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HIGH-RESOLUTION ANALYSIS OF THE $\nu_2+2\nu_3$ BAND OF HDO*

Hu Shui-ming(胡水明), He Sheng-gui(何圣贵), Zheng Jing-jing(郑晶晶),
Wang Xiang-huai(王湘淮), Ding Yun(丁　昀), and Zhu Qing-shi(朱清时)
Open Research Laboratory of Bond-Selective Chemistry, University of Science and Technology of China, Hefei 230026, *China*

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The Fourier transform spectrum of the $\nu_2 + 2\nu_3$ band of the HDO molecule was recorded with a resolution of 0.02 cm^{-1}. The spectrum was rotational analysed and the spectroscopic parameters of the (0,1,2) state were estimated in terms of Watson's effective rotational Hamiltonian model and also the model in the Padé–Borel approximation form. They reproduce the upper energy levels with an accuracy close to the experimental uncertainty of 0.001 cm^{-1}.

Keywords: ro-vibrational spectrum, Fourier transform spectroscopy, HDO molecule
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I. INTRODUCTION

The HDO molecule has been found to have a local mode nature of stretching vibrational states; for instance, the sequence of the $(V_1, 0, 0)^{\dagger}$ and $(0, 0, V_3)$ states were found to be approximately well isolated if some local resonances were neglected in some cases.[1−4] This is the reason why such states could be suitable intermediate states utilized in the bond-selective chemical reactions with the help of lasers.[5] In contrast with the H_2O or D_2O molecules, no definite polyad structure has been evidenced in HDO while dramatic high-order interactions seem to dominate the ro-vibrational energy structure of the molecule. Some states with a large difference of vibrational quantum numbers exhibit strong resonances among them, which can be hardly found in other small molecules.[6−8]

Although the highly accurate *ab initio* study can give a prediction of the energy levels with a good precision,[9,10] the effective Hamitonian (EH) analysis, by fitting the energy levels obtained from the experimental transitions, has been proven to be still very effective to model the ro-vibrational interactions in the molecule. A successful EH analysis can reproduce most of the experimental energy levels at a precision close to the experimental accuracy, and the comparison between the results of EH and those of *ab initio* method can give a better comprehension of the intramolecular dynamics.

The work presented here is part of our systematic high-resolution study of the absorption spectra of D_2O and HDO in the infrared region (see Refs.[6,11–13] and references therein). The sequence of the $\nu_2 + n\nu_3$ band of HDO, which has an additional bending vibrational quantum number compared to the corresponding strongest $n\nu_3$ band, is still much stronger than other adjacent bands. But in contrast with the well-isolated property of the $(0,0,V_3)$ states, it has been found that the $(0, 1, V_3)$ states suffer strong local resonances with other states. Toth[14] reported that the $(0, 1, 1)$ state had a strong resonance with the $(2, 0, 0)$ state, thus the intensity of the $2\nu_1$ band increased significantly. Campargue's group[8] studied some bands of HDO in the near infrared and visible range utilizing the intra-cavity laser absorption spectroscopy (ICLAS). They found strong local resonance between the "bright" $(0, 1, 4)$ state and the "dark" $(1, 4, 2)$ and $(0, 12, 0)$ states, and some sub-levels of the $(0, 1, 5)$ are evidently perturbed by nearby levels of other vibrational states. We also found strong local resonance in some sub-levels of the $(0, 1, 3)$ state.[15] The $\nu_2 + 2\nu_3$ band was first studied by Bykov *et al.*[16] with the ICLAS technique, but the accuracy of the line positions of 0.04 cm^{-1} was rather low. We restudied this band with a Fourier transform spectrometer at a much better resolution. Our analysis also indicates the misassignments in Ref.[16]. In this paper, we will present the EH analysis of this band and the comparison with the *ab initio* results.

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† (V_1, V_2, V_3) denotes the vibrational states of HDO where V_1, V_2 and V_3 represent the vibrational quantum numbers for the OD stretching, the bending, and the OH stretching, respectively.

II. EXPERIMENTAL DETAILS

The sample of $D_2^{16}O$ was purchased from Peking Chemical Industry, Ltd (China). The stated purity of the deuterium was 99.8%. The spectra were recorded at room temperature with the Bruker IFS 120HR Fourier transform interferometer (Hefei, China), which is equipped with a path length adjustable multi-pass gas cell, a tungsten source, a CaF_2 beam splitter, and a Ge diode detector. The unapodized resolution was 0.02 cm^{-1}, and the apodization function was Blackman–Harris 3-Term.

Since in the region under study there are many lines due to the H_2O and D_2O absorptions, two spectra were measured with different ratios of HDO to D_2O and H_2O. The first spectrum was recorded at a total pressure of 1000 Pa with the percentage of HDO being approximately 50% and the path length being 105 m. The corresponding conditions of the second spectrum were 1500 Pa, 15% and 69 m, respectively. The line positions were calibrated with the H_2O absorptions in this region from the GEISA97 database. The accuracy of the unblended line positions was estimated to be 0.001 cm^{-1}. For illustration, two small pieces of the recorded spectra are presented in Fig.1.

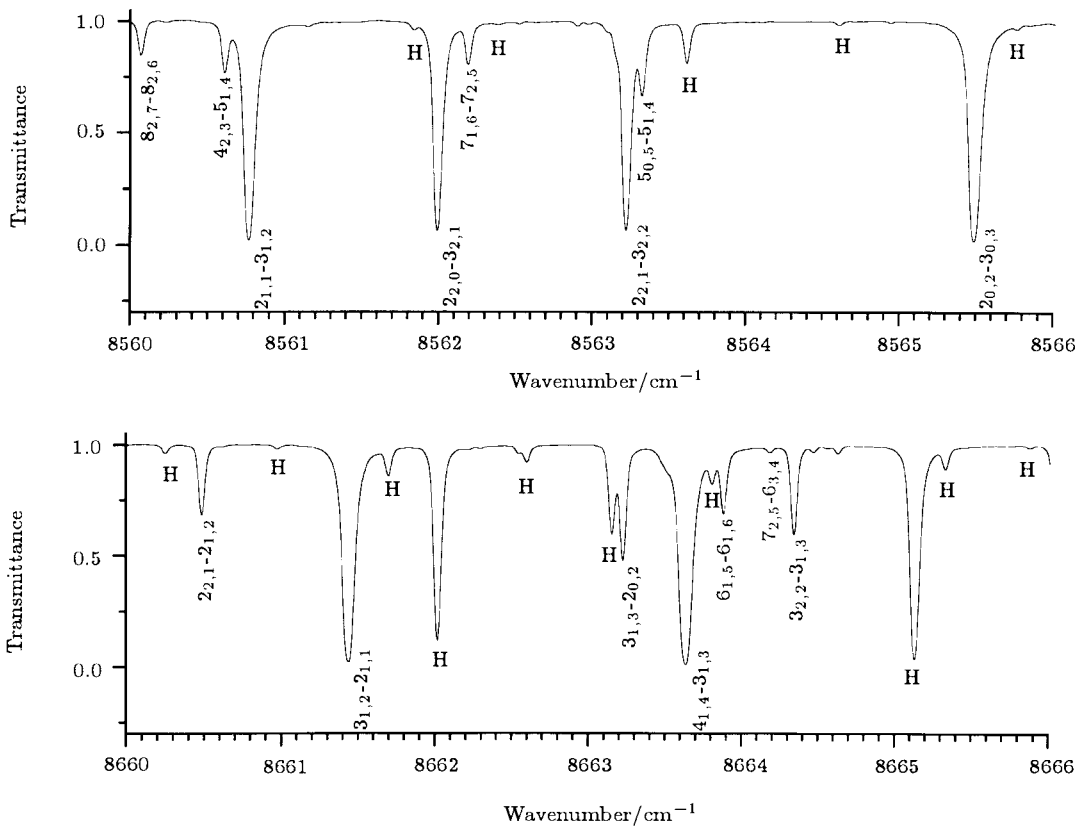


Fig.1. Part of the spectrum: transitions in the regions 8560–8566 cm^{-1} and 8660–8666 cm^{-1}. Assignments of HDO are given; lines marked by "H" belong to H_2O. See text for experimental details.

III. SPECTRUM ANALYSIS

A. Assignment of transitions

Since HDO is a prolate asymmetric top molecule and its symmetry group is isomorphic C_i type symmetry, any of its vibrational–rotational bands contains absorption lines arising from transitions of two types (both 'A' and 'B'). The recorded 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 Ref.[17]. As a result of the analysis, we assigned 750 transitions with $J^{max} = 16$ and $K_a^{max} = 8$ to the $\nu_2 + 2\nu_3$ band. The number of 'A' and 'B' type transitions are 436 and 314, respectively. The relative intensity of the two type transitions is about 3.0:1.

With these transitions assigned, 149 rotational energy levels of the $(0, 1, 2)$ state were obtained. They are listed with the experimental uncertainties in Ta-

ble 1. It can be found that for most of the energy levels obtained from more than three transitions from different ground-state levels, the experimental uncertainties are less than $0.001\,cm^{-1}$, on average $0.0007\,cm^{-1}$. It indicates the fine accuracy of the experimental line positions and the excellent quality of the spectrum compared with the result in Ref.[16].

Table 1. The rotational energy levels of the HDO (0,1,2) state.

J	K_a	K_c	Obs/cm^{-1}	$\Delta^{(a)}$	$\delta^{(b)}$	$n^{(c)}$	J	K_a	K_c	Obs/cm^{-1}	$\Delta^{(a)}$	$\delta^{(b)}$	$n^{(c)}$
0	0	0	8611.1020	4	7	2	9	0	9	9228.1784	9	6	6
1	0	1	8626.4927	–10	10	5	9	1	9	9228.4054	–1	0	4
1	1	1	8640.3602	–4	6	4	9	1	8	9338.5104	6	2	4
1	1	0	8643.4113	–3	1	4	9	2	8	9343.7269	–6	3	7
2	0	2	8656.8187	–7	2	6	9	2	7	9412.4010	0	5	7
2	1	2	8668.0859	7	4	8	9	3	7	9445.4755	11	2	8
2	1	1	8677.2297	–5	1	7	9	3	6	9469.9212	10	3	7
2	2	1	8718.6094	14	2	7	9	4	6	9552.6052	20	5	6
2	2	0	8719.0576	18	1	5	9	4	5	9556.0264	6	1	6
3	0	3	8701.2265	–12	2	8	9	5	5	9681.6655	15	1	6
3	1	3	8709.3976	–5	1	9	9	5	4	9681.8648	–4	8	7
3	1	2	8727.6226	–3	1	6	9	6	4	9837.3785		20	2
3	2	2	8764.7310	11	3	9	9	6	3	9837.3740		35	3
3	2	1	8766.9039	9	2	10	9	7	3	10018.7274	8	7	4
3	3	1	8840.8473	8	5	5	9	7	2	10018.7275	8	6	4
3	3	0	8840.8885	5	4	7	9	8	2	10224.0627	–1		1
4	0	4	8758.7233	–4	2	8	9	8	1	10224.0627	–1		1
4	1	4	8764.0270	–3	3	10	10	0	10	9358.3473	–6	2	4
4	1	3	8794.1328	–1	1	6	10	1	10	9358.4578	–15	3	6
4	2	3	8825.8430	10	2	9	10	1	9	9484.0968	–7	2	6
4	2	2	8831.9779	1	2	10	10	2	9	9487.0912	–6	8	6
4	3	2	8903.0382	–0	3	10	10	2	8	9573.9222	–25	7	7
4	3	1	8903.3232	–9	6	8	10	3	8	9598.2053	–286*	5	10
4	4	1	9007.1230	–8	4	4	10	3	7	9636.0334	6	2	4
4	4	0	9007.1264	–6	11	5	10	4	7	9708.6954	58*	2	6
5	0	5	8828.5566	–5	4	6	10	4	6	9715.9772	7	3	4
5	1	5	8831.6909	7	10	7	10	5	6	9837.3116	–12	4	6
5	1	4	8876.0704	–1	3	9	10	5	5	9837.8851	–43*	7	2
5	2	4	8901.6275	2	4	8	10	6	5	9991.9684	–21	12	2
5	2	3	8914.6526	1	2	10	10	7	4	10172.4593		28	3
5	3	3	8980.8838	–7	3	8	10	7	3	10172.4593		26	4
5	3	2	8981.9930	–7	2	8	11	0	11	9500.6711	–0	15	3
5	4	2	9084.7292	–16	7	4	11	1	11	9500.7193	–57*	18	3
5	4	1	9084.7585	–5	4	6	11	1	10	9641.3408	2	2	6
5	5	1	9216.3015	18	10	4	11	2	10	9642.9955	0	2	6
5	5	0	9216.3021	22	1	5	11	2	9	9747.9899	–50*	11	6
6	0	6	8910.4085	0	1	5	11	3	9	9764.7446	–112*	5	6
6	1	6	8912.1340	1	2	6	11	3	8	9818.6178	–4	6	5
6	1	5	8972.4951	6	2	9	11	4	8	9880.0154	142*	0	4
6	2	5	8991.7122	1	1	8	11	4	7	9893.7946	–2	9	3

Table 1. (*Continued*)

J	K_a	K_c	Obs/cm^{-1}	$\Delta^{(a)}$	$\delta^{(b)}$	$n^{(c)}$	J	K_a	K_c	Obs/cm^{-1}	$\Delta^{(a)}$	$\delta^{(b)}$	$n^{(c)}$
6	2	4	9014.7582	4	2	10	11	5	7	10008.7245	256*	2	3
6	3	4	9074.2987	−15	3	11	11	5	6	10010.1471	−14	5	5
6	3	3	9077.4588	−12	3	8	11	6	6	10162.1650	−8	30	6
6	4	3	9178.0556	−14	2	8	11	6	5	10162.2468	18	30	5
6	4	2	9178.1934	−19	7	6	12	0	12	9655.1361	10	16	2
6	5	2	9309.1455	11	5	6	12	1	12	9655.1606	−4	3	3
6	5	1	9309.1482	14	12	5	12	1	11	9810.3647	20	6	7
6	6	1	9466.9364	−27	17	4	12	2	11	9811.2539	8	0	4
6	6	0	9466.9380	−11	5	4	12	2	10	9933.7027	−127*	6	2
7	0	7	9004.2525	2	2	6	12	3	10	9944.5849	−57*	0	2
7	1	7	9005.1580	5	3	8	12	3	9	10016.5440	−1	15	3
7	1	6	9082.3089	9	2	9	12	4	9	10066.1802	290*	1	2
7	2	6	9095.6903	2	7	9	12	5	8	10195.7328	4	20	3
7	2	5	9131.6940	7	3	9	13	0	13	9821.7166	−5	20	2
7	3	5	9183.0869	−14	2	9	13	1	13	9821.7284	−11	20	2
7	3	4	9190.3695	−1	6	5	13	1	12	9991.2692		25	3
7	4	4	9287.1561	−5	4	10	13	2	12	9991.7312	−13	22	3
7	4	3	9287.6467	−7	5	7	13	3	11	10137.3342	−2	18	2
7	5	3	9417.6182	18	3	7	13	4	9	10303.2292			1
7	5	2	9417.6307	1	13	9	14	0	14	10000.3884	8	30	2
7	6	2	9574.8892	−5	7	6	14	1	14	10000.3944	8	2	3
7	6	1	9574.8894	−5	5	5	14	1	13	10184.1156	207*	2	4
7	7	1	9757.5134	9	8	6	14	2	13	10184.3510		27	3
7	7	0	9757.5134	9	8	4	14	2	12	10338.6593		15	3
8	0	8	9110.1562	7	1	5	14	3	11	10453.3339	3		1
8	1	8	9110.6154	4	3	5	15	0	15	10191.1124	−3	26	2
8	1	7	9204.5172	−2	11	9	15	1	15	10191.1153	−2	18	2
8	2	7	9213.1537	−1	1	9	16	0	16	10393.8352			1
8	2	6	9264.5939	4	7	10	16	1	16	10393.8410			1
8	3	6	9306.9430	−6	6	9	16	1	15	10605.6074	0		1
8	3	5	9321.1895	1	3	7							
8	4	5	9412.0318	1	4	9							
8	4	4	9413.4374	−0	3	8							
8	5	4	9541.7745	11	5	7							
8	5	3	9541.8339	9	3	9							
8	6	3	9698.3588	−10	7	4							
8	6	2	9698.3585	5	12	4							
8	7	2	9880.4148	−6	15	5							
8	7	1	9880.4148	−6	15	5							

(a) $\Delta = E_{\rm obs} - E_{\rm cal}$, in 10^{-4}cm^{-1}, differences between observed and calculated energy. Calculations are carried out with the parameters listed in column 2 of Table 2. Left blank if the level is not included in the fitting because of large experimental uncertainties.

(b) 1σ error of the observed energy, as blank when only one transition to this level has been found.

(c) Number of transitions used in deriving the up-level.

∗ Level not included in the fitting. See the text for details.

B. Effective Hamiltonian model and fitting of the energy levels

As in our earlier analysis of the asymmetric top molecules, the Watson 'A' type Hamiltonian[18] was used to fit the experimental energy levels:

$$\begin{aligned} H =&E_v + (A - \frac{B+C}{2})J_z^2 + \frac{B+C}{2}J^2 + \frac{B-C}{2}J_{xy}^2 \\ &- \Delta_k J_z^4 - \Delta_{jk} J_z^2 J^2 - \Delta_j J^4 \\ &- \delta_k\{J_z^2, J_{xy}^2\} - 2\delta_j J_{xy}^2 J^2 \\ &+ H_k J_z^2 + H_{kj} J_z^4 J^2 + H_{jk} J_z^2 J^4 + H_j J^6 \\ &+ h_k\{J_z^4, J_{xy}^2\} + h_{jk}\{J_z^2, J_{xy}^2\}J^2 + 2h_j J_{xy}^2 J^4 \\ &+ L_k J_z^8 + L_{kkj} J_z^6 J^2 + \ldots + P_k J_z^{10} + \ldots \end{aligned} \quad (1)$$

where $J_{xy}^2 = J_x^2 - J_y^2$, $J^2 = \sum_\alpha J_\alpha^2$, and $\{A, B\} = AB + BA$.

Because HDO is a very light tri-atomic molecule, to take into account the bending–rotation coupling of such molecules, Polyansky proposed another effective rotational Hamiltonian under the Padé–Borel (P–B) approximations.[19] The matrix elements of this effective rotational Hamiltonian can be calculated in the common $|jk\rangle$ basis of symmetric top with the formulae

$$\begin{aligned} \langle jk|W_V|jk\rangle =&E_V + \int_0^\infty \mathrm{d}t e^{-t}\frac{c_0c_1 + (c_1^2 - c_0c_2)t}{c_1 - c_2t}, \\ \langle jk|W_V|jk\pm 2\rangle =&\langle jk|J_{xy}^2|jk\pm 2\rangle \\ &\times \int_0^\infty \mathrm{d}t e^{-t}\frac{b_0b_1 + (b_1^2 - b_0b_2)t}{b_1 - b_2t}, \end{aligned} \quad (2)$$

where E_V is the vibrational energy and

$$\begin{aligned} c_0 =&\left[A - \frac{B+C}{2}\right]k^2 + \frac{B+C}{2}j(j+1), \\ c_1 =&-\Delta_k k^4 - \Delta_{jk}k^2 j(j+1) - \Delta_j j^2(j+1)^2, \\ 2c_2 =&H_k k^6 + H_{kj}k^4 j(j+1) \\ &+ H_{jk}k^2 j^2(j+1)^2 + H_j j^3(j+1)^3 \\ &+ L_k k^8 + L_{kkj}k^6 j(j+1) + \ldots \\ &+ P_k k^{10} + \ldots, \end{aligned} \quad (3)$$

$$\begin{aligned} b_0 =&\frac{B-C}{2}, \\ b_1 =&-\delta_k[k^2 + (k\pm 2)^2] - 2\delta_j j(j+1), \\ 2b_2 =&h_k[k^4 + (k\pm 2)^4] + h_{jk}[k^2 + (k\pm 2)^2]j \\ &\cdot(j+1) + 2h_j j^2(j+1)^2 \\ &+ l_k[k^6 + (k\pm 2)^6] \\ &+ l_{kj}[k^4 + (k\pm 2)^4]j(j+1) + \ldots \\ &+ p_k[k^8 + (k\pm 2)^8] + \ldots. \end{aligned} \quad (4)$$

In this work, we will utilize both types of EH models in fitting the energy levels of the $(0, 1, 2)$ state and try to decide which one would be more suitable.

For both EH models, we use the same set of energy levels to fit the effective Hamiltonian parameters. The results of the fitted parameters together with their standard deviation values of 1σ statistical confidence intervals are listed in Table 2. For a convenient comparison, the corresponding parameters from Ref.[16] are also listed in the same table.

Table 2. The spectroscopic constants (cm^{-1}) of the HDO (0,1,2) state[(a)]

	Watson	P–B	Ref.[16]
E_V	8611.10160(39)	8611.10237(108)	8611.095(9)
A	23.109004 (117)	23.110300 (271)	23.10537(338)
B	9.2291081 (463)	9.2281938 (783)	9.22826 (57)
C	6.1648097 (258)	6.1650789 (615)	6.16525 (36)
$\Delta_k(\times 10^2)$	1.877296 (764)	1.91756 (231)	1.8672 (331)
$\Delta_{jk}(\times 10^4)$	4.9479 (421)	4.2274 (549)	4.866 (297)
$\Delta_j(\times 10^4)$	4.47353 (428)	4.40050 (501)	4.288 (28)
$\delta_k(\times 10^3)$	3.03210 (506)	2.95821 (838)	2.478 (20)
$\delta_j(\times 10^4)$	1.66784 (220)	1.61246 (367)	1.674 (18)
$H_k(\times 10^4)$	0.92792 (234)	1.18615 (845)	0.789 (109)
$H_{kj}(\times 10^5)$	–1.8126 (197)	–2.2078 (195)	–2.494 (690)
$H_{jk}(\times 10^6)$	4.3942 (329)	3.6539 (335)	–
$H_j(\times 10^7)$	1.0349 (186)	0.6606 (197)	–
$h_k(\times 10^5)$	2.9764 (369)	3.4911 (797)	–
$h_{jk}(\times 10^6)$	1.5432 (289)	0.2748 (177)	–
$h_j(\times 10^8)$	5.1473 (973)	3.221 (134)	–
$L_k(\times 10^7)$	–3.0984 (324)	–1.6834 (453)	–2.78 (109)
$L_{kj}(\times 10^8)$	1.938 (289)	2.0212 (772)	–
$l_k(\times 10^8)$	–3.401 (364)	–2.326 (190)	–
$l_{kj}(\times 10^8)$	1.792 (147)	5.152 (209)	–

(a) Data in parentheses are the standard deviation values on last digit.

IV. DISCUSSION

The results were compared with the *ab initio* energy levels calculated by Schwenke *et al.*[9,10] The *ab initio* band centre has a deviation of $0.13\,cm^{-1}$, and for most of the observed rotational levels the difference is within $0.3\,cm^{-1}$. This also indicates the high accuracy of the *ab initio* calculations.

In our earlier studies,[1,6,11] we have shown that the Watson's EH model is rather easy and effective for the bands analysed. While Campargue *et al.* prefer to use the EH model in the P–B approximation form.[3,4,7,8,20] In the case of the $(0,1,2)$ state of HDO, shown in Table 2, for the rotational and centrifugal distortion parameters, the corresponding parameters of the two sets are very close. The standard deviation of the fitting under the Watson's EH model is $0.0010\,cm^{-1}$, while the corresponding value connected with the Polyansky's EH model is $0.0035\ cm^{-1}$. So we can accept that the first EH model is better in this case. We think the reason is that the second EH model can be better if the bending–rotation interaction is very strong; say, the bending quantum number V_2 or the rotational angular-momentum quantum number J is very high. Thus, in the case of $(0,1,2)$, where $V_2 = 1$ and $J \leq 16$, it seems not so essential to take into account the bending–rotation interactions. Furthermore, in the first EH model, the matrix elements have a linear dependence on the fitting parameters while having a nonlinear dependence in the second model. Therefore the fitting procedure is much easier for the former than the latter; quicker to reach the convergence, and less sensitive to the initial input values. Consequently, we prefer to use the usual Watson EH model in the present case. The rotational energy levels were calculated with the parameters of the Watson EH model listed in Table 2 and the differences between the calculated and observed values are listed in Table 1 as "Δ".

For most levels, "Δ" is within $0.002\,cm^{-1}$, typically $0.001\,cm^{-1}$, which is very close to the experimental uncertainty. But some of the energy levels, such as $J_{Ka,Kc} = 10_{3,8}$, are marked with asterisks in Table 1 and are excluded from the fitting procedure, because they are observed certainly. However, the differences between the observed and calculated energies are much larger than the experimental uncertainty. For $10_{3,8}$, the difference is the largest, $0.029\,cm^{-1}$. This indicates that such levels are perturbed by some nearby levels of other vibrational states with weak accidental resonances. Because the sensitivity is still far from enough for observing the extreme weak transitions to those "dark" states, the details about the perturbations cannot be determined from the spectrum. But it would be helpful to investigate the *ab initio* results in Ref.[9]. We found that some rotational levels of the $(0,3,1)$ and $(2,2,0)$ vibrational states are located close to those perturbed energy levels of the $(0,1,2)$ state. They are possibly the origin of the perturbations. But we can see that such resonance is very weak since the perturbed energy levels are just slightly shifted. In other words, the $(0,1,2)$ vibrational state can still be considered as a well-isolated state.

V. CONCLUSION

The spectrum of the $\nu_2 + 2\nu_3$ band of HDO has been recorded at an unapodized resolution of $0.02\,cm^{-1}$ with a Fourier transform spectrometer. A total of 149 rotational energy levels of the $(0,1,2)$ vibrational state were derived from 750 transitions with an experimental uncertainty of $0.001\,cm^{-1}$. The rovibrational parameters were fitted using both Watson's effective Hamiltonian and the effective Hamiltonian in the Padé–Borel approximation form. They reproduce the experimental energy levels with the root-mean-square deviations of 0.0010 and $0.0035\,cm^{-1}$, respectively. The analysis indicates that the $(0,1,2)$ vibrational state is well isolated from other states despite the fact that some evidence of weak accidental resonance was found for several rotational levels.

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