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High resolution spectroscopy of strongly interacting bands ν_4, ν_6, ν_7, ν_8, and ν_{10} of deuterated ethylene, C_2H_3D

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Rotational structure of strongly interacting bands ν_4, ν_6, ν_7, ν_8, and ν_{10} of the C_2H_3D molecule is spectroscopically studied. Spectra were recorded by Fourier spectrometer Brucker 125HR in the laboratory of physical and theoretical chemistry of Technical University of Braunschweig. 27950 transitions with maximum values of $J^{\max} = 40$ and $K_a^{\max} = 20$ were assigned to the studied bands. The effective Hamiltonian parameters were determined in the model including the ν_3 resonating state. The 4028 upper energy levels were used as incoming data. They are reproduced with root mean square deviation of $d_{\mathrm{rms}} = 1.7\cdot\ 10^{-4}\,\mathrm{cm}^{-1}$. Corresponding value for more than 24000 line positions is $d_{\mathrm{rms}} = 2.1\cdot\ 10^{-4}\,\mathrm{cm}^{-1}$.

Keywords: ethylene, high resolution spectroscopy, strongly interacting bands, Fourier-spectroscopy.

1. Introduction

Many organic molecules are the subject of interest in various fields of science, from biology to astrophysics. One such molecule is the ethylene molecule, which plays an important role both in plant life, acting as a hormone, and in animal metabolism. Ethylene is of great interest to the chemistry problems of the Earth's atmosphere [1], because it is one of the greenhouse gases. The presence of ethylene has been noted in the atmospheres of other planets in the solar system [2–5], as well as in objects outside the solar system [6]. In organic chemistry, ethylene can be seen as a prototype for understanding more complex organic molecules: to describe the corresponding absorption spectra and potential surface function (PSF). The latter determines the internal dynamics of the molecule, describing the interaction of atomic nuclei in different configurations. Having full information about the PSF parameters, it is possible to find the exact values of the eigenvalues of the Hamiltonian of the molecule due to the potential energy V contribution to the total energy of the molecule ($\hat{H} = \hat{T} + \hat{V}$). However, the determination of PSF parameters is possible only when using, along with highly accurate information about the parent molecule, relevant information about its various isotopologues, such as $cis-C_2H_2D_2$, $trans-C_2H_2D_2$, C_2HD_3, C_2H_3D.

As a consequence of the above, spectroscopic studies of various isotopic modifications of ethylene have been conducted for many years in various laboratories around the world. Not being able to give here a complete list of such works, we cite only some of the works carried out in recent years at the Tomsk Polytechnic University [7–17]. This paper is devoted to the study of the spectrum of deuterated ethylene C_2H_3D in the range $600-1300\,\mathrm{cm}^{-1}$, where strongly resonant bands ν_4, ν_6, ν_7, ν_8 and ν_{10} are localized.

2. General information about the molecule C_2H_3D

The symmetry of the molecule C_2H_3D (asymmetric top) is isomorphic to the dot group C_s, and the asymmetry parameter $\kappa \simeq -0.894$ (calculated as $(2B - A - C)/\,(A - C)$, where A, B and C — rotational parameters defined through the principal moments of inertia of the molecule in the Cartesian coordinate system with the origin in the center of mass). A schematic representation of the molecule is shown in Fig. 1. It should be noted that the axes of the coordinate system coincide with the principal axes of inertia. For the asymmetrically substituted isotopologue under consideration, the z-axis is neither the symmetry axis nor the major axis. For more information on the symmetry of the molecule, see Table 1. Columns 2, 3 show the characters of irreducible representations of the symmetry group C_s. Columns 4 and 5 contain information about the symmetry of the dimensionless vibrational coordinates q_λ, the components of the angular momentum operators J_α, and the components of the matrix of directional cosines $k_{Z\alpha}$. The last column contains the angular momentum components and the guiding cosines corresponding to the I^r representation of the asymmetric top molecule [18–22], used in this paper.

One useful conclusion about the asymmetric wavelength that can be drawn from Table 1 points to the following

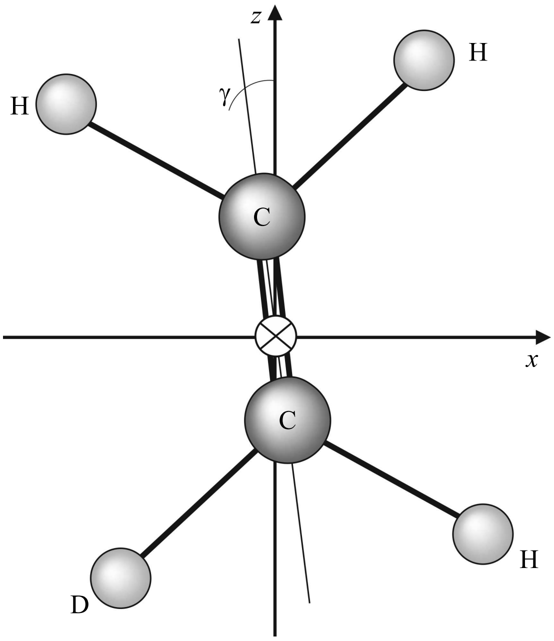

Figure 1. Schematic representation of the C_2H_3D molecule in the I^r-representation.

allowed types of transitions in the absorption bands of the molecule under study:

1. Hybrid bands in which transitions of a- and b-types are possible. Bands formed by transitions to excited symmetry states A''. Selection rules for such bands: $\Delta J = 0, \pm 1$; ΔK_a — any; ΔK_c — odd.
2. The c-type bands are formed by transitions from the ground state to the excited symmetry A' with selection rules: $\Delta J = 0, \pm 1$; ΔK_a — odd; ΔK_c — even.

The strong resonances between the upper states of the hybrid A'' bands and the A' bands, which will result in so-called d-type transitions in the latter, are also of interest when studying the absorption spectrum of the C_2H_3D molecule. The selection rules for this type of transition are as follows: $\Delta J = 0, \pm 1$; ΔK_a and ΔK_c — even.

Speaking of determining the selection rules for the band before analyzing the spectrum, it should be noted that its type, a, b or c, is determined by the nonzero matrix elements of the guide cosines k_{Zz}, k_{Zx} and k_{Zy}, respectively. The non-zero values can be determined by their resulting symmetry $\Gamma(k_{Z\alpha}) = A'' \otimes \gamma^{\nu_1} \otimes \gamma^{\nu_2}$. The symmetries of the lower possible vibrational state γ^{ν_1} (in our case, it is the ground vibrational state, for which $\gamma^{\nu_1} = A'$) and the upper vibrational state, i. e. the considered fundamental band, are used for this purpose. The direct product (denoted as $\otimes$) of irreducible representations of the point symmetry group C_s is well described, for example, in [23]. Thus, it can be demonstrated that transitions from the ground state to symmetry states A', and with them the corresponding bands, will lead to the resulting symmetry $\Gamma(k_{Z\alpha}) = A'$, which, according to Table 1, correspond to non-zero matrix elements k_{Zy}. This allows us to conclude about the c-type of such bands and the corresponding selection rules. The symmetry bands A'' turn out to be hybrid, with transitions of a- and b-types.

3. Effective Hamiltonian Model

To describe interacting vibrational-rotational states, as well as to describe any quantum system, it is necessary to know about the Hamiltonian of this system. A detailed study and description of the effective Hamiltonian for an isolated vibrational state was made in [24]. In the general case, in the presence of resonant interactions, the effective Hamiltonian has the form [25–28]:

$$H^{\text{vib-rot}} = \sum_{v,\tilde{v}} |v\rangle\langle\tilde{v}| H^{v\tilde{v}}, \tag{1}$$

where the summation goes over all interacting vibrational states. The diagonal contributions in (1) can be expressed as the Watson Hamiltonian:

$$\begin{aligned} H^{vv} &= E^v + [A^v - \frac{1}{2}(B^v + C^v)]J_z^2 \\ &+ \frac{1}{2}(B^v + C^v)J^2 + \frac{1}{2}(B^v - C^v)J_{xy}^2 \\ &- \Delta_K^v J_z^4 - \Delta_{JK}^v J_z^2 J^2 - \Delta_J^v J^4 - \delta_K^v [J_z^2, J_{xy}^2]_+ - 2\delta_J^v J^2 J_{xy}^2 \\ &+ H_K^v J_z^6 + H_{KJ}^v J_z^4 J^2 + H_{JK}^v J_z^2 J^4 + H_J^v J^6 + [J_{xy}^2, h_K^v J_z^4 \\ &+ h_{JK}^v J^2 J_z^2 + h_J^v J^4]_+ + L_K^v J_z^8 + L_{KKJ}^v J_z^6 J^2 + L_{JK}^v J_z^4 J^4 \\ &+ L_{KJJ}^v J_z^2 J^6 + L_J^v J^8 + [J_{xy}^2, l_K^v J_z^6 \\ &+ l_{KJ}^v J^2 J_z^4 + l_{JK}^v J^4 J_z^2 + l_J^v J^6]_+ + \ldots, \end{aligned} \tag{2}$$

where $J_{xy}^2 = J_x^2 - J_y^2$; $[\ldots, \ldots]_+$ — anticommutators; A^v, B^v and C^v — effective rotational constants of the vibrational state (v), and the rest — various orders of centrifugal distortion coefficients. The non-diagonal contributions, well described in [29], will be different depending on the symmetry of the interacting states. For the states of the same symmetry

$$H^{v\tilde{v}} = H_F^{v\tilde{v}} + H_{Cy}^{v\tilde{v}} \quad (v \neq \tilde{v}), \tag{3}$$

where

$$\begin{aligned} H_F^{v\tilde{v}} &= {}^{v\tilde{v}}F_0 + {}^{v\tilde{v}}F_K J^2 + {}^{v\tilde{v}}F_J J^2 \\ &+ {}^{v\tilde{v}}F_{KK} J_z^2 + {}^{v\tilde{v}}F_{KJ} J_z^2 J^2 + {}^{v\tilde{v}}F_{JJ} J^4 + \ldots \\ &+ {}^{v\tilde{v}}F_{xy}\left(J_x^2 - J_y^2\right) + {}^{v\tilde{v}}F_{Kxy}\left[J_z^2, \left(J_x^2 - J_y^2\right)\right]_+ \\ &+ {}^{v\tilde{v}}F_{Jxy} J^2 \left(J_x^2 - J_y^2\right) + \ldots \end{aligned} \tag{4}$$

and

$$\begin{aligned} H_{Cy}^{v\tilde{v}} &= iJ_y H_{(1y)}^{v\tilde{v}} + iH_{(1y)}^{v\tilde{v}} J_y \\ &+ [J_x, J_z]_+ H_{(2y)}^{v\tilde{v}} + H_{(2y)}^{v\tilde{v}} [J_x, J_z]_+ + \ldots. \end{aligned} \tag{5}$$

Table 1. Symmetry types and characters of irreducible representations of the symmetry group C_s (as applied to the molecule C_2H_3D)

Representation	E	$\sigma(xy)$	Vibrational coordinates	Rotational parameters	Rotational parameters (I^r)
1	2	3	4	5	6
A'	1	1	$q_1, q_2, q_3, q_5, q_6, q_9, q_{10}, q_{11}, q_{12}$ $q_9, q_{10}, q_{11}, q_{12}$	J_z, k_{Zz}	J_y, k_{Zy}
A''	1	-1	q_4, q_7, q_8	J_x, k_{Zx} J_y, k_{Zz}	J_x, k_{Zx} J_z, k_{Zz}

For the interacting states of different symmetries, the expression for the non-diagonal contributions has the form

$$H^{v\tilde{v}} = H^{v\tilde{v}}_{Cz} + H^{v\tilde{v}}_{Cx} \quad (v \neq \tilde{v}), \tag{6}$$

where

$$H^{v\tilde{v}}_{Cz} = iJ_z H^{v\tilde{v}}_{(1y)} + [J_x, J_y]_+ H^{v\tilde{v}}_{(2z)} + H^{v\tilde{v}}_{(2z)} [J_x, J_y]_+ + \dots \tag{7}$$

and

$$H^{v\tilde{v}}_{Cx} = iJ_x H^{v\tilde{v}}_{(1x)} + iH^{v\tilde{v}}_{(1x)} J_x + [J_y, J_z]_+ H^{v\tilde{v}}_{(2x)} + H^{v\tilde{v}}_{(2x)} [J_y, J_z]_+ + \dots . \tag{8}$$

It is also worth noting that in expressions (7) and (8)

$$H^{v\tilde{v}}_{(i\alpha)} = \frac{1}{2}{}^{v\tilde{v}}C^{(i\alpha)} + {}^{v\tilde{v}}C^{(i\alpha)}_K J_z^2 + \frac{1}{2}{}^{v\tilde{v}}C^{(i\alpha)}_J J^2 + {}^{v\tilde{v}}C^{(i\alpha)}_{KK} J_z^2 + {}^{v\tilde{v}}C^{(i\alpha)}_{KJ} J_z^2 J^2 + \frac{1}{2}{}^{v\tilde{v}}C^{(i\alpha)}_{JJ} J^4 + {}^{v\tilde{v}}C^{(i\alpha)}_{KKK} J_z^6 + {}^{v\tilde{v}}C^{(i\alpha)}_{KKJ} J_z^4 J^2 + {}^{v\tilde{v}}C^{(i\alpha)}_{KJJ} J_z^2 J^4 + \frac{1}{2}{}^{v\tilde{v}}C^{(i\alpha)}_{JJJ} J^6 + \dots \quad (\alpha = x, y, z). \tag{9}$$

4. Estimationof Coriolis Interaction Parameters

Because of the complexity of describing the experimental transitions in the vibrational states under consideration, it becomes necessary to take into account many strong interactions between the vibrational-rotational states of different vibrational states. This leads to the use of so many interaction parameters included in the Hamiltonian (1)−(9) that it becomes difficult to determine the parameters by numerical methods. It is possible to make the task easier if some of the variable parameters are fixed, which requires information about these parameters. The main parameters of the Coriolis interactions became candidates for the role of such fixed parameters, because theoretical estimation of their values is possible due to the knowledge of the quadratic power coefficients of the intramolecular potential function of the ethylene molecule obtained in [30]. The parameters of Coriolis interactions calculated on this basis are given in column 2 of Table 2.

Table 2. Parameters of Coriolis interactions $\xi^{\alpha}_{\lambda\mu}$ of the C_2H_3D molecule, calculated from data [30] on the quadratic part of the intramolecular potential function

α	λ	μ	Value, cm^{-1}	α	λ	μ	Value,cm^{-1}
1			2	1			2
y	3	10	0.1855	x	10	8	2.1020
y	3	6	0.4512	z	10	8	−0.2945
x	3	7	0.6043	x	10	4	1.0975
z	3	7	1.7488	z	10	4	1.5605
x	3	8	−0.0983	x	6	7	−0.2227
z	3	8	−1.5643	z	6	7	1.7403
x	3	4	0.4269	x	6	8	0.1209
z	3	4	1.9100	z	6	8	−2.9855
x	10	7	−0.9359	x	6	4	−0.6790
z	10	7	2.6224	z	6	4	−1.1293
y	10	6	−0.0343				

5. Analysis of experimental data

Fig. 2 shows the experimental spectra analyzed as part of this work. The spectra were recorded at the Technical University of Braunschweig (Germany) on a Brucker 125 HR spectrometer. All spectra were taken with an optical path length of 4 m. Survey spectra I and II (range of 590−1150 cm^{-1}), shown at the top of the figure, were recorded at 21.9°C and pressures of 4, 30 Pa, respectively. The instrumental resolution was 0.0015 cm^{-1}. Spectrum III (range of 1080−1350 cm^{-1}) at the bottom of the figure was taken at 22.1°C and a pressure of 230 Pa with a resolution of 0.0021 cm^{-1}. Spectrum I clearly shows *Q*-, *P*-, and *R*-branches of the ν_7 and ν_8 — most intense bands, the last of which completely overlaps the ν_4 band. Also, the *P*-branch of ν_{10} and theν_3-branch are marked in the figure.

To analyze the spectrum, the method of combination difference of the ground vibrational state was used: the rotational energies of the ground vibrational state were calculated based on the data from [31]. Table 3 contains statistical information on the results of the analysis of the absorption spectrum of the molecule under study. In particular, the total number of transitions attributed to both the hybrid bands ν_6, ν_{10}, and the bands ν_4, ν_7, ν_8,was

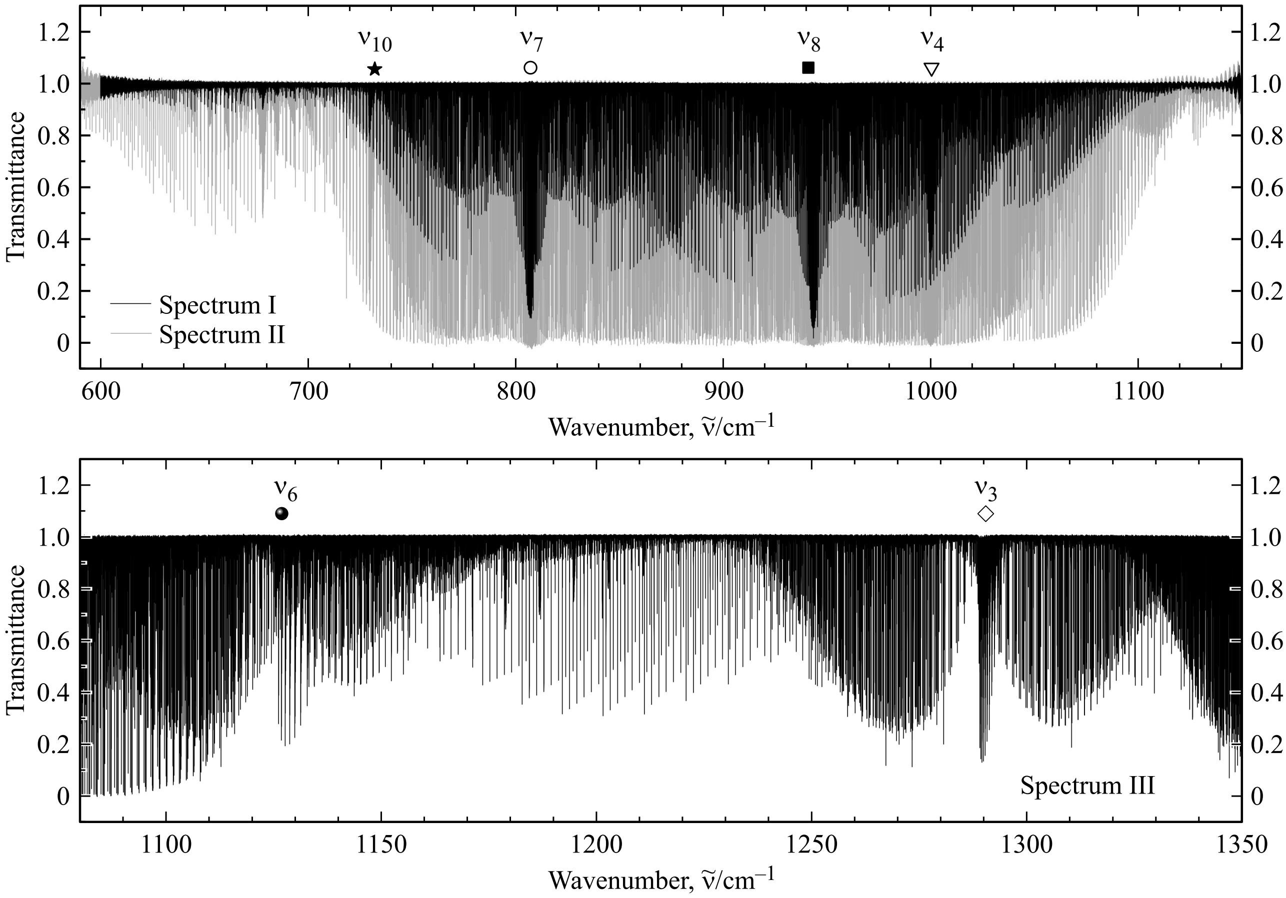

Figure 2. Overview spectrum of the molecule C_2H_3D. At the top, spectra I and II in the range of $590-1150\,\mathrm{cm}^{-1}$, at the bottom, spectrum III in the range of $1080-1350\,\mathrm{cm}^{-1}$.

Table 3. Statistical information on the results of spectrum analysis of the molecule C_2H_3D

Band	Centre, cm^{-1}	$J^{\max}$	$K_a^{\max}$	$N_t{}^{a)}$	$N_u{}^{b)}$	$m_1{}^{c)}$	$m_2{}^{c)}$	$m_3{}^{c)}$
1	2	3	4	5	6	7	8	9
$\nu_{10}(A')$, This paper	732.1426	31	20	4650	671	71.2	17.9	10.9
$\nu_{10}(A')$, [32]	732.1443	28	14					
$\nu_7(A'')$, This paper	806.4722	46	18	8500	1220	62.3	30.1	7.6
$\nu_7(A'')$, [32]	806.4725	35	14					
$\nu_8(A'')$, This paper	943.5032	50	26	6530	952	82.4	12.9	4.7
$\nu_8(A'')$, [32]	943.5033	35	14					
$\nu_4(A'')$, This paper	1000.0395	33	11	5450	781	68.3	9.8	21.9
$\nu_4(A'')$, [32]	1000.0399	35	14					
$\nu_6(A')$, This paper	1125.2769	42	21	2800	404	62.4	23.0	14.6
$\nu_6(A')$, [32]	1125.2769	30	13					
$\nu_6(A')$, [33]	1125.2769	27	20	947				
In total, this paper				27930	4028			
Total, [32]				18000				
$d_{\mathrm{rms}}{}^{d)}$, This paper	$1.7\cdot10^{-4}$							

Note. [a] N_t — the number of transitions.
[b] N_u — the number of upper state energies obtained.
[c] $m_i = n_i/N_u\cdot100\%$ (i=1, 2, 3); n_1, n_2, and n_3 — the number of upper-level energies for which the difference $\delta=E^{\{textexp}-E^{\mathrm{calc}}$ satisfies the conditions $\delta\le 2\cdot10^{-4}\,\mathrm{cm}^{-1}$, $2\cdot10^{-4}\,\mathrm{cm}^{-1}<\delta\le4\cdot10^{-4}\,\mathrm{cm}^{-1}$, $\delta>4\cdot10^{-4}\,\mathrm{cm}^{-1}$.
[d] u cm^{-1}.

Table 4. Spectroscopic parameters of the basic vibrational state of the molecule C_2H_5D (in cm^{-1})

Parameter	[31]	This paper
1	2	3
A	4.038999	4.00588802(69)
B	0.9202228	0.916325131(93)
C	0.7425594	0.74377235(19)
$\Delta_K \cdot 10^4$	0.8061	0.704840(38)
$\Delta_{JK} \cdot 10^4$	0.04692	0.060440(22)
$\Delta_J \cdot 10^4$	0.013524	0.0129547(33)
$\delta_K \cdot 10^4$	0.0910	0.081080(88)
$\delta_J \cdot 10^4$	0.003131	0.00284258(76)
$H_K \cdot 10^8$	0.673	0.5332(40)
$H_{KJ} \cdot 10^8$	-0.035	-0.0760(54)
$H_{JK} \cdot 10^8$	0.0034	0.0168(15)
$H_J \cdot 10^8$	0.00021	0.000320(25)
$h_K \cdot 10^8$		0.293(40)
$h_{JK} \cdot 10^8$		0.0118(10)
$h_J \cdot 10^8$		0.0001354(83)
$d_{\rm rms} \cdot 10^4$	20.11	1.036

27950. Also for the bands ν_4, ν_7, ν_8 many d-type transitions were found, which were mentioned in Section 2.

6. Ground state parameters

When using the ground state parameters from the [31], the experimental values of the combination differences began to deviate from those determined from the [31] work, and the difference between them exceeded the experimental error by several times. Moreover, this deviation was observed for energy levels with quantum numbers $J \geqslant 26$ and $K_a \geqslant 8$, which are not the limit for the experimental spectrum study in this paper. As a consequence, it became necessary to improve the parameters of the ground state.

To determine the parameters of the molecule ground state, information about the combinational differences of the ground vibrational state, obtained from the positions of the lines known from the experiment, is needed. Within this study, the experimental spectrum allowed more than 3000 combination differences with maximum quantum numbers $J_{\max}$=40 and $K_a^{\max}$=16 to determine the ground state parameters. Table 4 contains the results of the ground state parameters in column 3. From comparison with the parameters of work [31] (column 2 of Table 4), we can see quite satisfactory correlation of the parameters. The new parameters reproduce the experiment with an error of $d_{\rm rms} \cdot 10^4 = 1.036\,cm^{-1}$, which exceeds the reproduction accuracy of work [31] parameters by 20 times. The resulting set of ground state parameters was used further in the work, as well as for spectra reanalysis.

7. Determination of effective Hamiltonian parameters and discussion of results

As mentioned above, 27950 experimental lines of the spectrum of the molecule C_2H_3D were assigned to the vibrational states $(v_4{=}1)$, $(v_6{=}1)$, $(v_7{=}1)$, $(v_8{=}1)$ and $(v_{10}{=}1)$ under study, and they were used to determine rotational energies of upper vibrational states. A total of 4028 such energies have been identified. These energies were used to determine the parameters of the effective Hamiltonian by the least-squares method.

On the experimental spectrum shown earlier (Fig. 2), one can see that the bands in the studied range represent an almost continuous structure. The ν_3 band (center about $1290\,cm^{-1}$) is close by, further to the right are also the ν_{12} and $2\nu_{10}$ bands (centers about 1400 and $1460\,cm^{-1}$, respectively). As the wave number increases, the density of the other bands only increases. Thus, the task of describing the structure of the five bands under study and their interactions with neighboring bands can become infinite because of the need to consider each successive state, which interacts with each successive one, and so on. As is usually the case, to solve such a problem, one has to choose a physically reasonable simplification, in other words, find a finite number of states interacting with the five under study. Analysis of the vibrational-rotational structure of the states $v_4{=}1)$, $(v_6{=}1)$, $(v_7{=}1)$, $(v_8{=}1)$ and $(v_{10}{=}1)$ showed that it will be sufficient to select additionally only the ν_3 band from the whole cascade of bands in the range of large quantum numbers. The justification for this is, first, the fact that the distance between the last band ν_6 examined and the band ν_3 (approximately $165\,cm^{-1}$) is about half the distance between ν_6 and the next band in the range. Second, the experimental data reproduction using an analysis that considers only one additional state $(v_3{=}1)$ turned out to be quite satisfactory.

Thus, in this paper, an effective Hamiltonian was used, taking into account the five investigated states and an additional state (v_3). The vibrational-rotational energies of the latter were involved only those for which $J = 0$, 1, and 2. In the future, it is planned to analyze the shorter wavelength range, where the role of such an additional dark state will be taken by (v_6). In addition to the interaction of the states under study with the additional state (v_3), it was necessary to consider the interaction of five states $(v_4{=}1)$, $(v_6{=}1)$, $(v_7{=}1)$, $(v_8{=}1)$ and $(v_{10}{=}1)$ with each other, which makes it necessary to use a large number of resonance parameters. In turn, the correlation between a large number of such parameters and the centrifugal distortion parameters leads to an incorrect definition of the latter. This problem is circumvented by the fact that the values of the centrifugal parameters must be close to those for the main vibrational state [34]. Thus, by fixing the parameters on the values from Table 4, the procedure for determining the effective Hamiltonian parameters allowed us to refine the band

Table 5. Spectroscopic parameters of the states $(v_4 = 1)$, $(v_6 = 1)$, $(v_7 = 1)$, $(v_8 = 1)$ and $(v_{10} = 1)$ of the molecule C_2H_3D (in cm^{-1})

Parameter	$(000)^b$	$(v_{10} = 1)^c$	$(v_{10} = 1)^d$	$(v_7 = 1)^c$	$(v_7 = 1)^d$	$(v_8 = 1)^c$	$(v_8 = 1)^d$
1	2	3	4	5	6	7	8
E		732.142300(64)	732.1443	806.471982(31)	806.4725	943.503080(32)	943.5033
A	4.00588802	3.9887196(63)	4.044842	4.0453017(37)	3.967143	3.9659525(30)	4.007676
B	0.916325131	0.9158925(16)	0.903365	0.9138023(11)	0.924494	0.9111203(24)	0.911344
C	0.743772350	0.7423493(45)	0.743922	0.7449286(16)	0.744876	0.7445513(26)	0.744876
$\Delta_K \cdot 10^5$	7.0484	6.878519(79)	3.106	6.878519	10.026	6.878519	6.522
$\Delta_{JK} \cdot 10^5$	0.6044	0.60888(62)	0.820	0.60888	0.816	0.60888	0.365
$\Delta_J \cdot 10^5$	0.129547	0.12978(67)	−0.0311	0.12978	0.2355	0.12978	0.1285
$\delta_K \cdot 10^5$	0.8108	0.8108	−0.366	0.8108	0.243	0.8108	0.327
$\delta_J \cdot 10^5$	0.0284258	0.0284258	−0.1632	0.0284258	0.0731	0.0284258	0.0263
$H_K \cdot 10^9$	−5.332	−5.332		−5.332		−5.332	
$H_{KJ} \cdot 10^9$	−0.760	−0.760		−0.760		−0.760	
$H_{JK} \cdot 10^9$	0.168	0.168		0.168		0.168	
$H_J \cdot 10^9$	0.0032	0.0032		0.0032		0.0032	
$h_K \cdot 10^9$	2.930	2.930		2.930		2.930	
$h_{KJ} \cdot 10^9$	0.118	0.118		0.118		0.118	
$h_J \cdot 10^9$	0.001354	0.001354		0.001354		0.001354	

Table 5 (*continued*)

Parameter	$(v_4 = 1)^c$	$(v_4 = 1)^d$	$(v_6 = 1)^c$	$(v_6 = 1)^d$	$(v_6 = 1)^e$	$(v_3 = 1)^c$
1	9	10	11	12	13	14
E	1000.039364(30)	1000.0399	1125.276888(31)	1125.2769	1125.27674	1288.788159(90)
A	3.9579014(60)	3.944431	4.0346021(32)	4.002324	4.103782	4.0105827(49)
B	0.9138423(82)	0.908689	0.9180181(27)	0.922087	0.921948	0.9178315(77)
C	0.7445802(53)	0.744614	0.7426154(30)	0.740833	0.741003	0.7419887(86)
$\Delta_K \cdot 10^5$	6.878519	5.258	6.878519	8.256	14.93	6.878519
$\Delta_{JK} \cdot 10^5$	0.60888	0.570	0.60888	1.084	0.429	0.60888
$\Delta_J \cdot 10^5$	0.12978	0.1069	0.12978	0.1461	0.1551	0.12978
$\delta_K \cdot 10^5$	0.8108	0.866	0.8108	1.000	1.819	0.8108
$\delta_J \cdot 10^5$	0.0284258	0.0145	0.0284258	0.0371	0.0355	0.0284258
$H_K \cdot 10^9$	-5.332		-5.332		253.	-5.332
$H_{KJ} \cdot 10^9$	-0.760		-0.760		2.7	-0.760
$H_{JK} \cdot 10^9$	0.168		0.168		-2.7	0.168
$H_J \cdot 10^9$	0.0032		0.0032		0.32	0.0032
$h_K \cdot 10^9$	2.930		2.930			2.930
$h_{KJ} \cdot 10^9$	0.118		0.118			0.118
$h_J \cdot 10^9$	0.001354		0.001354			0.001354
$L_K \cdot 10^{11}$					-71.0	
$L_{KKJ} \cdot 10^{11}$					-49.3	
$L_{JK} \cdot 10^{11}$					16.2	
$L_{JJK} \cdot 10^{11}$					-1.93	
$L_J \cdot 10^{11}$					0.077	
$d_{rms} \cdot 10^4$	1.7					

Note. [a] In parentheses — confidence intervals 1σ. The parameters without confidence intervals were fixed at the values of the ground state parameters from column 2.

[b] Reproduced from Table 4. [c] Defined in this paper. [d] Reproduced from [32]. [e] Reproduced from [33].

Table 6. Resonance interaction parameters between the vibrational states (v_4=1), (v_6=1), (v_7=1), (v_8=1) and (v_{10}=1) of the molecule C_2H_3D (in cm^{-1})

Parameter	Value	Parameter	Value	Parameter	Value	Parameter	Value
${}^{1,2}C^{1y} \equiv (2C\xi^{y})^{1,2}$	0.1855						
${}^{1,3}F_{Kxy} \cdot 10^{4}$	-0.130(13)	${}^{1,3}F_{KKxy} \cdot 10^{6}$	-0.237(19)	${}^{1,3}F_{KKKxy} \cdot 10^{8}$	0.1083(72)		
${}^{1,3}C^{1y} \equiv (2C\xi^{y})^{1,3}$	0.4512	${}^{1,3}C^{1y}_{KK} \cdot 10^{5}$	-0.750(26)	${}^{1,3}C^{1y}_{KJ} \cdot 10^{6}$	-0.439(20)	${}^{1,3}C^{1y}_{KKK} \cdot 10^{7}$	0.2606(62)
${}^{1,3}C^{1y}_{KKJ} \cdot 10^{9}$	0.572(96)	${}^{1,3}C^{2y} \cdot 10^{2}$	0.311(40)	${}^{1,3}C^{2y}_{K} \cdot 10^{4}$	-0.203(21)	${}^{1,3}C^{2y}_{KK} \cdot 10^{6}$	0.403(17)
${}^{1,3}C^{2y}_{KKK} \cdot 10^{9}$	-0.913(33)						
${}^{2,3}F_{KJ} \cdot 10^{4}$	-0.253(31)	${}^{1,3}F_{JJxy} \cdot 10^{9}$	0.1485(18)				
${}^{2,3}C^{1y} \equiv (2C\xi^{y})^{2,3}$	-0.34	${}^{2,3}C^{2y}_{K} \cdot 10^{2}$	0.2009(77)				
${}^{2,3}C^{2y}_{KK} \cdot 10^{5}$	0.748(57)	${}^{2,3}C^{2y}_{KKK} \cdot 10^{7}$	-0.3141(97)				
${}^{2,3}C^{2y}_{KKJ} \cdot 10^{8}$	0.138(14)	${}^{2,3}C^{2y}_{KKK} \cdot 10^{7}$	-0.3141(97)				
${}^{1,3}C^{2} \cdot 10^{3}$	0.8410(77)	${}^{1,3}C^{2}_{J} \cdot 10^{5}$	0.2999(83)	${}^{1,3}C^{2}_{KJ} \cdot 10^{8}$	0.101(10)	${}^{1,3}C^{2}_{JJ} \cdot 10^{9}$	-0.487(31)
${}^{1,3}C^{2}_{KJJ} \cdot 10^{11}$	-0.1118(73)						
${}^{2,3}F_{J} \cdot 10^{2}$	0.1948(88)	${}^{2,3}F_{xy} \cdot 10^{2}$	0.3148(44)	${}^{2,3}F_{Kxy} \cdot 10^{5}$	-0.2213(84)	${}^{2,3}F_{Jxy} \cdot 10^{5}$	-0.1121(71)
${}^{2,3}F_{KJxy} \cdot 10^{8}$	0.401(20)	${}^{2,3}F_{JJxy} \cdot 10^{9}$	0.338(23)	${}^{2,3}F_{KKJxy} \cdot 10^{11}$	-0.823(27)	${}^{2,3}F_{KJJxy} \cdot 10^{12}$	-0.964(52)
${}^{1,4}C^{1} \equiv (2A\xi^{z})^{1,4}$	-1.6	${}^{1,4}C^{1}_{K} \cdot 10^{3}$	0.19252(72)	${}^{1,4}C^{1}_{J} \cdot 10^{4}$	-0.892(19)	${}^{1,4}C^{1}_{KKK} \cdot 10^{10}$	-0.831(72)
${}^{1,4}C^{1}_{KKJ} \cdot 10^{10}$	0.917(68)	${}^{1,4}C^{2} \cdot 10^{3}$	0.7636(95)	${}^{1,4}C^{2}_{K} \cdot 10^{5}$	-0.1365(85)		
${}^{2,4}C^{1}_{KK} \cdot 10^{6}$	0.7249(87)	${}^{2,4}C^{1}_{JJ} \cdot 10^{7}$	0.1863(54)	${}^{2,4}C^{1}_{KKJ} \cdot 10^{9}$	-0.464(22)	${}^{2,4}C^{1}_{KJJ} \cdot 10^{10}$	0.639(49)
${}^{2,4}C^{2} \cdot 10^{2}$	1.2517(59)	${}^{2,4}C^{2}_{KJ} \cdot 10^{8}$	-0.534(32)	${}^{2,4}C^{2}_{KJJ} \cdot 10^{11}$	0.227(18)	${}^{2,4}C^{2}_{JJJ} \cdot 10^{12}$	0.782(44)
${}^{3,4}C^{1}_{K} \cdot 10^{4}$	0.379(31)	${}^{3,4}C^{1}_{J} \cdot 10^{4}$	-0.1850(84)	${}^{3,4}C^{1}_{KK} \cdot 10^{6}$	-0.1145(86)	${}^{3,4}C^{1}_{KJ} \cdot 10^{7}$	-0.346(29)
${}^{3,4}C^{1}_{JJ} \cdot 10^{8}$	-0.125(25)	${}^{3,4}C^{1}_{KKK} \cdot 10^{9}$	-0.334(26)	${}^{3,4}C^{2} \cdot 10^{3}$	-0.276(22)	${}^{3,4}C^{2}_{KKK} \cdot 10^{11}$	-0.353(20)
${}^{3,4}C^{2}_{KJJ} \cdot 10^{12}$	0.755(43)						
${}^{1,5}C^{1} \equiv (2C\xi^{y})^{1,5}$	-0.2						
${}^{2,5}C^{1} \equiv (2A\xi^{z})^{2,5}$	2.4	${}^{2,5}C^{1}_{J} \cdot 10^{3}$	-0.11402(99)	${}^{2,5}C^{1}_{KK} \cdot 10^{7}$	-0.2016(94)	${}^{2,5}C^{1}_{KJ} \cdot 10^{7}$	0.2151(94)
${}^{2,5}C^{1}_{JJ} \cdot 10^{7}$	0.1095(70)	${}^{2,5}C^{1}_{JJJ} \cdot 10^{11}$	-0.947(52)	${}^{2,5}C^{2} \cdot 10^{2}$	0.7069(81)	${}^{2,5}C^{2}_{K} \cdot 10^{5}$	0.5279(85)
${}^{2,5}C^{2}_{J} \cdot 10^{6}$	0.6654(84)	${}^{2,5}C^{2}_{KK} \cdot 10^{7}$	-0.196(11)	${}^{2,5}C^{2}_{KJ} \cdot 10^{8}$	-0.765(18)	${}^{2,5}C^{2}_{KKK} \cdot 10^{10}$	0.244(49)
${}^{2,5}C^{2}_{KKJ} \cdot 10^{10}$	0.349(13)	${}^{2,5}C^{2}_{KJJ} \cdot 10^{11}$	0.1008(37)				
${}^{3,5}C^{1} \equiv (2A\xi^{z})^{3,5}$	1.4						
${}^{4,5}C^{1} \equiv (2B\xi^{x})^{4,5}$	-1.4	${}^{4,5}C^{1}_{K} \cdot 10^{3}$	0.2105(35)	${}^{4,5}C^{1}_{KK} \cdot 10^{6}$	0.1656(81)	${}^{4,5}C^{1}_{KJ} \cdot 10^{8}$	-0.1526(44)
${}^{4,5}C^{1}_{JJ} \cdot 10^{7}$	0.367(38)	${}^{4,5}C^{1}_{KKK} \cdot 10^{9}$	0.312(18)	${}^{4,5}C^{1}_{KKJ} \cdot 10^{9}$	0.305(17)	${}^{4,5}C^{2} \cdot 10^{1}$	-0.3925(15)
${}^{4,5}C^{2}_{J} \cdot 10^{5}$	0.8650(89)	${}^{4,5}C^{2}_{KJ} \cdot 10^{7}$	-0.1161(27)	${}^{4,5}C^{2}_{JJ} \cdot 10^{9}$	0.316(94)	${}^{4,5}C^{2}_{KKK} \cdot 10^{10}$	0.1493(62)
${}^{4,5}C^{2}_{JJJ} \cdot 10^{12}$	0.647(54)						
${}^{1,6}C^{1} \equiv (2C\xi^{y})^{1,6}$	-0.4	${}^{1,6}C^{1}_{J} \cdot 10^{5}$	-0.592(31)	${}^{1,6}C^{1}_{KK} \cdot 10^{7}$	-0.780(67)	${}^{1,6}C^{1}_{KJ} \cdot 10^{7}$	-0.942(27)
${}^{1,6}C^{1}_{JJ} \cdot 10^{8}$	0.309(14)	${}^{1,6}C^{2} \cdot 10^{2}$	-0.3089(51)	${}^{1,6}C^{2}_{K} \cdot 10^{5}$	-0.2170(89)	${}^{1,6}C^{2}_{J} \cdot 10^{5}$	0.2931(80)
${}^{2,6}C^{1} \equiv (2A\xi^{z})^{2,6}$	1.6	${}^{2,6}C^{1}_{KJ} \cdot 10^{7}$	0.258(12)	${}^{2,6}C^{1}_{JJ} \cdot 10^{7}$	-0.786(26)	${}^{2,6}C^{2}_{J} \cdot 10^{6}$	-0.933(59)
${}^{2,6}C^{2}_{KJ} \cdot 10^{7}$	0.1458(36)	${}^{2,6}C^{2}_{KKJ} \cdot 10^{10}$	-0.159(10)				
${}^{3,6}C^{1} \equiv (2A\xi^{z})^{3,6}$	-2.7	${}^{3,6}C^{1}_{K} \cdot 10^{3}$	0.158232(99)	${}^{3,6}C^{1}_{JJ} \cdot 10^{8}$	-0.517(36)	${}^{3,6}C^{2} \cdot 10^{3}$	0.496(10)
${}^{3,6}C^{2}_{J} \cdot 10^{6}$	0.583(25)	${}^{3,6}C^{2}_{KJJ} \cdot 10^{12}$	-0.343(22)	${}^{3,6}C^{2}_{JJJ} \cdot 10^{12}$	-0.1078(48)		
${}^{4,6}C^{1} \equiv (2B\xi^{x})^{4,6}$	0.6						
${}^{5,6}F_{J} \cdot 10^{2}$	0.5426(95)	${}^{5,6}F_{KJ} \cdot 10^{5}$	0.2473(93)	${}^{5,6}F_{xy} \cdot 10^{3}$	0.895(84)	${}^{5,6}F_{Jxy} \cdot 10^{6}$	-0.951(71)

centers together with the rotational parameters and the resonance interaction parameters. The results of this study, namely, the parameters of the effective Hamiltonian, are presented in Tables 5 and 6. For comparison, Table 5 also shows the values of the corresponding parameters from the works [32,33]. There is a certain correlation between the results of this work and those of [32,33], but the results of this work allow us to reproduce the energy structure and positions of the spectrum lines with much greater accuracy. Table 7 shows a portion of the vibrational-rotational levels of the investigated states up to $J = 10$, as well as the experimental and calculated errors of determination in columns 3 and 4.

8. Conclusion

In this paper, we analyzed the high-resolution infrared spectrum of the molecule C_2H_3D in the range of $600-1300\,\mathrm{cm}^{-1}$, with the resonating bands ν_4, ν_6, ν_7, ν_8 and ν_{10} as the object of analysis. Experimental transitions of 27950 with maximum quantum numbers $J^{\max} = 40$ and $K_a^{\max} = 20$ were assigned to the studied bands. The theoretical model of the effective Hamiltonian included both the interaction of the five states under study with each other and their interaction with the state $(v_3 = 1)$. The obtained parameters reproduce the experimental data with an error of $d_{\mathrm{rms}} = 1.7 \cdot 10^{-4}\,\mathrm{cm}^{-1}$ for the 4028 upper energy levels

Table 7. The vibrational-rotational energy levels of the states (v_4=1), (v_6=1), (v_7=1), (v_8=1) and (v_{10}=1) of the molecule C_2H_3D (in cm^{1})

Band	ν_{10}			ν_7			ν_8			ν_4			ν_6		
$J\ K_a\ K_c$	E	Δ	δ	E	Δ	δ	E	Δ	δ	E	Δ	δ	E	Δ	δ
1	2	3	4	2	3	4	2	3	4	2	3	4	2	3	4
0 0 0				806.47216	-	18				1000.03951	-	14	1125.27692	-	3
1 0 1				808.14163	4	12	945.15908	1	3	1001.69771	5	8	1126.93980	-	- 1
1 1 1				811.33938	2	10	948.17848	2	2	1004.72813	7	3	1130.12136	-	- 6
1 1 0				811.51753	3	12	948.34517	4	4	1004.89784	4	4	1130.30231	2	1
2 0 2				811.47341	4	12	948.46426	1	0	1005.00728	6	7	1130.25819	3	5
2 1 2				814.50012	1	12	951.32372	3	4	1007.87492	4	5	1133.26636	4	1
2 1 1				815.03446	3	12	951.82369	4	0	1008.38403	4	5	1133.80900	3	4
2 2 1				824.62339	3	3	960.88203	3	2	1017.47470	3	3	1143.35207	5	0
2 2 0				824.63061	3	4	960.88873	3	1	1017.48164	7	4	1143.35944	10	-12
3 0 3				816.45301	3	12	953.40533	2	4	1009.95428	5	2	1135.21695	2	4
3 1 3				819.23671	5	7	956.03731	9	- 5	1012.59077	4	6	1137.97917	3	8
3 1 2				820.30513	2	11	957.03717	2	1	1013.60880	5	4	1139.06416	3	7
3 2 2				829.63080	4	4	965.84971	2	1	1022.44921	4	2	1148.34060	1	0
3 2 1				829.66679	2	6	965.88319	3	2	1022.48377	4	4	1148.37795	3	1
3 3 1	769.41886	12	- 2	846.04838	5	- 4	981.36807	2	- 1	1038.02651	2	- 1	1164.69685	17	-16
3 3 0	769.41886	12	13	846.04856	3	- 4	981.36822	2	- 2	1038.02667	3	1	1164.69685	17	3
4 0 4				823.05921	1	11	959.96249	5	5	1016.51848	4	3	1141.79422	2	7
4 1 4				825.54420	4	9	962.31475	4	4	1018.87076	5	6	1144.25441	2	5
4 1 3				827.32360	3	8	963.98006	3	0	1020.56650	5	1	1146.06157	1	3
4 2 3				836.30168	3	4	972.46794	3	2	1029.07634	4	2	1154.98594	5	5
4 2 2				836.40900	2	4	972.56785	3	1	1029.17953	3	3	1155.09751	2	- 6
4 3 2	775.99825	11	- 3	852.73688	2	- 4	988.00425	2	0	1044.67205	4	1	1171.36208	-	2
4 3 1	775.99940	13	11	852.73813	2	- 5	988.00542	3	- 1	1044.67333	4	- 2	1171.36357	-	-11
4 4 1	797.33382	12	3	875.67530	11	-10	1009.71317	10	- 1	1066.45739	11	0	1194.22943	4	- 7
4 4 0	797.33382	12	3	875.67530	11	-10	1009.71317	10	- 2	1066.45739	11	0	1194.22943	4	- 7
5 0 5				831.26512	3	7	968.11077	2	5	1024.67409	4	5	1149.96216	1	4
5 1 5				833.41613	2	7	970.14982	3	6	1026.70879	4	6	1152.08557	-	8
5 1 4				836.08158	4	- 6	972.64468	4	0	1029.24918	5	1	1154.79275	1	2
5 2 4				844.63119	1	3	980.73214	3	3	1037.35138	4	5	1163.28323	3	3
5 2 3				844.87913	3	4	980.96299	3	1	1037.58983	3	1	1163.54063	4	2
5 3 3	784.22720	18	9	861.10303	1	- 5	996.30441	3	- 1	1052.98415	4	- 1	1179.69942	3	- 3
5 3 2	784.23122	8	6	861.10811	2	- 3	996.30913	3	0	1052.98911	5	- 2	1179.70482	3	- 3
5 4 2	805.55873	5	11	884.03146	21	- 6	1018.00657	5	- 1	1074.76232	4	- 4	1202.55917	2	- 4
5 4 1	805.55873	5	8	884.03146	21	- 9	1018.00657	5	- 4	1074.76232	4	0	1202.55917	2	0
5 5 1	833.01067	11	7	913.48064	6	-15	1045.92059	5	- 4	1102.76525	5	3	1231.94143	3	- 6
5 5 0	833.01067	11	8	913.48064	6	-15	1045.92059	5	- 4	1102.76525	5	3	1231.94143	3	- 6
6 0 6				841.04053	1	6	977.82198	3	7	1034.39203	5	0	1159.68968	1	4
6 1 6				842.84432	2	4	979.53573	4	10	1036.09774	8	10	1161.46502	1	4
6 1 5				846.56799	2	6	983.02077	5	4	1039.64625	5	2	1165.24604	6	2
6 2 5				854.61333	2	1	990.63657	4	1	1047.26848	4	2	1173.22590	2	3
6 2 4				855.10105	2	1	991.09090	2	2	1047.73750	2	0	1173.73199	2	1
6 3 4	794.10742	16	1	871.14961	4	- 4	1006.27105	3	2	1062.96526	3	2	1189.71115	13	0
6 3 3	794.11961	9	7	871.16476	3	- 3	1006.28513	2	0	1062.98011	3	- 4	1189.72743	2	-12
6 4 3	815.43241	8	7	894.06429	4	- 6	1027.96320	4	- 1	1084.73295	3	- 4	1212.56001	18	- 9
6 4 2	815.43252	7	5	894.06443	4	- 9	1027.96335	3	- 2	1084.73310	2	- 2	1212.56001	18	10
6 5 2	842.88175	29	38	923.50227	3	- 11	1055.87067	3	- 6	1112.72887	9	0	1241.93481	3	- 4
6 5 1	842.88175	29	-48	923.50227	3	- 11	1055.87067	3	- 6	1112.72887	9	0	1241.93481	3	- 4
6 6 1	876.46072	7	4	959.43296	3	- 15	1089.99059	4	-10	1146.94344	4	0	1277.81780	5	- 4
6 6 0	876.46072	7	4	959.43296	3	- 15	1089.99059	4	-10	1146.94344	4	0	1277.81780	5	- 4

Note. Δ — value of the experimental error in units of $10^{-5}\,\mathrm{cm}^{-1}$ (Δ is missing in cases where the upper energy levels were determined from one transition), δ — difference $E^{\mathrm{exp}} - E^{\mathrm{calc}}$ also in units of $10^{-5}\,\mathrm{cm}^{-1}$.

Table 7 (*continued*)

Band	ν_{10}			ν_7			ν_8			ν_4			ν_6		
$J\ K_a\ K_c$	E	Δ	δ	E	Δ	δ	E	Δ	δ	E	Δ	δ	E	Δ	δ
1	2	3	4	2	3	4	2	3	4	2	3	4	2	3	4
7 0 7				852.35509	2	4	989.06773	3	9	1045.64341	5	2	1170.94578	4	10
7 1 7				853.82327	3	5	990.46493	3	9	1047.02990	5	8	1172.38451	6	14
7 1 6				858.76850	2	3	995.09499	6	5	1051.74390	3	0	1177.40677	5	- 1
7 2 6				866.24094	3	0	1002.17450	2	2	1058.82063	4	1	1184.80653	1	2
7 2 5				867.09743	2	1	1002.97277	3	1	1059.64428	4	1	1185.69460	3	2
7 3 5	805.64118	8	5	882.87900	5	- 4	1017.90619	2	0	1074.61761	7	2	1201.40003	10	- 1
7 3 4	805.67139	10	7	882.91667	2	- 3	1017.94128	3	2	1074.65445	4	- 2	1201.44015	3	6
7 4 4	826.95706	11	3	905.77670	3	- 6	1039.58548	5	- 1	1096.37184	3	- 4	1224.23477	31	-34
7 4 3	826.95755	9	3	905.77727	4	-10	1039.58604	3	- 3	1096.37243	3	- 1	1224.23477	31	34
7 5 3	854.40036	15	11	935.20044	10	- 9	1067.48298	3	1	1124.35712	20	3	1253.59800	2	- 7
7 5 2	854.40036	15	-17	935.20044	10	- 9	1067.48298	3	0	1124.35712	20	4	1253.59800	2	- 6
7 6 2	887.97789	8	1	971.11795	3	-10	1101.59714	6	- 4	1158.56529	3	- 1	1289.47440	3	- 4
7 6 1	887.97789	8	1	971.11795	3	-10	1101.59714	6	- 4	1158.56529	3	- 1	1289.47440	3	- 4
7 7 1	927.69390	5	3	1013.49711	2	-11	1141.92322	7	- 7	1198.98404	5	5	1331.84063	2	0
7 7 0	927.69390	5	3	1013.49711	2	-11	1141.92322	7	- 7	1198.98404	5	5	1331.84063	2	0
8 0 8				865.18216	1	2	1001.82291	3	7	1058.40262	7	- 3	1183.70323	5	- 2
8 1 8				866.34252	2	0	1002.92986	4	- 1	1059.49746	3	8	1184.83570	2	12
8 1 7				872.66516	2	0	1008.85061	3	11	1065.52488	3	- 1	1191.25592	2	1
8 2 7				879.50571	3	8	1015.33804	4	- 2	1071.99972	4	5	1198.01640	5	9
8 2 6				880.88580	2	- 9	1016.62519	3	1	1073.32694	4	1	1199.44612	2	2
8 3 6	818.82974	6	9	896.29290	3	- 4	1031.21134	2	0	1087.94260	3	0	1214.76707	1	2
8 3 5	818.89572	6	8	896.37514	3	0	1031.28791	2	0	1088.02294	3	- 2	1214.85479	3	- 1
8 4 5	840.13507	7	- 1	919.17192	2	- 6	1052.87616	5	0	1109.68174	3	- 5	1237.58572	10	8
8 4 4	840.13660	4	5	919.17378	2	- 4	1052.87790	5	- 1	1109.68359	3	- 5	1237.58791	14	- 7
8 5 4	867.56865	28	0	948.57778	10	- 7	1080.75910	15	- 3	1137.65160	19	-12	1266.93304	2	- 9
8 5 3	867.56909	31	- 3	948.57778	10	- 9	1080.75910	15	- 1	1137.65160	19	-10	1266.93304	2	- 6
8 6 3	901.14236	8	2	984.46481	2	- 7	1114.86495	3	- 7	1171.85083	4	- 1	1302.79994	2	- 2
8 6 2	901.14236	8	2	984.46481	2	- 7	1114.86495	3	- 7	1171.85083	4	- 1	1302.79994	2	- 2
8 7 2	940.85559	6	0	1026.84312	2	- 6	1155.18553	3	- 8	1212.26346	2	2	1345.15984	1	0
8 7 1	940.85559	6	0	1026.84312	2	- 6	1155.18553	3	- 8	1212.26346	2	2	1345.15984	1	0
8 8 1	986.73512	3	- 1	1075.63545	2	- 1	1201.71789	4	-11	1258.87742	2	3	1393.98926	2	3
8 8 0	986.73512	3	- 1	1075.63545	2	- 1	1201.71789	4	-11	1258.87742	2	3	1393.98926	2	3
9 0 9				879.50164	1	0	1016.06852	4	9	1072.65054	7	- 8	1197.94224	2	1
9 1 9				880.39488	2	3	1016.92290	4	0	1073.49268	2	7	1198.81023	3	11
9 1 8				888.23596	2	- 2	1024.26721	6	12	1080.96788	3	- 1	1206.77056	7	- 4
9 2 8				894.39839	3	- 2	1030.11847	4	- 2	1086.79668	3	4	1212.84578	4	14
9 2 7				896.47565	4	0	1032.05739	4	3	1088.79439	3	- 1	1214.99552	2	2
9 3 7	833.67355	7	7	911.39194	5	- 3	1046.18693	2	- 1	1102.94066	4	0	1229.81300	5	- 3
9 3 6	833.80431	10	8	911.55445	2	- 2	1046.33837	2	0	1103.09953	3	- 1	1229.98627	4	1
9 4 6	854.96912	2	2	934.25343	3	- 3	1067.83816	3	2	1124.66585	3	- 6	1252.61736	7	- 5
9 4 5	854.97294	5	4	934.25820	4	- 4	1067.84270	5	- 4	1124.67061	2	- 2	1252.62255	7	4
9 5 5	882.38815	27	0	963.63710	5	- 6	1095.70107	9	- 7	1152.61474	21	-13	1281.94225	7	- 7
9 5 4	882.38887	26	-17	963.63716	4	- 7	1095.70113	8	- 6	1152.61474	21	- 6	1281.94225	7	1
9 6 4	915.95488	5	- 4	999.46768	5	- 7	1129.79549	5	- 2	1186.80138	4	- 4	1317.79585	2	- 3
9 6 3	915.95488	5	- 5	999.46768	5	- 7	1129.79549	5	- 2	1186.80138	4	- 4	1317.79585	2	- 2
9 7 3	955.66199	7	- 1	1041.85751	3	- 2	1170.10853	2	- 3	1227.20578	3	- 2	1360.14720	4	3
9 7 2	955.66199	7	- 1	1041.85751	3	- 2	1170.10853	2	- 3	1227.20578	3	- 2	1360.14720	4	3
9 8 2	1001.57994	6	- 1	1090.63999	1	- 1	1216.63545	4	- 5	1273.81401	3	0	1408.97030	2	4
9 8 1	1001.57994	6	- 1	1090.63999	1	- 1	1216.63545	4	- 5	1273.81401	3	0	1408.97030	2	4
9 9 1	1053.55499	11	- 7	1145.80840	3	1	1269.37358	6	- 1	1326.61276	2	- 2	1464.24059	-	7
9 9 0	1053.55499	11	- 7	1145.80840	3	1	1269.37358	6	- 1	1326.61276	2	- 2	1464.24059	-	7
10 0 10				895.30098	2	- 1	1031.79235	5	10	1088.37527	2	- 3	1213.65027	3	0
10 1 10				895.97268	8	0	1032.43693	4	- 1	1089.00832	5	9	1214.30050	2	14

Table 7 (*continued*)

Band	ν_{10}			ν_7			ν_8			ν_4			ν_6		
J K_a K_c	E	Δ	δ	E	Δ	δ	E	Δ	δ	E	Δ	δ	E	Δ	δ
1	2	3	4	2	3	4	2	3	4	2	3	4	2	3	4
10 1 9				905.45466	4	- 1	1041.32018	2	12	1098.04751	4	4	1223.92323	4	- 2
10 2 9	834.18754	6	5	910.90877	3	- 3	1046.50613	5	1	1103.20163	5	7	1229.28402	3	14
10 2 8	836.69156	10	- 7	913.86725	3	0	1049.27004	5	6	1106.04687	4	0	1232.34233	10	0
10 3 8	850.17207	7	2	928.17532	2	- 3	1062.83212	1	- 2	1119.61086	5	- 1	1246.53662	1	1
10 3 7	850.41173	10	9	928.47230	3	- 1	1063.10902	2	1	1119.90124	4	0	1246.85319	4	1
10 4 7	871.46168	5	-14	951.02474	2	- 2	1084.47464	2	- 2	1141.32722	3	- 3	1269.33239	4	- 5
10 4 6	871.47068	8	2	951.03585	3	- 1	1084.48504	2	- 3	1141.33838	2	- 6	1269.34465	3	- 6
10 5 6	898.86054	6	- 4	980.38135	5	- 3	1112.31125	4	- 6	1169.24870	9	- 7	1298.62814	9	-10
10 5 5	898.86213	6	- 7	980.38155	6	- 4	1112.31144	5	- 4	1169.24888	7	- 4	1298.62814	9	13
10 6 5	932.41669	9	- 1	1016.11776	5	- 6	1146.39012	7	- 1	1203.41851	5	- 7	1334.46383	2	- 2
10 6 4	932.41669	9	- 4	1016.11776	5	- 7	1146.39012	7	- 1	1203.41851	5	- 7	1334.46383	2	- 2
10 7 4	972.11342	6	- 3	1058.54023	6	- 1	1186.69318	8	3	1243.81209	7	- 3	1376.80378	3	1
10 7 3	972.11342	6	- 3	1058.54023	6	- 1	1186.69318	8	3	1243.81209	7	- 3	1376.80378	3	1
10 8 3	1018.10156	6	- 3	1107.31223	2	0	1233.21300	4	- 2	1290.41281	2	- 1	1425.61869	19	2
10 8 2	1018.10156	6	- 3	1107.31223	2	0	1233.21300	4	- 2	1290.41281	2	- 1	1425.61869	19	2
10 9 2	1070.02718	5	1	1162.46899	3	3	1285.94526	2	4	1343.20140	2	4	1480.88249	4	6
10 9 1	1070.02718	5	1	1162.46899	3	3	1285.94526	2	4	1343.20140	2	4	1480.88249	4	6
10 10 1	1128.18521	4	- 3	1223.97525	4	5	1344.89328	1	1	1402.17781	2	- 3	1542.56909	-	3
10 10 0	1128.18521	4	- 3	1223.97525	4	5	1344.89328	1	1	1402.17781	2	- 3	1542.56909	-	3

Note. Δ — value of the experimental error in units of $10^{-5}\,\text{cm}^{-1}$ (Δ is missing in cases where the upper energy levels were determined from one transition), δ — difference $E^{\text{exp}} - E^{\text{calc}}$ also in units of $10^{-5}\,\text{cm}^{-1}$.

and with an error $d_{\text{rms}} = 2.1 \cdot 10^{-4}\,\text{cm}^{-1}$ for over 24000 line positions.

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Conflict of interest

The authors declare that they have no conflict of interest.

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