QUANTUM MECHANICAL CALCULATION OF ELECTRONIC STRUCTURE OF MOLECULE $C_{60}H$

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In the work by method of Wolfsberg - Helmholz (VH) has carried out the quantum mechanical calculation of electronic structure of nano-dimensional $C_{60}H$ - molecule in basis of Slater functions. Are determined, that in molecule $C_{60}H$ effective charges of atoms of carbon identical. Values of electronic energy, potential of ionization, effective charges of atoms of carbon and hydrogen of a molecule $C_{60}H$ are found.

In work the quantum mechanical calculation of electronic structure nano-electronic structure nano-dimensional molecule $C_{60}H$ by method Wolfsberg - Helmholz (WH) it is carried out. The molecule $C_{60}H$ presents the closed sphere, consisted of twenty correct hexagons and twelve correct pentagons in the tops of which there are atoms of carbon [1, 2]. The atom of hydrogen is in the center of sphere (Fig. 1).

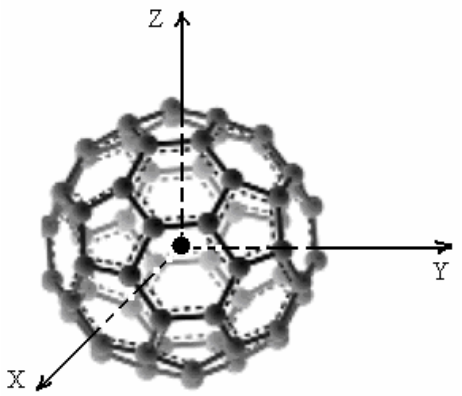

Figure 1. A molecule $C_{60}H$.

It is known, that method WH is one of simple semi-empirical variants of a molecular orbital (MO) method. It is considered that everyone electron in a molecule in MO method moves in the definite effective field, created by nucleus and other electrons independently of others. The states of electrons in a molecule are described by the one-electronic wave function named by molecular orbital. It is multicentered function, i.e. distances of electron from various nuclear of atoms are included in it. There are different variants of molecular orbital search. One of them is the search of molecular orbitals U_i in the form of linear combinations of atomic orbitals, included in a molecule (method MO LCAO):

$$U_i = \sum_{q=1}^{m} C_{qi}\chi_q \qquad (1)$$

where C_{qi} are unknown coefficients, χ_q are atomic orbitals, chosen as basic functions. In the work the essential Slater atomic orbitals are used in the capacity of basic functions (SAO) [3]:

$$\chi_q \equiv \chi_{nlm}(\xi,\vec{r}) = \frac{(2\xi)^{n+\frac{1}{2}}}{\sqrt{(2n)!}} r^{n-1} e^{-\xi r} S_{lm}(\theta,\varphi). \qquad (2)$$

where $S_{lm}(\theta,\varphi)$ are essential spherical functions. The following formulas are used for calculation of exponential parameter ξ [4]:

$$\xi_i = \frac{Z-\gamma_i}{n} \qquad (3)$$

$$\gamma_i = \sum_{j\neq i}^{N} \left\{1+\left(\frac{3n_j^2-\ell_j(\ell_j+1)}{3n_i^2-\ell_i(\ell_i+1)}\right)^2\right\}^{-3/2} \qquad (4)$$

where Z is serial number of atom, N is number of electrons in atom, n_i and ℓ_i are principal and orbital quantum numbers of considered electron, n_j and ℓ_j are the principal and orbital quantum numbers of the other electrons.

In quantum mechanical calculations of electronic structure of molecules we are usually limited by consideration of atom valent electrons and molecular orbitals are presented in the form of linear combinations SAO of these valent electrons. In the work $2s$ –, $2p_x$ –, $2p_y$ –, $2p_z$ – SAO of carbon atoms and $1s$ – of hydrogen atom are used for construction molecular orbitals of molecule $C_{60}H$. Thus, $m=4\times60+1=241$ of essential SAO are used in the capacity of basic functions. Using formulas (2), (3) and (4) the analytical expressions of basic SAO are defined:

$$\chi_1 = 2s(C_1) = \frac{1{,}015141}{\sqrt{\pi}} \cdot re^{-1{,}456771r}\cos\theta \qquad (5)$$

$$\chi_2 = 2p_x(C_1) = \frac{1{,}090819}{\sqrt{\pi}} \cdot re^{-1{,}682113r}\sin\theta\cos\varphi \qquad (6)$$

$$\chi_3 = 2p_y(C_1) = \frac{1{,}090819}{\sqrt{\pi}} \cdot re^{-1{,}682113r}\sin\theta\sin\varphi \qquad (7)$$

$$\chi_4 = 2p_z(C_1) = \frac{1{,}090819}{\sqrt{\pi}} \cdot re^{-1{,}682113r}\cos\theta \qquad (8)$$

$$\chi_5 = 1s(H) = \frac{1}{\sqrt{\pi}} \cdot e^{-r} \qquad (9)$$

In formulas (5) - (9) r, θ, φ - spherical coordinates of electron.

Coefficients C_{qi} in the formula (1) are found by the solution of the following system of equations:

$$\sum_q (H_{pq} - \varepsilon_i S_{pq}) C_{qi} = 0 \qquad (10)$$

Here the following designations are used:

$$H_{pq} = \int \chi_p^* \hat{H}_{ef} \chi_q dV \qquad (11)$$

$$S_{pq} = \int \chi_p^* \chi_q dV \qquad (12)$$

S_{pq} are overlap integrals between atomic orbitals χ_p and χ_q. $\hat{H}_{ef}$ is the effective Hamilton operator for one electron, moving in the definite effective field independently on other electrons:

$$\hat{H}_{ef} = -\frac{1}{2}\nabla^2 + U(r) \qquad (13)$$

Obvious expression of the effective Hamilton operator is unknown, that's why values of matrix elements H_{pq} can 't be calculated and they are estimated by different methods. The values of potentials of atom ionization are used in WG method for H_{pq} estimation. Diagonal elements H_{qq} of this matrix are taken by equal potentials of ionization of corresponding valency atom states. Nondiagonal elements are calculated, using the following expression [5]:

$$H_{pq} = 0.5 \cdot K \cdot S_{pq}(H_{pp} + H_{qq}) \qquad (14)$$

The value of coefficient K is found by the comparison with experimental data or theoretically from the condition of minimum of molecule electronic energy.

As it is seen from formulas (10) and (14) for quantum mechanical calculation of molecules by method WH, it is necessary to know the values of overlap integrals. The formulas, known from the corresponding scientific literature [6, 7] are used for calculation of overlap integrals. It is necessary to introduce the quantum numbers n, ℓ, m of corresponding atomic orbitals, the values of exponential parameter ξ and Cartesian coordinates of atoms in molecular system of coordinates for carrying out of computer calculations of overlap integrals on these formulas. For calculation of matrix elements H_{pq} the following values of ionization potentials of valency states *2s* –, *2p* – atoms of carbon and *1s* – atom of hydrogen are used [8].

$$(2s|C|2s) = -0{,}772096 \text{ a.u.},$$

$$(2p|C|2p) = -0{,}419161 \text{ a.u},$$

$$(1s|H|1s) = -0{,}4997861 \text{ a.u.}$$

Knowing values of matrix elements H_{pq} and S_{pq}, it is possible to solve equation system (10) and to calculate orbital energies ε_i, electronic energy $E = \sum_i \varepsilon_i$, values of ionization potential I of molecule $C_{60}H$ and values of coefficients C_{qi} in approximation WH. Using values of coefficients C_{qi}, it is possible to calculate the effective atom charges in a molecule $C_{60}H$ with the help of the following formula [9]:

$$q_A = n_A^o - \sum_i n_i \sum_{q \in A} |C_{qi}|^2 . \qquad (15)$$

Here n_A^o is positive charge of A atom after giving the valency electrons for band formation (for carbon atoms: $n_A^o = 4$, for hydrogen atom $n_A^o = 1$), n_i is number of electrons on i-th molecular orbital. Summation on i is carried out on molecular orbital, captured by electrons.

The values of electronic energy, value of potential of ionization, value of effective charges of carbon and hydrogen atoms of molecule $C_{60}H$ are found with the help of computer calculations**.** It is defined, that values of effective charges of carbon atoms are approximately identical:

$$E = -137{,}851353 \text{ a.u.},$$

$$I = 11{,}339642 \text{ eV},$$

$$q_A(C) = 0{,}8383 \text{ a.u. } (A = 1 \div 60)$$

$$q_{61}(H) = 0{,}4104 \text{ a.u.}$$

Quantum mechanical calculation of electronic structure of molecule $C_{60}H$ is carried out by the program, developed by employees of Department of Chemical Physics of Nanomaterials of Baku States University in Delphi Studio, working in operational system MS Windows XP.

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$C_{60}H$ - MOLEKULUNUN ELEKTRON QURULUŞUNUN KVANT MEXANİKİ HESABLANMASI

İşdə nanoölçülü $C_{60}H$ - molekulunun elektron quruluşu Volfsberq - Helmhols (VH) metodu ilə Sleyter funksiyaları bazisində kvant mexaniki hesablanmışdır. Müəyyən edilmişdir ki, $C_{60}H$ molekulunda karbon atomlarının effektiv yükləri təqribən eynidir. $C_{60}H$ molekulunun elektron enerjisi, ionlaşma potensialının qiyməti, karbon və hidrogen atomlarının effektiv yüklərinin qiymətləri tapılmışdır.

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КВАНТОВОМЕХАНИЧЕСКИЙ РАСЧЕТ ЭЛЕКТРОННОЙ СТРУКТУРЫ МОЛЕКУЛЫ $C_{60}H$

В работе с помощью метода Вольфсберга – Гельмгольца проведен квантовомеханический расчет электронной структуры наноразмерной молекулы $C_{60}H$ в базисе Слейтеровских функций. Определено, что в молекуле $C_{60}H$ эффективные заряды атомов углерода одинаковы. Найдены значения электронной энергии, потенциал ионизации, эффективные заряды атомов углерода и водорода молекулы $C_{60}H$.

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