would not have distinguished between the two orientations, since that symbol would be the same for both settings. For special purposes larger unit cells may be selected.

ORTHORHOMBIC SYSTEM

In the orthorhombic system there are six settings of the same unit cell, since we are confined by convention to a right-handed system of axes (i.e. one in which the positive directions of the x-, y- and z-axes (or a-, b-, c-) are taken in a right-handed screw order). In some cases, but not in all, the particular setting can be determined from the symbol. In class 222 the single-face-centred lattice is taken as C in the standard setting; also, where one symmetry axis is different from those in the two other directions, the unique direction is taken as the z-axis. In class $mm2$ the unique axis is taken as the standard z-axis, but there has been no consistent choice of the x- and y-axes to make the symmetry symbols in the space-group symbol read in the priority order of the rule given above. In the present work the choice made in the former *International Tables* (1935) has been adopted. Where the lattice is centred on a face parallel to the unique axis this face is taken as (100), and the lattice symbol used is A. In class mmm the single-face-centred lattice is taken as C. Apart from this, there is no consistent choice of axes, and the choice made in the former *International Tables* (1935) has been adopted.

The five permutations of the standard **abc** orientation shown at the head of the columns are not unique; the right-hand screw rule is obeyed if instead of **cab**, for example (meaning $\mathbf{a}'=\mathbf{c}$, $\mathbf{b}'=\mathbf{a}$, $\mathbf{c}'=\mathbf{b}$), we write $\bar{\mathbf{c}}\bar{\mathbf{a}}\mathbf{b}$, $\mathbf{c}\bar{\mathbf{a}}\bar{\mathbf{b}}$, or $\bar{\mathbf{c}}\mathbf{a}\bar{\mathbf{b}}$. The corresponding space-group symbol would be unaltered, although the transformation matrix would be different (sections 2.5, 4.9) in such a case. The space-group symbols for the five alternative settings are obtained by permutation of the standard symbol (and its interleaving symmetry symbols, separately) in accordance with the transformation of axes. Thus if the symmetry corresponding to **a** in the standard setting is a glide plane b or c, and if the transformation is $\mathbf{a}'=\mathbf{c}$, $\mathbf{b}'=\mathbf{a}$, $\mathbf{c}'=\mathbf{b}$, the same symmetry element will now refer to the new **b** (formerly **a**) and the corresponding glide will be c or a respectively. Thus, permuting the symbol *Ibam* (No. 72) would give *Imcb*. It follows that the permuted symbol does not necessarily obey the priority rule. In order that it should do so, it would have to be rearranged to read *Imaa*.

ncb

TETRAGONAL SYSTEM

In the tetragonal system there are no alternative settings of the same unit cell. But if the x- and y-axes are turned through 45° about the z-axis an alternative unit cell of double volume is obtained, and the symbols of these are given. Since the alternative unit cell is a centred one, interleaving symmetry elements are present in all tetragonal space groups. These are not, however, given in the table, since there is no question of alternative settings of the same unit cell.

The priority rule given on p. 543 has not been consistently followed in formulating the standard symbols for tetragonal space groups. For example, b is used rather than a where there are intersecting glide planes parallel to {100}, and c is used rather than a or b where there are interleaving and intersecting glide planes parallel to {100}. Here the nomenclature of the 1935 *Tables* has been retained, in order to avoid the considerable changes that would otherwise be required.

TRIGONAL AND HEXAGONAL SYSTEMS

Again in the trigonal and hexagonal systems there are no alternative settings of the same unit cell. But if the x-, y- and u-axes are turned through 90° about the z-axis, an alternative unit cell of triple volume is obtained; this is the setting denoted by the letter H in the former *International Tables* (1935) which is replaced for systematic purposes in the present volume by the use of the positional notation. If orthohexagonal axes are used the alternative unit cell is centred on the C-face. Consequently all trigonal and hexagonal space groups have interleaving elements of symmetry; but these are not given in the table since there is no question of alternative settings of the same unit cell.

CUBIC SYSTEM

The question of alternative settings does not arise in this system.

The priority rule is again not consistently followed in the formulation of standard symbols. For example, where there are interleaving and intersecting glide planes parallel to {011}, n has been used rather than a, b or c in space groups with a primitive lattice, but c is used rather than a, b or n in those with a face-centred lattice. The nomenclature of the 1935 *Tables* is retained here.

TABLE 6.2.1

Index of Three-dimensional Space-group Symbols for Various Settings

TRICLINIC SYSTEM

No. of space group	Schoenflies symbol	Symbol for all settings of the same unit cell
1	C_1^1	$P1$
2	C_i^1	$P\bar{1}$

MONOCLINIC SYSTEM

No. of space group	Schoenflies symbol	Symbols for various settings of the same unit cell					
		z-axis unique (1st setting)			*y*-axis unique (2nd setting)		
		Standard short symbol	Full symbols		Standard short symbol	Full symbols	
			a b c **a′ c′ b̄′**	**b a c** **b̄′ c′ a′**		**a c b** **a′ b′ c′**	**b c a** **c′ b′ a′**
3	C_2^1	$P2$	$P112$	$P112$	$P2$	$P121$	$P121$
4	C_2^2	$P2_1$	$P112_1$	$P112_1$	$P2_1$	$P12_11$	$P12_11$
5	C_2^3	$B2$	$B112$ 2_1	$A112$ 2_1	$C2$	$C121$ 2_1	$A121$ 2_1
6	C_s^1	Pm	$P11m$	$P11m$	Pm	$P1m1$	$P1m1$
7	C_s^2	Pb	$P11b$	$P11a$	Pc	$P1c1$	$P1a1$
8	C_s^3	Bm	$B11m$ a	$A11m$ b	Cm	$C1m1$ a	$A1m1$ c
9	C_s^4	Bb	$B11b$ n	$A11a$ n	Cc	$C1c1$ n	$A1a1$ n
10	C_{2h}^1	$P2/m$	$P11\frac{2}{m}$	$P11\frac{2}{m}$	$P2/m$	$P1\frac{2}{m}1$	$P1\frac{2}{m}1$
11	C_{2h}^2	$P2_1/m$	$P11\frac{2_1}{m}$	$P11\frac{2_1}{m}$	$P2_1/m$	$P1\frac{2_1}{m}1$	$P1\frac{2_1}{m}1$
12	C_{2h}^3	$B2/m$	$B11\frac{2}{m}$ $\frac{2_1}{a}$	$A11\frac{2}{m}$ $\frac{2_1}{b}$	$C2/m$	$C1\frac{2}{m}1$ $\frac{2_1}{a}$	$A1\frac{2}{m}1$ $\frac{2_1}{c}$
13	C_{2h}^4	$P2/b$	$P11\frac{2}{b}$	$P11\frac{2}{a}$	$P2/c$	$P1\frac{2}{c}1$	$P1\frac{2}{a}1$
14	C_{2h}^5	$P2_1/b$	$P11\frac{2_1}{b}$	$P11\frac{2_1}{a}$	$P2_1/c$	$P1\frac{2_1}{c}1$	$P1\frac{2_1}{a}1$
15	C_{2h}^6	$B2/b$	$B11\frac{2}{b}$ $\frac{2_1}{n}$	$A11\frac{2}{a}$ $\frac{2_1}{n}$	$C2/c$	$C1\frac{2}{c}1$ $\frac{2_1}{n}$	$A1\frac{2}{a}1$ $\frac{2_1}{n}$

TABLE 6.2.1 (*continued*). ORTHORHOMBIC SYSTEM

No. of space group	Schoenflies symbol	Standard full symbol **a b c**	Symbols for various settings of the same unit cell					
			a b c (standard)	**c a b**	**b c a**	**a $\bar{c}$ b**	**b a $\bar{c}$**	**$\bar{c}$ b a**
16	$D_2^1=V^1$	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$
17	$D_2^2=V^2$	$P222_1$	$P222_1$	$P2_122$	$P22_12$	$P22_12$	$P222_1$	$P2_122$
18	$D_2^3=V^3$	$P2_12_12$	$P2_12_12$	$P22_12_1$	$P2_122_1$	$P2_122_1$	$P2_12_12$	$P22_12_1$
19	$D_2^4=V^4$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
20	$D_2^5=V^5$	$C222_1$ $2_12_12_1$	$C222_1$ $2_12_12_1$	$A2_122$ $2_12_12_1$	$B22_12$ $2_12_12_1$	$B22_12$ $2_12_12_1$	$C222_1$ $2_12_12_1$	$A2_122$ $2_12_12_1$
21	$D_2^6=V^6$	$C222$ 2_12_12	$C222$ 2_12_12	$A222$ 22_12_1	$B222$ 2_122_1	$B222$ 2_122_1	$C222$ 2_12_12	$A222$ 22_12_1
22	$D_2^7=V^7$	$F222$ $2_12_12_1$	$F222$ $2_12_12_1$	$F222$ $2_12_12_1$	$F222$ $2_12_12_1$	$F222$ $2_12_12_1$	$F222$ $2_12_12_1$	$F222$ $2_12_12_1$
23	$D_2^8=V^8$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$
24	$D_2^9=V^9$	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222
25	C_{2v}^1	$Pmm2$	$Pmm2$	$P2mm$	$Pm2m$	$Pm2m$	$Pmm2$	$P2mm$
26	C_{2v}^2	$Pmc2_1$	$Pmc2_1$	$P2_1ma$	$Pb2_1m$	$Pm2_1b$	$Pcm2_1$	$P2_1am$
27	C_{2v}^3	$Pcc2$	$Pcc2$	$P2aa$	$Pb2b$	$Pb2b$	$Pcc2$	$P2aa$
28	C_{2v}^4	$Pma2$	$Pma2$	$P2mb$	$Pc2m$	$Pm2a$	$Pbm2$	$P2cm$
29	C_{2v}^5	$Pca2_1$	$Pca2_1$	$P2_1ab$	$Pc2_1b$	$Pb2_1a$	$Pbc2_1$	$P2_1ca$
30	C_{2v}^6	$Pnc2$	$Pnc2$	$P2na$	$Pb2n$	$Pn2b$	$Pcn2$	$P2an$
31	C_{2v}^7	$Pmn2_1$	$Pmn2_1$	$P2_1mn$	$Pn2_1m$	$Pm2_1n$	$Pnm2_1$	$P2_1nm$
32	C_{2v}^8	$Pba2$	$Pba2$	$P2cb$	$Pc2a$	$Pc2a$	$Pba2$	$P2cb$
33	C_{2v}^9	$Pna2_1$	$Pna2_1$	$P2_1nb$	$Pc2_1n$	$Pn2_1a$	$Pbn2_1$	$P2_1cn$
34	C_{2v}^{10}	$Pnn2$	$Pnn2$	$P2nn$	$Pn2n$	$Pn2n$	$Pnn2$	$P2nn$
35	C_{2v}^{11}	$Cmm2$ $ba2$	$Cmm2$ $ba2$	$A2mm$ $2cb$	$Bm2m$ $c2a$	$Bm2m$ $c2a$	$Cmm2$ $ba2$	$A2mm$ $2cb$

TABLE 6.2.1 (*continued*). ORTHORHOMBIC SYSTEM (*continued*)

No. of space group	Schoenflies symbol	Standard full symbol **a b c**	Symbols for various settings of the same unit cell					
			a b c (standard)	**c a b**	**b c a**	**a c̄ b**	**b a c̄**	**c̄ b a**
36	C_{2v}^{12}	$Cmc2_1$ $bn2_1$	$Cmc2_1$ $bn2_1$	$A2_1ma$ 2_1cn	$Bb2_1m$ $n2_1a$	$Bm2_1b$ $c2_1n$	$Ccm2_1$ $na2_1$	$A2_1am$ 2_1nb
37	C_{2v}^{13}	$Ccc2$ $nn2$	$Ccc2$ $nn2$	$A2aa$ $2nn$	$Bb2b$ $n2n$	$Bb2b$ $n2n$	$Ccc2$ $nn2$	$A2aa$ $2nn$
38	C_{2v}^{14}	$Amm2$ $nc2_1$	$Amm2$ $nc2_1$	$B2mm$ 2_1na	$Cm2m$ $b2_1n$	$Am2m$ $n2_1b$	$Bmm2$ $cn2_1$	$C2mm$ 2_1an
39	C_{2v}^{15}	$Abm2$ $cc2_1$	$Abm2$ $cc2_1$	$B2cm$ 2_1aa	$Cm2a$ $b2_1b$	$Ac2m$ $b2_1b$	$Bma2$ $cc2_1$	$C2mb$ 2_1aa
40	C_{2v}^{16}	$Ama2$ $nn2_1$	$Ama2$ $nn2_1$	$B2mb$ 2_1nn	$Cc2m$ $n2_1n$	$Am2a$ $n2_1n$	$Bbm2$ $nn2_1$	$C2cm$ 2_1nn
41	C_{2v}^{17}	$Aba2$ $cn2_1$	$Aba2$ $cn2_1$	$B2cb$ 2_1an	$Cc2a$ $n2_1b$	$Ac2a$ $b2_1n$	$Bba2$ $nc2_1$	$C2cb$ 2_1na
42	C_{2v}^{18}	$Fmm2$ $bc2_1$ $ca2_1$ $nn2$	$Fmm2$ $bc2_1$ $ca2_1$ $nn2$	$F2mm$ 2_1ca 2_1ab $2nn$	$Fm2m$ $b2_1a$ $c2_1b$ $n2n$	$Fm2m$ $c2_1b$ $b2_1a$ $n2n$	$Fmm2$ $ca2_1$ $bc2_1$ $nn2$	$F2mm$ 2_1ab 2_1ca $2nn$
43	C_{2v}^{19}	$Fdd2$ $dd2_1$	$Fdd2$ $dd2_1$	$F2dd$ 2_1dd	$Fd2d$ $d2_1d$	$Fd2d$ $d2_1d$	$Fdd2$ $dd2_1$	$F2dd$ 2_1dd
44	C_{2v}^{20}	$Imm2$ $nn2_1$	$Imm2$ $nn2_1$	$I2mm$ 2_1nn	$Im2m$ $n2_1n$	$Im2m$ $n2_1n$	$Imm2$ $nn2_1$	$I2mm$ 2_1nn
45	C_{2v}^{21}	$Iba2$ $cc2_1$	$Iba2$ $cc2_1$	$I2cb$ 2_1aa	$Ic2a$ $b2_1b$	$Ic2a$ $b2_1b$	$Iba2$ $cc2_1$	$I2cb$ 2_1aa
46	C_{2v}^{22}	$Ima2$ $nc2_1$	$Ima2$ $nc2_1$	$I2mb$ 2_1na	$Ic2m$ $b2_1n$	$Im2a$ $n2_1b$	$Ibm2$ $cn2_1$	$I2cm$ 2_1an
47	$D_{2h}^1=V_h^1$	$P\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$Pmmm$	$Pmmm$	$Pmmm$	$Pmmm$	$Pmmm$	$Pmmm$
48	$D_{2h}^2=V_h^2$	$P\frac{2}{n}\frac{2}{n}\frac{2}{n}$	$Pnnn$	$Pnnn$	$Pnnn$	$Pnnn$	$Pnnn$	$Pnnn$
49	$D_{2h}^3=V_h^3$	$P\frac{2}{c}\frac{2}{c}\frac{2}{m}$	$Pccm$	$Pmaa$	$Pbmb$	$Pbmb$	$Pccm$	$Pmaa$
50	$D_{2h}^4=V_h^4$	$P\frac{2}{b}\frac{2}{a}\frac{2}{n}$	$Pban$	$Pncb$	$Pcna$	$Pcna$	$Pban$	$Pncb$
51	$D_{2h}^5=V_h^5$	$P\frac{2_1}{m}\frac{2}{m}\frac{2}{a}$	$Pmma$	$Pbmm$	$Pmcm$	$Pmam$	$Pmmb$	$Pcmm$

TABLE 6.2.1 (*continued*). ORTHORHOMBIC SYSTEM (*continued*)

No. of space group	Schoenflies symbol	Standard full symbol **a b c**	Symbols for various settings of the same unit cell					
			a b c (standard)	**c a b**	**b c a**	**a c̄ b**	**b a c̄**	**c̄ b a**
52	$D_{2h}^{6}=V_h^6$	$P\frac{2}{n}\frac{2_1}{n}\frac{2}{a}$	*Pnna*	*Pbnn*	*Pncn*	*Pnan*	*Pnnb*	*Pcnn*
53	$D_{2h}^{7}=V_h^7$	$P\frac{2}{m}\frac{2}{n}\frac{2_1}{a}$	*Pmna*	*Pbmn*	*Pncm*	*Pman*	*Pnmb*	*Pcnm*
54	$D_{2h}^{8}=V_h^8$	$P\frac{2_1}{c}\frac{2}{c}\frac{2}{a}$	*Pcca*	*Pbaa*	*Pbcb*	*Pbab*	*Pccb*	*Pcaa*
55	$D_{2h}^{9}=V_h^9$	$P\frac{2_1}{b}\frac{2_1}{a}\frac{2}{m}$	*Pbam*	*Pmcb*	*Pcma*	*Pcma*	*Pbam*	*Pmcb*
56	$D_{2h}^{10}=V_h^{10}$	$P\frac{2_1}{c}\frac{2_1}{c}\frac{2}{n}$	*Pccn*	*Pnaa*	*Pbnb*	*Pbnb*	*Pccn*	*Pnaa*
57	$D_{2h}^{11}=V_h^{11}$	$P\frac{2}{b}\frac{2_1}{c}\frac{2_1}{m}$	*Pbcm*	*Pmca*	*Pbma*	*Pcmb*	*Pcam*	*Pmab*
58	$D_{2h}^{12}=V_h^{12}$	$P\frac{2_1}{n}\frac{2_1}{n}\frac{2}{m}$	*Pnnm*	*Pmnn*	*Pnmn*	*Pnmn*	*Pnnm*	*Pmnn*
59	$D_{2h}^{13}=V_h^{13}$	$P\frac{2_1}{m}\frac{2_1}{m}\frac{2}{n}$	*Pmmn*	*Pnmm*	*Pmnm*	*Pmnm*	*Pmmn*	*Pnmm*
60	$D_{2h}^{14}=V_h^{14}$	$P\frac{2_1}{b}\frac{2}{c}\frac{2_1}{n}$	*Pbcn*	*Pnca*	*Pbna*	*Pcnb*	*Pcan*	*Pnab*
61	$D_{2h}^{15}=V_h^{15}$	$P\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	*Pbca*	*Pbca*	*Pbca*	*Pcab*	*Pcab*	*Pcab*
62	$D_{2h}^{16}=V_h^{16}$	$P\frac{2_1}{n}\frac{2_1}{m}\frac{2_1}{a}$	*Pnma*	*Pbnm*	*Pmcn*	*Pnam*	*Pmnb*	*Pcmn*
63	$D_{2h}^{17}=V_h^{17}$	$C\frac{2}{m}\frac{2}{c}\frac{2}{m}$	*Cmcm* *bnn*	*Amma* *ncn*	*Bbmm* *nna*	*Bmmb* *cnn*	*Ccmm* *nan*	*Amam* *nnb*
64	$D_{2h}^{18}=V_h^{18}$	$C\frac{2}{m}\frac{2}{c}\frac{2_1}{a}$	*Cmca* *bnb*	*Abma* *ccn*	*Bbcm* *naa*	*Bmab* *ccn*	*Ccmb* *naa*	*Acam* *bnb*
65	$D_{2h}^{19}=V_h^{19}$	$C\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Cmmm* *ban*	*Ammm* *ncb*	*Bmmm* *cna*	*Bmmm* *cna*	*Cmmm* *ban*	*Ammm* *ncb*
66	$D_{2h}^{20}=V_h^{20}$	$C\frac{2}{c}\frac{2}{c}\frac{2}{m}$	*Cccm* *nnn*	*Amaa* *nnn*	*Bbmb* *nnn*	*Bbmb* *nnn*	*Cccm* *nnn*	*Amaa* *nnn*
67	$D_{2h}^{21}=V_h^{21}$	$C\frac{2}{m}\frac{2}{m}\frac{2}{a}$	*Cmma* *bab*	*Abmm* *ccb*	*Bmcm* *caa*	*Bmam* *cca*	*Cmmb* *baa*	*Acmm* *bcb*
68	$D_{2h}^{22}=V_h^{22}$	$C\frac{2}{c}\frac{2}{c}\frac{2}{a}$	*Ccca* *nnb*	*Abaa* *cnn*	*Bbcb* *nan*	*Bbab* *ncn*	*Cccb* *nna*	*Acaa* *bnn*
69	$D_{2h}^{23}=V_h^{23}$	$F\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Fmmm* *bca* *cab* *nnn*	*Fmmm* *bca* *cab* *nnn*	*Fmmm* *bca* *cab* *nnn*	*Fmmm* *cab* *bca* *nnn*	*Fmmm* *cab* *bca* *nnn*	*Fmmm* *cab* *bca* *nnn*

TABLE 6.2.1 (*continued*). ORTHORHOMBIC SYSTEM (*continued*)

No. of space groups	Schoenflies symbols	Standard full symbol **a b c**	Symbols for various settings of the same unit cell					
			a b c (standard)	**c a b**	**b c a**	**a c̄ b**	**b a c̄**	**c̄ b a**
70	$D_{2h}^{24}=V_h^{24}$	$F_{d\,d\,d}^{2\,2\,2}$	*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*
71	$D_{2h}^{25}=V_h^{25}$	$I_{m\,m\,m}^{2\,2\,2}$	*Immm* *nnn*	*Immm* *nnn*	*Immm* *nnn*	*Immm* *nnn*	*Immm* *nnn*	*Immm* *nnn*
72	$D_{2h}^{26}=V_h^{26}$	$I_{b\,a\,m}^{2\,2\,2}$	*Ibam* *ccn*	*Imcb* *naa*	*Icma* *bnb*	*Icma* *bnb*	*Ibam* *ccn*	*Imcb* *naa*
73	$D_{2h}^{27}=V_h^{27}$	$I_{b\,c\,a}^{2\,2\,2}$	*Ibca* *cab*	*Ibca* *cab*	*Ibca* *cab*	*Icab* *bca*	*Icab* *bca*	*Icab* *bca*
74	$D_{2h}^{28}=V_h^{28}$	$I_{m\,m\,a}^{2\,2\,2}$	*Imma* *nnb*	*Ibmm* *cnn*	*Imcm* *nan*	*Imam* *ncn*	*Immb* *nna*	*Icmm* *bnn*

NOTE

Table 6.2.1 can profitably be used for the identification of a space group from any form of the diffraction symbol in the low-symmetry systems (see pp. 52 and 346, and section 4.4). This is best illustrated by an example.

Example

An orthorhombic crystal gives only the following reflections:

hkl: $h+l=2n$ $\qquad$ $h0l$: $h=2n$; $(l=2n)$
$0kl$: $(l=2n)$ $\qquad$ $hk0$: $(h=2n)$; $k=2n$

The diffraction symbol is therefore *mmmB.ab* (point group *mm*2 or *mmm*).

If the point group is *mm*2, the only possible space group is found by inspection of Table 6.2.1 to be No. 41, setting **c a b**, symbol *B*2*ab*, the standard symbol for which is *Aba*2.

If the point group is *mmm*, the only possible space group is No. 64, setting **a c b**, symbol *Bmab*, the standard symbol for which is *Cmca*.

To use the standard setting in either case the axes (indices, co-ordinates, etc.) would have to be transformed as shown in sections 2.5 and 4.9.

TABLE 6.2.1 (*continued*). TETRAGONAL SYSTEM

No. of space group	Schoenflies symbol	Symbols		No. of space group	Schoenflies symbol	Symbols	
		a b c (standard)	**(a±b) (b∓a) c**			**a b c** (standard)	**(a±b) (b∓a) c**
75	C_4^1	$P4$	$C4$	99	C_{4v}^1	$P4mm$	$C4mm$
76	C_4^2	$P4_1$	$C4_1$	100	C_{4v}^2	$P4bm$	$C4mb$
77	C_4^3	$P4_2$	$C4_2$	101	C_{4v}^3	$P4_2cm$	$C4_2mc$
78	C_4^4	$P4_3$	$C4_3$	102	C_{4v}^4	$P4_2nm$	$C4_2mn$
79	C_4^5	$I4$	$F4$	103	C_{4v}^5	$P4cc$	$C4cc$
80	C_4^6	$I4_1$	$F4_1$	104	C_{4v}^6	$P4nc$	$C4cn$
				105	C_{4v}^7	$P4_2mc$	$C4_2cm$
81	S_4^1	$P\bar{4}$	$C\bar{4}$	106	C_{4v}^8	$P4_2bc$	$C4_2cb$
82	S_4^2	$I\bar{4}$	$F\bar{4}$	107	C_{4v}^9	$I4mm$	$F4mm$
				108	C_{4v}^{10}	$I4cm$	$F4mc$
83	C_{4h}^1	$P4/m$	$C4/m$	109	C_{4v}^{11}	$I4_1md$	$F4_1dm$
84	C_{4h}^2	$P4_2/m$	$C4_2/m$	110	C_{4v}^{12}	$I4_1cd$	$F4_1dc$
85	C_{4h}^3	$P4/n$	$C4/a$				
86	C_{4h}^4	$P4_2/n$	$C4_2/a$	111	$D_{2d}^1=V_d^1$	$P\bar{4}2m$	$C\bar{4}m2$
87	C_{4h}^5	$I4/m$	$F4/m$	112	$D_{2d}^2=V_d^2$	$P\bar{4}2c$	$C\bar{4}c2$
88	C_{4h}^6	$I4_1/a$	$F4_1/d$	113	$D_{2d}^3=V_d^3$	$P\bar{4}2_1m$	$C\bar{4}m2_1$
				114	$D_{2d}^4=V_d^4$	$P\bar{4}2_1c$	$C\bar{4}c2_1$
89	D_4^1	$P422$	$C422$	115	$D_{2d}^5=V_d^5$	$P\bar{4}m2$	$C\bar{4}2m$
90	D_4^2	$P42_12$	$C422_1$	116	$D_{2d}^6=V_d^6$	$P\bar{4}c2$	$C\bar{4}2c$
91	D_4^3	$P4_122$	$C4_122$	117	$D_{2d}^7=V_d^7$	$P\bar{4}b2$	$C\bar{4}2b$
92	D_4^4	$P4_12_12$	$C4_122_1$	118	$D_{2d}^8=V_d^8$	$P\bar{4}n2$	$C\bar{4}2n$
93	D_4^5	$P4_222$	$C4_222$	119	$D_{2d}^9=V_d^9$	$I\bar{4}m2$	$F\bar{4}2m$
94	D_4^6	$P4_22_12$	$C4_222_1$	120	$D_{2d}^{10}=V_d^{10}$	$I\bar{4}c2$	$F\bar{4}2c$
95	D_4^7	$P4_322$	$C4_322$	121	$D_{2d}^{11}=V_d^{11}$	$I\bar{4}2m$	$F\bar{4}m2$
96	D_4^8	$P4_32_12$	$C4_322_1$	122	$D_{2d}^{12}=V_d^{12}$	$I\bar{4}2d$	$F\bar{4}d2$
97	D_4^9	$I422$	$F422$				
98	D_4^{10}	$I4_122$	$F4_122$				

TABLE 6.2.1 (*continued*). TETRAGONAL SYSTEM (*continued*)

No. of space group	Schoenflies symbol	Short symbols		Full symbols	
		a b c (standard)	**(a±b) (b∓a) c**	**a b c**	**(a±b) (b∓a) c**
123	D_{4h}^{1}	$P4/mmm$	$C4/mmm$	$P\frac{4}{m}\frac{2}{m}\frac{2}{m}$	$C\frac{4}{m}\frac{2}{m}\frac{2}{m}$
124	D_{4h}^{2}	$P4/mcc$	$C4/mcc$	$P\frac{4}{m}\frac{2}{c}\frac{2}{c}$	$C\frac{4}{m}\frac{2}{c}\frac{2}{c}$
125	D_{4h}^{3}	$P4/nbm$	$C4/amb$	$P\frac{4}{n}\frac{2}{b}\frac{2}{m}$	$C\frac{4}{a}\frac{2}{m}\frac{2}{b}$
126	D_{4h}^{4}	$P4/nnc$	$C4/acn$	$P\frac{4}{n}\frac{2}{n}\frac{2}{c}$	$C\frac{4}{a}\frac{2}{c}\frac{2}{n}$
127	D_{4h}^{5}	$P4/mbm$	$C4/mmb$	$P\frac{4}{m}\frac{2_1}{b}\frac{2}{m}$	$C\frac{4}{m}\frac{2}{m}\frac{2_1}{b}$
128	D_{4h}^{6}	$P4/mnc$	$C4/mcn$	$P\frac{4}{m}\frac{2_1}{n}\frac{2}{c}$	$C\frac{4}{m}\frac{2}{c}\frac{2_1}{n}$
129	D_{4h}^{7}	$P4/nmm$	$C4/amm$	$P\frac{4}{n}\frac{2_1}{m}\frac{2}{m}$	$C\frac{4}{a}\frac{2}{m}\frac{2_1}{m}$
130	D_{4h}^{8}	$P4/ncc$	$C4/acc$	$P\frac{4}{n}\frac{2_1}{c}\frac{2}{c}$	$C\frac{4}{a}\frac{2}{c}\frac{2_1}{c}$
131	D_{4h}^{9}	$P4_2/mmc$	$C4_2/mcm$	$P\frac{4_2}{m}\frac{2}{m}\frac{2}{c}$	$C\frac{4_2}{m}\frac{2}{c}\frac{2}{m}$
132	D_{4h}^{10}	$P4_2/mcm$	$C4_2/mmc$	$P\frac{4_2}{m}\frac{2}{c}\frac{2}{m}$	$C\frac{4_2}{m}\frac{2}{m}\frac{2}{c}$
133	D_{4h}^{11}	$P4_2/nbc$	$C4_2/acb$	$P\frac{4_2}{n}\frac{2}{b}\frac{2}{c}$	$C\frac{4_2}{a}\frac{2}{c}\frac{2}{b}$
134	D_{4h}^{12}	$P4_2/nnm$	$C4_2/amn$	$P\frac{4_2}{n}\frac{2}{n}\frac{2}{m}$	$C\frac{4_2}{a}\frac{2}{m}\frac{2}{n}$
135	D_{4h}^{13}	$P4_2/mbc$	$C4_2/mcb$	$P\frac{4_2}{m}\frac{2_1}{b}\frac{2}{c}$	$C\frac{4_2}{m}\frac{2}{c}\frac{2_1}{b}$
136	D_{4h}^{14}	$P4_2/mnm$	$C4_2/mmn$	$P\frac{4_2}{m}\frac{2_1}{n}\frac{2}{m}$	$C\frac{4_2}{m}\frac{2}{m}\frac{2_1}{n}$
137	D_{4h}^{15}	$P4_2/nmc$	$C4_2/acm$	$P\frac{4_2}{n}\frac{2_1}{m}\frac{2}{c}$	$C\frac{4_2}{a}\frac{2}{c}\frac{2_1}{m}$
138	D_{4h}^{16}	$P4_2/ncm$	$C4_2/amc$	$P\frac{4_2}{n}\frac{2_1}{c}\frac{2}{m}$	$C\frac{4_2}{a}\frac{2}{m}\frac{2_1}{c}$
139	D_{4h}^{17}	$I4/mmm$	$F4/mmm$	$I\frac{4}{m}\frac{2}{m}\frac{2}{m}$	$F\frac{4}{m}\frac{2}{m}\frac{2}{m}$
140	D_{4h}^{18}	$I4/mcm$	$F4/mmc$	$I\frac{4}{m}\frac{2}{c}\frac{2}{m}$	$F\frac{4}{m}\frac{2}{m}\frac{2}{c}$
141	D_{4h}^{19}	$I4_1/amd$	$F4_1/ddm$	$I\frac{4_1}{a}\frac{2}{m}\frac{2}{d}$	$F\frac{4_1}{d}\frac{2}{d}\frac{2}{m}$
142	D_{4h}^{20}	$I4_1/acd$	$F4_1/ddc$	$I\frac{4_1}{a}\frac{2}{c}\frac{2}{d}$	$F\frac{4_1}{d}\frac{2}{d}\frac{2}{c}$

ADDITIONAL NOTE

There is also some ambiguity in using the symbol C4mb for group No. 100 referred to the *C*-lattice because the glide plane parallel to (110) in the *C*-orientation has a translation of $(a+b)/4$, for which there is at present no separate symbol. Correspondingly in No. 102, for which the symbol $C4_2mn$ is used, the glide plane parallel to (110) has a translation of $[(a+b)/4+c/2]$. Corresponding glide planes occur in Nos. 104, 106, 117, 118, 125, 126, 127, 128, 133, 134, 135 and 136 when referred to the *C*-lattice.

TABLE 6.2.1 (*continued*)

TRIGONAL SYSTEM				HEXAGONAL SYSTEM			
No. of space group	Schoenflies symbol	Short symbol	Full symbol	No. of space group	Schoenflies symbol	Short symbol	Full symbol
143	C_3^1	$P3$		168	C_6^1	$P6$	
144	C_3^2	$P3_1$		169	C_6^2	$P6_1$	
145	C_3^3	$P3_2$		170	C_6^3	$P6_5$	
146	C_3^4	$R3$		171	C_6^4	$P6_2$	
				172	C_6^5	$P6_4$	
147	C_{3i}^1	$P\bar{3}$		173	C_6^6	$P6_3$	
148	C_{3i}^2	$R\bar{3}$		174	C_{3h}^1	$P\bar{6}$	
149	D_3^1	$P312$		175	C_{6h}^1	$P6/m$	
150	D_3^2	$P321$		176	C_{6h}^2	$P6_3/m$	
151	D_3^3	$P3_112$		177	D_6^1	$P622$	
152	D_3^4	$P3_121$		178	D_6^2	$P6_122$	
153	D_3^5	$P3_212$		179	D_6^3	$P6_522$	
154	D_3^6	$P3_221$		180	D_6^4	$P6_222$	
155	D_3^7	$R32$		181	D_6^5	$P6_422$	
156	C_{3v}^1	$P3m1$		182	D_6^6	$P6_322$	
157	C_{3v}^2	$P31m$		183	C_{6v}^1	$P6mm$	
158	C_{3v}^3	$P3c1$		184	C_{6v}^2	$P6cc$	
159	C_{3v}^4	$P31c$		185	C_{6v}^3	$P6_3cm$	
160	C_{3v}^5	$R3m$		186	C_{6v}^4	$P6_3mc$	
161	C_{3v}^6	$R3c$		187	D_{3h}^1	$P\bar{6}m2$	
162	D_{3d}^1	$P\bar{3}1m$	$P\bar{3}1\frac{2}{m}$	188	D_{3h}^2	$P\bar{6}c2$	
163	D_{3d}^2	$P\bar{3}1c$	$P\bar{3}1\frac{2}{c}$	189	D_{3h}^3	$P\bar{6}2m$	
164	D_{3d}^3	$P\bar{3}m1$	$P\bar{3}\frac{2}{m}1$	190	D_{3h}^4	$P\bar{6}2c$	
165	D_{3d}^4	$P\bar{3}c1$	$P\bar{3}\frac{2}{c}1$	191	D_{6h}^1	$P6/mmm$	$P\frac{6}{m}\frac{2}{m}\frac{2}{m}$
166	D_{3d}^5	$R\bar{3}m$	$R\bar{3}\frac{2}{m}$	192	D_{6h}^2	$P6/mcc$	$P\frac{6}{m}\frac{2}{c}\frac{2}{c}$
167	D_{3d}^6	$R\bar{3}c$	$R\bar{3}\frac{2}{c}$	193	D_{6h}^3	$P6_3/mcm$	$P\frac{6_3}{m}\frac{2}{c}\frac{2}{m}$
				194	D_{6h}^4	$P6_3/mmc$	$P\frac{6_3}{m}\frac{2}{m}\frac{2}{c}$

TABLE 6.2.1 (*continued*). CUBIC SYSTEM

No. of space group	Schoenflies symbol	Short symbol	Full symbol	No. of space group	Schoenflies symbol	Short symbol	Full symbol
195	T^1	$P23$		213	O^7	$P4_132$	
196	T^2	$F23$		214	O^8	$I4_132$	
197	T^3	$I23$		215	T_d^1	$P\bar{4}3m$	
198	T^4	$P2_13$		216	T_d^2	$F\bar{4}3m$	
199	T^5	$I2_13$		217	T_d^3	$I\bar{4}3m$	
200	T_h^1	$Pm3$	$P\frac{2}{m}\bar{3}$	218	T_d^4	$P\bar{4}3n$	
201	T_h^2	$Pn3$	$P\frac{2}{n}\bar{3}$	219	T_d^5	$F\bar{4}3c$	
202	T_h^3	$Fm3$	$F\frac{2}{m}\bar{3}$	220	T_d^6	$I\bar{4}3d$	
203	T_h^4	$Fd3$	$F\frac{2}{d}\bar{3}$	221	O_h^1	$Pm3m$	$P\frac{4}{m}\bar{3}\frac{2}{m}$
204	T_h^5	$Im3$	$I\frac{2}{m}\bar{3}$	222	O_h^2	$Pn3n$	$P\frac{4}{n}\bar{3}\frac{2}{n}$
205	T_h^6	$Pa3$	$P\frac{2_1}{a}\bar{3}$	223	O_h^3	$Pm3n$	$P\frac{4_2}{m}\bar{3}\frac{2}{n}$
206	T_h^7	$Ia3$	$I\frac{2_1}{a}\bar{3}$	224	O_h^4	$Pn3m$	$P\frac{4_2}{n}\bar{3}\frac{2}{m}$
207	O^1	$P432$		225	O_h^5	$Fm3m$	$F\frac{4}{m}\bar{3}\frac{2}{m}$
208	O^2	$P4_232$		226	O_h^6	$Fm3c$	$F\frac{4}{m}\bar{3}\frac{2}{c}$
209	O^3	$F432$		227	O_h^7	$Fd3m$	$F\frac{4_1}{d}\bar{3}\frac{2}{m}$
210	O^4	$F4_132$		228	O_h^8	$Fd3c$	$F\frac{4_1}{d}\bar{3}\frac{2}{c}$
211	O^5	$I432$		229	O_h^9	$Im3m$	$I\frac{4}{m}\bar{3}\frac{2}{m}$
212	O^6	$P4_332$		230	O_h^{10}	$Ia3d$	$I\frac{4_1}{a}\bar{3}\frac{2}{d}$

7. DICTIONARY OF CRYSTALLOGRAPHIC TERMS FOR VOLUME I IN ENGLISH, FRENCH, GERMAN, RUSSIAN AND SPANISH

List of terms in English which are similar (easily recognisable*) in all the five languages

Amplitude
analogous
anisotropy
antilogous
asymmetry
atom

Bipyramid

Centre of symmetry
centro-symmetry
class
co-ordinate
crystal
crystallography
cubic

Diffraction
dodecahedron

Elements (symmetry)
enantiomorphism

Form
Fourier analysis

Gnomonic projection
goniometer
group
group theory

Hemihedry
hexagonal
holohedry

Identity operation
index, indices
intensity
inversion
isomorphism
isostructural
isotropy

Laue method
Laue symmetry

Matrix
molecule
monoclinic

Nomenclature

Octahedron
optical activity
optical ellipsoid
optical indicatrix
orientation
orthogonal
orthorhombic

Parallel
pedion
piezoelectricity
pinacoid
polar axis
polarity
prism
projection
pseudo-symmetry
pyramid
pyroelectricity

Radius vector
rhombohedron

Scalenohedron
spectrum, spectra
stereogram
stereographic projection
structure
structure factor
symbol
symmetry
system
synthesis

Temperature
tetrahedron
tetragonal
triclinic
trigonal

X-rays (Röntgen rays)

Zone

**In the case of Russian, a knowledge of alphabetical equivalents is assumed*

7. DICTIONARY OF CRYSTALLOGRAPHIC TERMS

ENGLISH	FRENCH	GERMAN	RUSSIAN	SPANISH
Acute bisectrix angle	bissectrice aigüe angle	spitze Bisektrix Winkel	острая бисектриса угол	bisectriz aguda angulo
atomic scattering factor	facteur de structure atomique	(Atom-) Formfaktor (atomarer) Streufaktor	атомный фактор (рассеяния)	factor atómico
axial angle	angle des axes	Achsenwinkel	осевой угол	angulo axil o axial
axial ratio	rapport des axes	Achsenverhältnis	отношение осевых единиц	relación axil o axial (relación paramétrica)
axis (of symmetry)	axe (de symétrie)	(Symmetrie-) Achse	ось (симметрии)	eje (de simetría)
alternating axis (rotation plus reflection)	axe alterne	Drehspiegelachse	зеркальная ось	eje de rotación reflejada
inversion axis (rotation plus inversion)	axe inverse	(Dreh-) Inversionsachse	инверсионная ось	eje de inversión
rotation axis	axe de rotation	Dreh(ungs)achse	простая (поворотная) ось	eje de rotación
screw axis	axe hélicoïdal	Schraubenachse	винтовая ось	eje helicoidal
Basal plane	base	Basisfläche	базис (плоскость базиса)	plano básico o basal
biaxial crystal	cristal biaxe	(optisch) zweiachsiger Kristall	двуосный кристалл	cristal biáxico
Cleavage	clivage	Spaltbarkeit	спайность	exfoliación
close-packed structure	assemblage compact	dichteste (dichte) Packung (Kugelpackung)	плотнейшая упаковка (структура плотнейшей упаковки)	estructura compacta
composition plane	plan d'accolement	Verwachsungsfläche	плоскость срастания (в двойниках)	plano de composición
cube diagonal	diagonale du cube	Würfeldiagonale (Raumdiagonale)	диагональ куба	diagonal del cubo
cube edge	arête du cube	Würfelkante	ребро куба	arista del cubo
cube face	face du cube	Würfelfläche	грань куба	cara del cubo
cube face diagonal	diagonale de la face du cube	Würfelflächendiagonale	диагональ грани куба	diagonal de la cara del cubo
Debye factor	facteur de Debye	Debye-Faktor	температурный (Дебайский) фактор	factor de Debye o de temperatura
density	densité	Dichte	плотность	densidad
Electron density	densité électronique	Elektronendichte	электронная плотность	densidad electrónica
equation	équation	Gleichung	уравнение	ecuación
equivalent positions	positions équivalentes	gleichwertige Lagen	эквивалентные положения	posiciones equivalentes
general equivalent positions	positions équivalentes générales	allgemeine Punktlagen	общие эквивалентные положения	posiciones generales equivalentes
special equivalent positions	positions équivalentes spéciales	spezielle Punktlagen	частные эквивалентные положения	posiciones especiales equivalentes
etch figures	figures de corrosion	Ätzfiguren	фигуры раз'едания	figuras de corrosión
extinctions (absent reflections)	extinctions (réflexions absentes)	Auslöschungen	погасания (отсутствующие рефлексы)	extinciones

7. DICTIONARY OF CRYSTALLOGRAPHIC TERMS

ENGLISH	FRENCH	GERMAN	RUSSIAN	SPANISH
Face (crystal)	face (du cristal)	Fläche (Kristallfläche)	грань (кристалла)	cara
Geometrical structure factor	facteur de structure (géométrique)	(geometrischer) Strukturfaktor	структурный фактор	factor de estructura
group	groupe	Gruppe	группа (симметрии)	grupo
one-dimensional group	groupe unidimensionel	eindimensionale Gruppe	одномерная группа	grupo monodimensional
plane group	groupe plan	Ebenengruppe	плоская группа	grupo plano
point group	groupe ponctuel	Punktgruppe	точечная группа	grupo puntual
space group	groupe spatial	Raumgruppe	пространственная группа	grupo espacial
sub-group	sous-groupe	Untergruppe	(субгруппа) подгруппа	subgrupo
super-group	super-groupe	Obergruppe	сверхгруппа	supergrupo
three-dimensional group	groupe tridimensionnel	dreidimensionale Gruppe	трехмерная группа	grupo tridimensional o espacial
two-dimensional group	groupe bidimensionnel	zweidimensionale Gruppe	двухмерная группа	grupo didimensional o plano
translation group	groupe de translations	Translationsgruppe	группа переносов (трансляционная группа)	grupo de translación
Habit	faciès	Habitus	габитус	hábito
Interaxial angles	angles des axes	Achsenwinkel (kristallographische)	углы между осями	ángulos de los ejes
interfacial angles	angles des faces	Flächenwinkel	углы между гранями	ángulos de las caras
interplanar spacing	espacement des plans réticulaires (distance interréticulaire)	Netzebenenabstand	межплоскостное расстояние	espaciado
Lattice	réseau	Gitter	решетка	red
lattice complex	complexe réticulaire	Gitterkomplex	совокупность гомологических точек в решетке	complejo reticular
lattice constant	constante réticulaire	Gitterkonstante	параметр решетки	constante reticular
body-centred space lattice	réseau spatial centré	raum- (innen-) zentriertes Gitter	об'емно-центрированная решетка	red espacial centrada
Bravais lattice	réseau de Bravais	Bravais-Gitter	решетка Бравэ	red de Bravais
direct lattice	réseau direct	direktes Gitter	прямая решетка	red directa
face centred space lattice	réseau à faces centrées	flächenzentriertes Raumgitter (flz. Gitter)	решетка с центрированными гранями (гранецентрированная решетка)	red de caras centradas
reciprocal lattice	réseau réciproque	reziprokes Gitter	обратная решетка	red recíproca
Laue photograph	cliché de Laue	Laue-Aufnahme(Lauebild)	Лауэграмма	Lauegrama (diagrama de Laue)
line	ligne	Linie	линия	línea
glide line	ligne de symétrie translatoire	Gleitlinie	линия скольжения	línea de deslizamiento
reflection line	ligne de réflexion	Reflexionslinie	линия отражения	línea de reflexión

ENGLISH	FRENCH	GERMAN	RUSSIAN	SPANISH
Modulus	module	Modul	модуль	módulo
compression modulus	de compression	Kompressionsmodul	модуль сжатия	de compresión
elastic modulus	d'élasticité	Elastizitätsmodul	модуль упругости	elástico
hydrostatic modulus	hydrostatique	Hydrostatischesmodul	гидростатический модуль	hidrostático
torsion modulus	de torsion	Torsionsmodul	модуль скручивания	de torsión
multiplicity	multiplicité	Vielfachheit (Vielfältigkeit)	мультиплетность (повторяемость)	multiplicidad
Net	réseau plan	Netz (Netzebene)	плоская сетка	retícula
Optical rotatory power	pouvoir rotatoire	optisches Drehvermögen	вращательная способность	poder rotatorio
Parametral plane	plan paramétrique	Einheitsfläche	параметрическая плоскость	plano paramétrico
perpendicular	perpendiculaire	senkrecht	перпендикуляр	perpendicular
phase angle	angle de phase	Phasenwinkel	фаза (фазовый угол)	fase
plane	plan	Ebene	плоскость	plano
glide plane	plan de symétrie avec glissement	Gleitspiegelebene (Gleitebene)	плоскость скольжения (плоскость скользящего отражения)	plano de deslizamiento
mirror plane (reflection plane)	miroir (plan de symétrie; plan de réflexion)	Spiegelebene (Reflexionsebene)	зеркальная плоскость (отражающая плоскость)	plano de simetría (plano de reflexión)
point	point	Punkt	точка	punto
reflection point	point de réflexion	Reflexionspunkt	точка отражения	punto de reflexión
point symmetry	symétrie ponctuelle	Punktsymmetrie	точечная симметрия (симметрия конечных фигур)	simetría puntual
primitive triplet	triplet primitif	primitives Tripel	примитивная тройка (сопряженных трансляций)	triplete primitivo (parámetros fundamentales)
principal directions	directions principales	Hauptachsen (der Indikatrix)	основные направления	direcciones principales
projection	projection	Projektion	проекция	proyección
clinographic projection	projection oblique	schiefwinklige Projektion	аксонометрическая проекция	proyección clinográfica
gnomonic projection	projection gnomonique	gnomonische Projektion	гномоническая проекция	proyección gnomónica
orthogonal projection	projection orthogonale	rechtwinklige Projektion	ортогональная проекция	proyección ortogonal
stereographic projection	projection stéréographique	stereographische Projektion	стереографическая проекция	proyección estereográfica
Reflecting power	pouvoir réflecteur	Reflexionsvermögen	отражающая способность	poder reflector
reflection	réflexion	Reflexion	отражение	reflexión
reflection line	ligne de réflexion	Reflexionsstab	линия отражения	línea de reflexión
reflection plane	plan de réflexion	Reflexionsebene	отражающая плоскость	plano de reflexión
reflection point	point de réflexion	Reflexionspunkt	точка отражения	punto de reflexión
rhombohedron	rhomboèdre	Rhomboeder	ромбоэдр	romboedro
obverse rhombohedron } reverse rhombohedron }	see page 20. (Equivalent terms in various languages confused.)			
rotation	rotation	Drehung	вращение	rotación
rotation axis	axe de rotation	Drehachse	ось вращения	eje de rotación
rotation point	point de rotation	Drehpunkt	точка вращения	punto de rotación

7. DICTIONARY OF CRYSTALLOGRAPHIC TERMS

ENGLISH	FRENCH	GERMAN	RUSSIAN	SPANISH
Scattered wave	onde diffusée	gestreute Welle (Streuwelle)	рассеянная волна	onda difundida
scattering power	pouvoir diffusant	Streuvermögen	рассеивающая способность	poder de difusión
single crystal	cristal unique (monocristal)	Einkristall	одиночный кристалл (монокристалл)	cristal único
space	espace	Raum	пространство	espacio
spacing (interplanar)	espacement (interréticulaire)	Netzebenenabstand	межплоскостное расстояние	espaciado (reticular)
sphere of reflection	sphère de réflexion	Ewald'sche Ausbreitungskugel (Reflexionskugel)	сфера отражения	esfera de reflexión
structure-sensitive (texture-sensitive)	conditionné par la structure	strukturempfindlich (texturempfindlich)	структурночувствительный (текстурночувствительный)	sensible a la estructura
susceptibility	susceptibilité	Suszeptibilität	восприимчивость	susceptibilidad
diamagnetic	diamagnétique	diamagnetisch	диамагнитная	diamagnética
paramagnetic	paramagnétique	paramagnetisch	парамагнитная	paramagnética
symmetry	symétrie	Symmetrie	симметрия	simetría
symmetry axis	axe de symétrie	Symmetrieachse	ось симметрии	eje de simetría
symmetry line	ligne de symétrie	Symmetriestab	линия симметрии	línea de simetría
symmetry operation	opération de symétrie	Symmetrieoperation	операция симметрии	operación de simetría
symmetry plane	plan de symétrie	Symmetrieebene	плоскость симметрии	plano de simetría
Thermal vibration	vibration thermique	Schwingung (thermische Vibration)	температурное колебание	vibración térmica
transformation	transformation	Transformation	преобразование	transformación
transformation matrix	matrice de transformation	Transformations-Matrix	матрица преобразования	matriz de transformación
translation	translation	Translation	перенос (трансляция)	translación
twin	macle	Zwilling	двойник	macla
twinning	maclage	Zwillingsbildung	двойникование	maclado (formación de macla)
Uniaxial crystal	cristal uniaxe	(optisch) einachsiger Kristall	одноосный кристалл	cristal uniáxico
unit cell	maille élémentaire	Zelle (Einheitszelle; Elementarparallelepiped)	единичная (элементарная) ячейка	celda (celdilla unidad; paralelepípedo elemental)
Volume	volume	Volumen	об'ем	volumen
X-ray methods	méthodes de rayons X	Röntgenstrahlen-Methode	Рентгеновские методы	métodos de rayos X
Laue method	méthode de Laue	Laue-Methode	метод Лауэ	método de Laue
moving-film method	méthode à film mobile	bewegend-Film-Methode	метод „разворачивания" слоевой линии	método de la película movil
oscillation method	méthode du cristal oscillant	Schwenkmethode	метод качания (колебания)	método del cristal oscilante
powder method	méthode des poudres	Pulvermethode (Debye-Scherrer-Methode)	метод порошка (метод Дебай-Шеррера)	método del polvo cristalino
rotation method	méthode du cristal tournant	Drehkristall-Methode	метод вращения	método del cristal giratorio
Zone axis	axe de zone	Zonenachse (Zonenrichtung)	Ось зоны	eje de zona

Y

INTERNATIONAL TABLES FOR X-RAY CRYSTALLOGRAPHY

VOLUME

I

INTERNATIONAL TABLES FOR X-RAY CRYSTALLOGRAPHY

VOLUME I