MILLIMETER VIBRATIONAL – ROTATIONAL TRANSITIONS OF GOSH-CONFORMER OF ISOPROPYL ALCOHOL MOLECULE AT J<50

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The search of millimeter rotational and vibrational-rotational transitions of gosh-conformer of isopropyl alcohol molecule up to J≤50 (rotational principal quantum number) is carried out using the spectra of gosh-conformer of isopropyl alcohol molecule earlier identified by authors and their inclusions in inverse spectroscopic task. 51 millimeter rotational and vibrational-rotational transitions in main vibrational state up to J≤50 are identified. The reduced Hamiltonian used in total format, well enough describes the rotational and vibrational-rotational transitions of gosh-conformer of isopropyl alcohol molecule complicated by internal rotation. This work is supported by the Science Development Foundation under the President of the Republic of Azerbaijan. Grant № EİF-BGM-2-BRFTF-1-2012/2013-07/04/1.

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INTRODUCTION

The investigations of rotational spectrum of isopropyl alcohol (trans – conformer) in centimeter range has been began by Imanov, Abdurakhmanov, Yolchiyev [1] and later by Hirota [2]. The works by investigation of rotational and vibrational-rotational transitions of gosh-conformer of isopropyl alcohol molecule have been began by Hirota [3]. The gosh-conformers of isopropyl alcohol molecule in our works [4,7,8,10] are investigated with use of reduced Hamiltonian. In these works the rotational, quartic and sixthtic constants are improved with accuracy and the internal rotation parameters are defined. The millimeter spectrum of isopropyl alcohol is recorded on hybrid spectrometer and the catalog more than 7000 spectral lines is written. The accuracy of measurement of spectral line frequencies is in the limit 0,05-0,15 MHz and depends on intensity and inter-disposition of spectral lines. The spectroscopically pure sample of isopropyl alcohol by OP-2 OCCh 11-5 type (99,4% of the main product) is used without further purification. Quade - Lin Hamiltonian is reduced for more detailed study of rotational and vibrational-rotational spectrum and more correct definition of parameters of gosh-conformer internal rotation of isopropyl alcohol molecule in [10]. 340 transitions are identified using this Hamiltonian. However, in this work all parameters of internal rotation and sixthtic constants of centrifugal perturbation we can’t define because of the lack of experiment material.

CALCULATION

The task of the continuation of identification with high J of rotational and vibrational-rotational spectra of gosh-conformer of isopropyl alcohol molecule is investigated in the present work. Hamiltonian in matrix form used in the present work, has the following form:

$$H = \begin{vmatrix} \langle s|H|s\rangle \langle s|H|a\rangle \\ \\ \langle a|H|s\rangle \langle a|H|a\rangle \end{vmatrix} \tag{1}$$

where

$$\langle s|H|s\rangle = A_s J_x^2 + B_s J_y^2 + C_s J_s^2 - \Delta_j^s J^4 - \Delta_{jk}^s J^2 J_z^2 - \Delta_k^s J_z^4 - 0.5(\delta_j^s J^2 + \delta_k^s J_z^2, J_+^2 + J_-^2) +$$

$$+ H_j^s J^6 + H_{jk}^s J^4 J_z^2 + H_{kj}^s J^2 J_z^4 + H_k^s J_z^6 + 0.5(h_J^s J^4 + h_{jk}^s J^2 J_z^2 + h_k^s J_z^4, J_+^2 + J_-^2)$$

$$\langle a|H|a\rangle = \Delta + A_a J_x^2 + B_a J_y^2 + C_a J_z^2 - \Delta_j^a J^4 - \Delta_{jk}^a J^2 J_z^2 - \Delta_k^a J_z^4 - 0.5(\delta_j^a J^2 + \delta_k^a J_z^2, J_+^2 + J_-^2) +$$

$$+ H_j^a J^6 + H_{jk}^a J^4 J_z^2 + H_{kj}^a J^2 J_z^4 + H_k^a J_z^6 + 0.5(h_j^a J^4 + h_{jk}^a J^2 J_z^2 + h_k^a J_z^4, J_+^2 + J_-^2)$$

$$\langle s|H|a\rangle = 0.5 R_{yx}^{sa} \{J_y, J_x\}_+ + 0.5 R_{zx}^{sa} \{J_z, J_x\}_+ + i P_{yJ}^{sa} J^2 J_y + i P_{zJ}^{sa} J^2 J_z + i0.5 P_{yx}^{sa} \left\{J_y, J_x^2\right\}_+$$

$$+ i0.5 P_{zx}^{sa} \left\{J_z, J_x^2\right\}_+$$

$\langle a|H|s\rangle = \langle s|H^*|a\rangle$, $R_{\alpha x}^{as} = -R_{\alpha x}^{sa}, P_{\alpha j}^{as} = -P_{\alpha j}^{sa}, P_{\alpha x}^{as} = -P_{\alpha x}^{sa}$, where: $\alpha = z, y$

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$A_s, B_s, C_s, A_a, B_a, C_a$ are rotational constants correspondingly for symmetrical and antisymmetrical state, $\Delta^s_j, \Delta^s_{jk}, \Delta^s_k, \delta^s_j, \delta^s_k, \Delta^a_j, \Delta^a_{jk}, \Delta^a_k, \delta^a_j, \delta^a_k$ are quartic members of centrifugal perturbation correspondingly for symmetrical and antisymmetrical state $H^s_j, H^s_{jk}, H^s_{kj}, H^s_k, h^s_j, h^s_{jk}, h^s_k, H^a_j, H^a_{jk}, H^a_{kj}, H^a_k, h^a_j, h^a_{jk}, h^a_k$ are sixthtic members of centrifugal perturbation correspondingly for symmetrical and antisymmetrical state, Δ, $R^{sa}_{yx}, R^{sa}_{zx}, P^{sa}_{yj}, P^{sa}_{zj}, P^{sa}_{yx}, P^{sa}_{zx}$ are parameters obtained in the result of interaction of two states (symmetrical and antisymmetrical ones), i.e. by other words the internal rotation parameters.

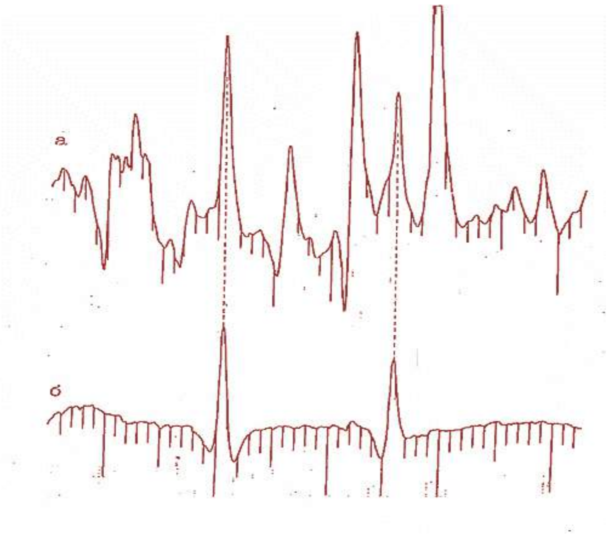

Fig. 1. The record of isopropyl alcohol molecule with Stark modulation (a) and modulation by RF -MW double resonances (b) at pumping $a12_{-1}$–$a12_{-2}$ 7.586 MHz, probing transitions $a12_0$–$a12_{-2}$ 43580.759 MHz and $a12_1$–$a12_{-1}$ 43614.287 MHz.

Table 1

The millimeter rotational transitions of isopropanol molecule (gosh-form)

Transitions	Experimental frequencies (MHz)	$N_{ex.} - \nu_{th}$ (MHz)	Transitions	Experimental frequencies (MHz)	$N_{ex.} - \nu_{th}$ (MHz)
J τ - J τ			J τ - J τ		
1	2	3	1	2	3
a 13 7 - a 13 4	42582.600	0.3270	s 37 9 - a 37 8	70319.610	70319.610
a 13 4 - a 13 2	39246.290	0.0093	a 38 38 - s 38 37	48093.760	48093.760
a 14 11 - a 14 9	33927.910	-0.3944	s 38 14 - a 38 13	56222.980	56222.980
a 14 14 - s 14 13	49068.870	0.3848	s 38 8 - a 38 7	77843.080	77843.080
s 15 5 - s 15 2	76019.900	-0.3373	s 37 33 - s 38 33	61782.500	61782.500
a 15 6 - a 15 4	39365.218	-0.2971	a 39 39 - s 39 38	48523.790	-0.1832
a 16 7 - a 16 5	40175.580	0.0080	a 39 32 - s 39 33	39889.330	-0.3088
a 16 6 - a 16 4	33306.820	0.2464	s 39 15 - a 39 14	56347.150	-0.2687
a 17 12 - a 17 10	38787.410	-0.3613	s 39 11 - a 39 10	71443.890	-0.0096
a 18 18 - a 18 15	42695.040	0.2290	s 39 18 - s 39 17	50303.060	-0.0686
s 18 8 - s 18 6	34136.650	-0.2608	a 40 40 - s 40 39	49000.480	0.2199
s 23 10 - s 23 8	51080.970	0.1346	a 40 33 - s 40 34	40097.640	0.1361
s 25 11 - a 25 10	47216.680	-0.3317	a 41 38 - s 41 39	69013.090	-0.0528
s 26 13 - s 26 11	47840.700	0.0572	s 41 13 - a 41 12	72387.160	0.0994
s 27 1 - a 27 0	57154.070	0.1360	a 42 35 - s 42 36	40612.280	-0.2570
a 27 12 - a 27 10	53221.120	-0.2651	a 42 19 - a 42 18	69923.840	-0.2982
s 27 2 - a 27 -1	57154.070	0.1328	a 43 43 - s 43 42	50752.130	-0.2008
s 28 26 - s 28 24	45142.950	0.0405	s 43 17 - a 43 16	64953.530	0.3053
s 30 13 - s 30 11	62196.240	0.3642	s 43 15 - a 43 14	73060.020	0.1277
s 32 27 - s 32 25	64516.870	0.3885	s 44 20 - a 44 19	76780.910	0.1036
a 33 29 - a 33 26	41672.700	0.0403	s 44 32 - a 43 33	76834.760	0.0138
a 33 17 - a 33 14	64180.390	0.2463	a 45 38 - s 45 39	41686.610	0.0907
a 35 17 - s 35 16	53131.420	-0.3419	a 47 47 - s 47 46	54045.310	-0.0571
s 36 34 - a 36 33	46967.540	0.2280	a 48 41 - s 48 42	43212.040	0.1084
a 37 30 - s 37 31	39556.270	-0.2362	a 48 33 - s 47 34	69768.440	-0.0657
s 37 11 - a 37 10	63299.790	-0.0874			

Here $\tau = K_{-1} - K_1$ where K_{-1}, K_1 are projections of total angular moments on molecular axis for states of symmetric tops (extended and thinned symmetric tops).

CONCLUSION

51 millimeter rotational and vibrational-rotational transitions of gosh-conformer of isopropyl alcohol molecule up to J≤50 are identified.

All earlier identified rotational and vibrational-rotational transitions of gosh-conformer of isopropyl alcohol molecule up to J≤50 in frequency range 25 – 78 GHz and 240-496GHz are included in the solution of inverse problem.

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