

# High-Resolution Fourier-Transform Intracavity Laser Absorption Spectroscopy of D<sub>2</sub>O in the Region of the $4\nu_1 + \nu_3$ Band

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The high-resolution absorption spectrum of the D<sub>2</sub>O molecule was recorded with the Fourier-transform intracavity laser absorption spectrometer in the region 12 570–12 820 cm<sup>-1</sup> where the band  $4\nu_1 + \nu_3$  is located. Transitions belonging to the  $4\nu_1 + \nu_3$  band, and the bands  $3\nu_1 + 2\nu_3$  and  $3\nu_1 + 2\nu_2 + \nu_3$ , of which the up states are strongly interacted with that of the  $4\nu_1 + \nu_3$ , were assigned in the recorded spectrum. Up state energy levels were fitted to derive effective spectroscopic parameters, which reproduce majority of the assigned transitions within the experimental accuracy. © 2002 Elsevier Science (USA)

*Key Words:* intracavity laser absorption spectroscopy, vibration–rotation spectra, D<sub>2</sub>O molecule, spectroscopic parameters.

## 1. INTRODUCTION

The high-resolution spectroscopy of water molecule and its isotopes is of theoretical and practical interests. Although the very accurate *ab initio* study can give a good prediction of the energy levels and transition intensities (1, 2), which is very helpful in the spectral assignment (3), the effective Hamiltonian (EH) analysis by fitting the energy levels obtained from the experimental transitions is still very effective to model the rovibrational interactions in the molecule. As a rule, a successful EH analysis can reproduce most of the experimental energy levels within the experimental uncertainty, and the comparison between the results of EH and *ab initio* calculations can be instructive in understanding the intramolecular dynamics. However, when the vibrational quantum number  $\nu$  increases, some difficulties arise in the EH analysis. For the water molecule, which is a light asymmetric top, many high-order interactions exist in the vibrational polyads, and they mix up so many vibration states that one can hardly include all of them in the EH analysis. And more basically, because the EH analysis is based on the fitting procedure of the experimental transitions or energy levels derived from them, more experimental data are need since the volume of the interacting states increases with  $\nu$ . But in the contrast, available experimental data are usually even less since the intensities of the transitions decrease rapidly. Thus a high-sensitivity recording of the spectrum is critical in the study of the highly excited vibrational states of water.

Among various spectroscopic methods, intracavity laser absorption spectroscopy (ICLAS) is ultrasensitive and has been widely used. The detailed description of ICLAS and references to early contributions can be found elsewhere (4). The equivalent absorption pathlength in ICLAS is

$$L_{eq} = c \cdot t_g \cdot l/L, \quad [1]$$

where  $c$  is the speed of light and  $l/L$  is the ratio of the length of the intracavity sample cell with respect to the total length of the laser cavity. We have claimed that to introduce the Fourier-transform method in the ICLAS measurement, FT-ICLAS, would promise some attractive advantages versus ordinary grating spectrometer based ICLAS (5). FT-ICLAS will be efficient and reliable, since it can provide an accurately calibrated spectrum in a wide region instead of some small pieces which should be calibrated separately. It can provide a resolution up to 10<sup>-3</sup> cm<sup>-1</sup> which can be comparable with the separation between the longititude modes in the broadband laser. And as a result of the multichannel property of the FT measurement, it can also effectively reduce the seeding noise of the multimode laser.

The present contribution, is devoted to the study of the rotational structure of the energy levels for the D<sub>2</sub>O molecule in the  $4\nu_1 + \nu_3$  region employing the FT-ICLAS technique. It is the continuation of our earlier studies of the fine rotational structures of the deuterated species of H<sub>2</sub>O in the infrared region, Refs. (6, 7) and references there in. A brief description of the experiment is given in Section 2, theoretical EH model can be found in Section 3, and the results and discussions are presented in Section 4.

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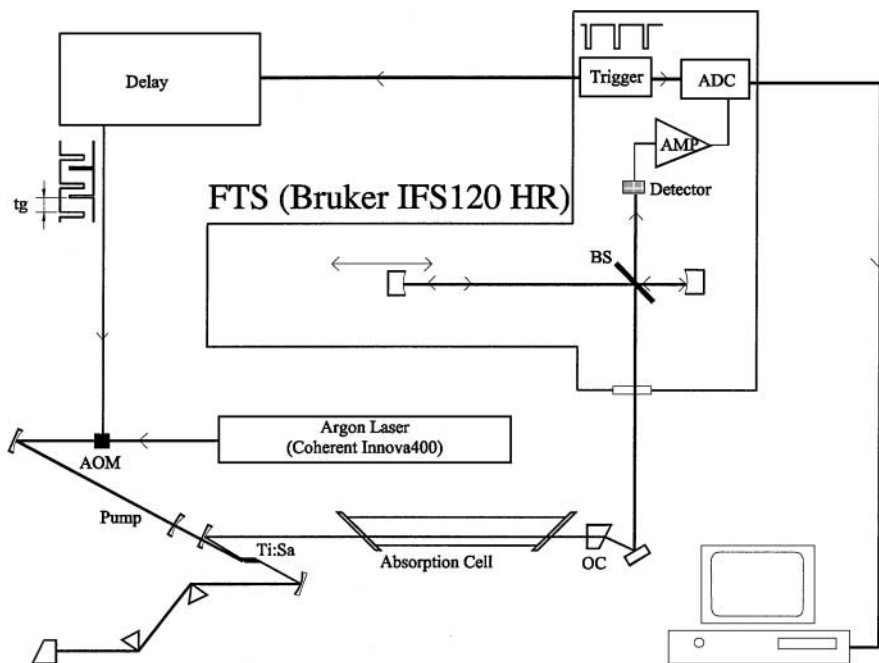


FIG. 1. Configuration of FT-ICLAS; see text or Ref. (5) for details.

## 2. EXPERIMENTAL DETAILS

The details of the FT-ICLAS setup built in Hefei can be found elsewhere (5, 8). Here we just give a brief description. Fig. 1 depicts the experimental configuration. A Bruker IFS 120HR Fourier-transform spectrometer is used to record the laser emission from a homemade 1.9-m-long standing wave Ti : Sapphire laser which is pumped by a Coherent Innova 400 Argon ion laser. A 0.8-m-long sample cell is placed inside the Ti : Sapphire laser cavity. A rectangular wave signal, generated by a function generator and synchronized with the sampling pulse of the FT interferometer, was used to drive an acoustic-optics modulator (AOM) to chop the pumping laser. The generation time,  $t_g$ , is defined as the delay of the sampling pulse of the FT interferometer with respect to the AOM chopping pulse.

The Bruker IFS 120HR interferometer was equipped with a quartz beam-splitter and a Si-diode detector. Electrical filters were applied to improve the signal noise ratio, thus the  $t_g$  value should be considered as a “effective” one and depends on the width of the emission laser pulse and also the electrical filters applied (5). The unapodized resolution  $0.05 \text{ cm}^{-1}$  ( $1/\text{MOPD}$ (Maximal Optical Path Difference)) is comparable with the Doppler width  $0.036 \text{ cm}^{-1}$  of  $\text{D}_2\text{O}$  at this region. Box-car apodization function and Mertz phase correction were used in Fourier transformation.

The spectrum was recorded at room temperature. No attempt had been carried out to exclude the atmospheric absorption by the residual air inside the Ti : Sapphire laser cavity. The sample of  $\text{D}_2\text{O}$  was purchased from PeKing Chemical Industry, Ltd. (China). The stated abundance of deuterium is 99.8%.  $\text{D}_2\text{O}$  gas

was filled in the sample cell at 9 Torr. Some lines of HDO in this region were also found in the spectrum because we did not perform a long time deuterating of the sample cell. The pulse width of the laser emission was about  $150 \mu\text{s}$  which would lead to a maximal equivalent absorption length of 19 kilometers if the Eq. 1 is evaluated.

By tuning the Ti : Sapphire laser, several spectra with different centers were obtained and the whole spectrum in the region of  $12\,570\text{--}12\,820 \text{ cm}^{-1}$  was obtained by combining all these spectra together after the baseline correction. The spectrum calibration was carried out with the  $\text{H}_2\text{O}$  lines in this region which is tabulated in the HITRAN96 database. They have also been recorded by Toth [9]. The precision of the position of the unblended lines is estimated to be better than  $0.01 \text{ cm}^{-1}$ . The accuracy was also confirmed by the combination differences analysis (see in Section 4) where the typical deviation is  $0.004 \text{ cm}^{-1}$ . For illustration, Fig. 2 shows two small parts of the spectrum.

## 3. HAMILTONIAN MODEL AND INITIAL APPROXIMATION FOR THE PARAMETERS

The  $4\nu_1 + \nu_3$  band of the  $\text{D}_2\text{O}$  molecule, being a part of the so-called  $\nu = 5$  ( $\nu = \nu_1 + \nu_2/2 + \nu_3$ ) polyad, suffers strong resonance perturbations from other vibrational states in this polyad. On this reason we used the following Hamiltonian model in the analysis,

$$H^{eff} = \sum_{\nu\nu'} |v\rangle \langle v'| H^{\nu\nu'}, \quad [2]$$

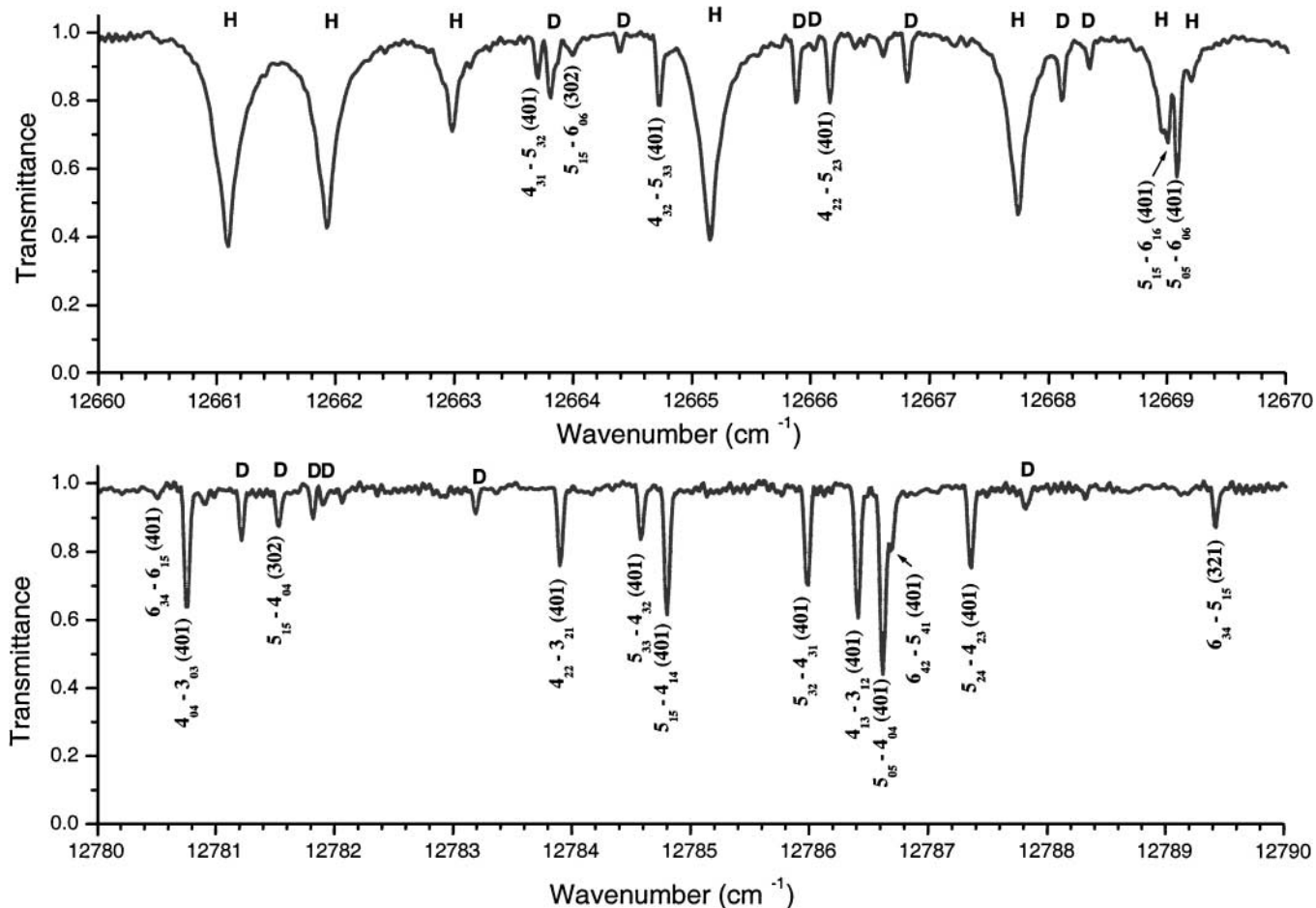


FIG. 2. FT-ICLAS spectrum of D<sub>2</sub>O in the region 12660–12670 and 12780–12790 cm<sup>-1</sup>. Assignments of D<sub>2</sub>O are given; lines marked by “D” and “H” belong to HDO and H<sub>2</sub>O, respectively. See text for experimental details.

where the diagonal operators  $H^{vv}$  are the usual Watson’s rotational operators (10),

$$\begin{aligned}
 H^{vv} = & E^v + \left[ A^v - \frac{1}{2}(B^v + C^v) \right] J_z^2 + \frac{1}{2}(B^v + C^v) J^2 \\
 & + \frac{1}{2}(B^v - C^v) J_{xy}^2 - \Delta_K^v J_z^4 - \Delta_{JK}^v J_z^2 J^2 - \Delta_J^v J^4 \\
 & - \delta_K^v [J_z^2, J_{xy}^2]_+ - 2\delta_J^v J^2 J_{xy}^2 + H_K^v J_z^6 + H_{KJ}^v J_z^4 J^2 \\
 & + H_{JK}^v J_z^2 J^4 + H_J^v J^6 + [J_{xy}^2, h_K^v J_z^4 + h_{JK}^v J^2 J_z^2 \\
 & + h_J^v J^4]_+ + L_K^v J_z^8 + L_{KKJ}^v J_z^6 J^2 + L_{KJ}^v J_z^4 J^4 \\
 & + L_{KJJ}^v J_z^2 J^6 + L_J^v J^8 + [J_{xy}^2, l_K^v J_z^6 + l_{KJ}^v J^4 J_z^2 \\
 & + l_J^v J^2 J^4 + l_J^v J^6]_+ + P_K^v J_z^{10} + \dots \quad [3]
 \end{aligned}$$

Operators  $H^{vv'}$  ( $v \neq v'$ ) describe resonance interactions. Since D<sub>2</sub>O is an asymmetric top molecule, the symmetry of which is isomorphic to the C<sub>2v</sub> symmetry group, its vibrational wave functions ( $\nu_1 \nu_2 \nu_3$ ) with even values of quantum number  $\nu_3$  have the symmetry A<sub>1</sub>, and others have the symmetry B<sub>2</sub>. As the

consequence, two types of resonance operators  $H^{vv'}$  ( $v \neq v'$ ) may be presented in the Hamiltonian (2):

(a) Fermi type resonance interactions which connect vibrational states of the same symmetry are described by the operators  $H_F^{vv'}$ ,

$$\begin{aligned}
 H_F^{vv'} = & F_0^{vv'} + F_K^{vv'} J_z^2 + F_J^{vv'} J^2 + \dots + F_{xy}^{vv'} J_{xy}^2 \\
 & + F_{xyK}^{vv'} [J_{xy}^2, J_z^2]_+ + F_{xyJ}^{vv'} J_{xy}^2 J^2 \\
 & + F_{xyJK}^{vv'} J^2 [J_{xy}^2, J_z^2]_+ + F_{xyJJ}^{vv'} J_{xy}^2 J^4 + \dots; \quad [4]
 \end{aligned}$$

(b) Coriolis type interactions which connect states of different symmetries are described by the operators  $H_C^{vv'}$ ,

$$\begin{aligned}
 H_C^{vv'} = & C_y^{vv'} iJ_y + C_{yK}^{vv'} [iJ_y, J_z^2]_+ + C_{yJK}^{vv'} [iJ_y, J_z^2]_+ J^2 \\
 & + \dots + C_{xz}^{vv'} [J_x, J_z]_+ + C_{xzK}^{vv'} [[J_x, J_z]_+, J_z^2]_+ \\
 & + C_{xzJ}^{vv'} [J_x, J_z]_+ J^2 + C_{xzJK}^{vv'} J^2 [[J_x, J_z]_+, J_z^2]_+ \\
 & + \dots + C_{yxy}^{vv'} [iJ_y, J_{xy}]_+ + \dots \quad [5]
 \end{aligned}$$

TABLE 1  
Band Centers of D<sub>2</sub>O

$\nu_1\nu_2\nu_3$	band center <sup>a</sup>	ref	$\nu_1\nu_2\nu_3$	band center <sup>a</sup>	ref
0 1 0	1178.38	[11]	2 2 0	7593.12	[16]
0 2 0	2336.84	[12]	1 2 1	7672.92	[16]
1 0 0	2671.65	[12]	0 2 2	7825.37	[16]
0 0 1	2787.72	[12]	3 0 0	7852.93	[16]
0 3 0	3474.32	[13]	2 0 1	7899.82	[16]
1 1 0	3841.42	[13]	1 0 2	8054.06	[16]
0 1 1	3956.01	[13]	0 0 3	8220.18	[16]
1 2 0	4990.83	[14]	1 3 1	8788.60	[17]
0 2 1	5105.38	[14]	0 3 2	8934.60	[17]
2 0 0	5291.72	[14]	3 1 0	9005.35	[17]
1 0 1	5373.90	[14]	2 1 1	9050.36	[17]
0 0 2	5529.44	[14]	1 1 2	9201.90	[17]
1 3 0	6119.04	[15]	3 0 1	10358.56	[7]
0 3 1	6235.08	[15]			
2 1 0	6452.98	[15]			
1 1 1	6533.24	[15]			
0 1 2	6687.00	[15]			

<sup>a</sup> In units of cm<sup>-1</sup>.

In Eqs. [3]–[5] the following notations are used:  $J_{xy}^2 = J_x^2 - J_y^2$ , and  $J^2 = \sum_{\alpha} J_{\alpha}^2$ .

It should be mentioned that, although the  $v = 5$  polyad consists of 21 vibrational states; (500), (401), (302), (203), (104),

(005), (420), (321), (222), (123), (024), (340), (241), (142), (043), (260), (161), (062), (180), (081), and (0100), practically only the  $4\nu_1 + \nu_3$  band appears in the experimental spectrum. For this reason two questions arise under the present study:

(1) How to correctly estimate the initial values of the parameters of the Hamiltonian [2]–[5]?

(2) How many interacting states should be taken into account in that Hamiltonian?

Both of these problems can be solved in the same way as in our previous contribution (7). Namely, to estimate the initial values of the vibrational energies of the  $v = 5$  polyad, we first fitted the vibrational energies of the lower polyads of the D<sub>2</sub>O molecule. In this case, the band centers listed in Table 1 were applied in the fit to derive the harmonic frequencies, anharmonic parameters, and pure vibrational resonance interaction coefficients. Then these parameters were used to estimate the band centers of the  $v = 5$  polyad. These estimated band centers, which are also presented in Table 2, would be taken as the initial values used in the fit of the rovibrational energies derived from the experimental data.

The rotational parameters  $A^v$ ,  $B^v$ , and  $C^v$  of the  $(\nu_1 0 \nu_3)$  and  $(\nu_1 2 \nu_3)$  vibrational states were estimated by the simple

TABLE 2  
Spectroscopic Parameters of the (401), (302), (321), (420), (142), and (043) Vibrational States of the D<sub>2</sub>O Molecule (in cm<sup>-1</sup>)<sup>a</sup>

Parameter	(401)	(302)	(321)	(420)	(142)	(043)
$E$	12742.498(98)	12737.644(22)	12615.334(43)	12608.96	12504.99	12678.22
$A$	14.0331(113)	13.7533(246)	16.84322(606)	17.183	22.535	21.510
$B$	6.915523(782)	6.87907(648)	7.095	7.030	7.371	7.436
$C$	4.51989(161)	4.56426(103)	4.487	4.474	4.461	4.474
$\Delta_K \times 10^3$	5.514(312)	9.25347	21.986	21.986	67.1	67.1
$\Delta_{JK} \times 10^3$	-1.52324	-1.52324	-2.368	-2.368	-4.033	-4.033
$\Delta_J \times 10^3$	0.309983	0.309983	0.3682	0.3682	0.421	0.421
$\delta_K \times 10^3$	0.34708	0.34708	1.3004	1.3004	3.18	3.18
$\delta_J \times 10^3$	0.123109	0.123109	0.1531	0.1531	0.183	0.183
$H_K \times 10^5$	1.8449	1.8449	8.80	8.80	44.7	44.7
$H_{KJ} \times 10^5$	-0.2457	-0.2457	-0.629	-0.629	-3.64	-3.64
$H_{JK} \times 10^5$	-0.02149	-0.02149	-	-	0.276	0.276
$H_J \times 10^5$	0.006513	0.006513	0.0106	0.0106	0.015	0.015
$h_K \times 10^5$	0.3790	0.3790	1.073	1.073	6.11	6.11
$h_{JK} \times 10^5$	-0.00528	-0.00528	-	-	0.00508	0.00508
$h_J \times 10^5$	0.003226	0.003226	0.00518	0.00518	0.00735	0.00735
$L_K \times 10^7$	-0.5964	-0.5964	-3.01	-3.01	-	-
$L_{KKJ} \times 10^7$	0.151	0.151	-	-	-	-
$L_{KJ} \times 10^7$	0.0384	0.0384	-	-	-	-
$L_{KJJ} \times 10^7$	0.00054	0.00054	-	-	-	-
$L_J \times 10^7$	-0.000168	-0.000168	-	-	-	-
$l_K \times 10^7$	-0.173	-0.173	-	-	-	-
$l_J \times 10^7$	-0.0000836	-0.0000836	-	-	-	-
$P_K \times 10^9$	0.1516	0.1516	-	-	-	-

<sup>a</sup> Values in parentheses are thye  $1\sigma$  statistical confidence intervals. Parameters presented without confidence intervals were fixed and not fitted (see text, for details).

formula

$$P^{v_1 v_2 v_3} = P^{0v_2 0} + v_1(P^{100} - P^{000}) + v_3(P^{001} - P^{000}), \quad [6]$$

where  $P$  denotes any of the parameters  $A^v$ ,  $B^v$ , or  $C^v$ ; the values of the parameters of the (000), (100), (001), and (020) vibrational states were taken from Refs. (11) and (12). As further analysis had shown, the states (043) and (142) should be taken into account in the Hamiltonian as well. The initial values of the rotational parameters of these two states were roughly estimated on the basis of interpolation of corresponding parameters of the (000), (010), (020), and (030) vibrational states and following corrections in accordance with Eq. [6].

All the values of the centrifugal distortion coefficients of the ( $v_1 0 v_3$ ) and ( $v_1 2 v_3$ ) vibrational states were taken to be equal to the values of corresponding coefficients of the (000) and (020) states in Ref. (12), respectively. As to the values of centrifugal distortion coefficients of the (043) and (142) states, they were estimated from the interpolation of corresponding coefficients of the (000), (010), and (020) vibrational states. All the initial values of Coriolis-type parameters were set to zero.

#### 4. ANALYSIS AND DISCUSSION

The observed transitions were assigned using the ground state combination differences method, and the ground state rotational energies were calculated on the basis of the parameters from

(12). As a result of the analysis, we assigned 183 transitions with  $J^{max.} = 12$  and  $K_a^{max.} = 5$  to the  $4\nu_1 + \nu_3$  band. A list of the experimental energy levels of this vibrational state is presented in Table 4. Since the (401) state is strongly perturbed by other states of the  $v = 5$  polyad, 10 and 4 transitions were assigned to the  $3\nu_1 + 2\nu_3$  and  $3\nu_1 + 2\nu_2 + \nu_3$  bands, respectively. They are also presented in Table 5.

Because the total number of the vibrational states of the  $v = 5$  polyad (namely, 21) is considerably larger than the number of bands appeared in the spectrum, only those vibrational states which have direct influence on the ‘‘appeared’’ rovibrational levels were taken into account in Hamiltonian [3]. As the analysis has shown, six vibrational states should be considered in the present study: (401), (302), (321), (420), (142), and (043). However, the last three bands do not appear in the spectrum but accidentally perturb individual rovibrational transitions belonging to the first three bands.

The parameters obtained from the fit are presented in Tables 2 and 3 together with their  $1\sigma$  statistical confidence intervals. Those parameters presented in Table 2 without confidence intervals were fixed to their values estimated by the way discussed above. To illustrate the ability of derived parameters to reproduce the initial experimental data, the difference between the experimental data and the calculated values, which are derived from the parameters listed in Tables 2 and 3, are presented in Table 4 and also in Table 5. One can see that majority of the experimental energies/transitions were reproduced within the experimental uncertainties.

TABLE 3  
Parameters of Resonance Interactions between Some States of the  $\nu = 5$  Polyad of D<sub>2</sub>O<sup>a</sup>

Parameter	Value	Parameter	Value	Parameter	Value
Fermi Type Interactions					
$F_0^{401321}$	2.381(569)	$F_K^{401321}$	-0.4684(184)		
$F_{xy}^{401321} \times 10$	0.3994(583)	$F_{xyJ}^{401321} \times 10^3$	-1.439(146)	$F_{xyJJ}^{401321} \times 10^5$	0.4304(588)
$F_0^{401043}$	5.630(741)	$F_K^{401043}$	-0.6044(770)	$F_J^{401043}$	-0.04525(358)
Coriolis Type Interactions					
$C_y^{302401}$	0.37310(381)	$C_{yK}^{302401} \times 10^2$	-1.4915(758)	$C_{yJK}^{302401} \times 10^2$	-0.01618(102)
$C_{xz}^{302401}$	-0.24045(781)	$C_{xxJK}^{302401} \times 10^4$	-0.5808(195)		
$C_{xz}^{420401}$	0.1899(109)	$C_{xxK}^{420401} \times 10^2$	-0.2687(210)	$C_{xxJ}^{420401} \times 10^2$	-0.1445(151)
$C_{yxy}^{142401} \times 10^2$	0.18983(780)				

<sup>a</sup> Values in parentheses are the  $1\sigma$  statistical confidence intervals.

TABLE 4  
Obtained Experimental Rovibrational Term Values for the (401) Vibrational State of the D<sub>2</sub>O Molecule (in cm<sup>-1</sup>)<sup>a</sup>

<i>J</i>	<i>K<sub>a</sub></i>	<i>K<sub>c</sub></i>	<i>E</i>	Δ	δ	<i>J</i>	<i>K<sub>a</sub></i>	<i>K<sub>c</sub></i>	<i>E</i>	Δ	δ	<i>J</i>	<i>K<sub>a</sub></i>	<i>K<sub>c</sub></i>	<i>E</i>	Δ	δ
1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	3	4
0	0	0	12743.018		-13	4	3	2	12932.248	1	0	6	3	3	13064.897	5	14
1	0	1	12754.250	2	4	4	3	1	12932.715	7	1	6	4	3	13117.479	5	0
1	1	1	12761.507	4	4	4	4	1	12989.195	25	7	6	4	2	13117.808	4	-1
1	1	0	12763.902	3	1	4	4	0	12989.195	25	-1	6	5	2	13190.410	4	4
2	0	2	12777.612	4	-16	5	0	5	12901.598	7	15	6	5	1	13190.410	4	-5
2	1	2	12781.920	6	1	5	1	5	12902.109	3	-4	7	0	7	13028.938	5	4
2	1	1	12789.071	8	-3	5	1	4	12934.954	8	2	7	1	7	13029.052		7
2	2	1	12810.266	2	4	5	2	4	12945.460	6	-9	7	1	6	13084.879	1	0
2	2	0	12810.783		5	5	2	3	12958.425	9	-1	7	2	6	13087.829		7
3	0	3	12809.693	9	-10	5	3	3	12990.459	3	0	7	2	5	13120.410	7	-1
3	1	3	12812.307	3	-4	5	3	2	12992.253	5	6	7	3	5	13140.878	6	-6
3	1	2	12826.431	4	4	5	4	2	13047.396	2	2	7	3	4	13151.075	6	2
3	2	2	12844.461	3	-4	5	4	1	13047.465	3	2	7	4	4	13199.445	3	1
3	2	1	12846.887	3	-6	5	5	1	13120.445	3	0	7	4	3	13200.565	3	-4
3	3	1	12886.120	2	-3	5	5	0	13120.445	3	-1	8	0	8	13106.105	4	-5
3	3	0	12886.189	3	3	6	0	6	12960.884	8	2	8	1	8	13106.233	3	-3
4	0	4	12851.202		13	6	1	6	12961.264	4	-9	9	0	9	13192.444	5	4
4	1	4	12852.452	4	-4	6	1	5	13003.939	1	-1	9	1	9	13192.301	8	5
4	1	3	12875.374	4	-5	6	2	5	13011.630	3	1	10	0	10	13287.390		-8
4	2	3	12889.635	9	-2	6	2	4	13034.412	1	2	11	0	11	13391.570	5	8
4	2	2	12896.148	4	8	6	3	4	13060.078	8	-2	12	0	10	13504.655	2	-2

<sup>a</sup> Δ is the experimental uncertainty of the energy value, equal to one standard deviation in units of 10<sup>-3</sup> cm<sup>-1</sup>; δ is the difference  $E^{exp.} - E^{calc.}$ , also in units of 10<sup>-3</sup> cm<sup>-1</sup>; Δ is not quoted when the energy value was obtained from only one transition.

TABLE 5  
The Rovibrational Transitions Assigned to the 3ν<sub>1</sub> + 2ν<sub>3</sub> and 3ν<sub>1</sub> + 2ν<sub>2</sub> + ν<sub>3</sub> Bands of D<sub>2</sub>O

Upper state			Lower state			Band	Line position, exp., in cm <sup>-1</sup>	Line position, calc., in cm <sup>-1</sup>	δ <sup>a)</sup> in 10 <sup>-3</sup> cm <sup>-1</sup>
<i>J'</i>	<i>K'<sub>a</sub></i>	<i>K'<sub>c</sub></i>	<i>J</i>	<i>K<sub>a</sub></i>	<i>K<sub>c</sub></i>				
1	2	3	4	5	6				
6	3	4	6	3	3	321	12614.211	12614.209	2
6	3	4	7	1	7	321	12653.888	12653.888	0
5	1	5	6	0	6	302	12663.991	12663.998	-7
4	1	4	5	0	5	302	12677.752	12677.751	1
3	1	3	4	0	4	302	12691.496	12691.485	11
2	1	2	3	0	3	302	12705.251	12705.245	6
1	1	1	2	0	2	302	12720.276	12720.285	-9
1	1	1	0	0	0	302	12756.163	12756.163	0
2	1	2	1	0	1	302	12763.570	12763.575	-5
3	1	3	2	0	2	302	12770.601	12770.593	8
5	1	5	4	0	4	302	12781.525	12781.533	-8
6	3	4	5	1	5	321	12789.416	12789.412	4
7	1	7	6	0	6	302	12791.133	12791.131	2
6	4	2	5	2	3	321	12802.737	12802.740	-3

<sup>a</sup> The δ is the difference between experimental and calculated values of line position.

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