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journal homepage: www.elsevier.com/locate/jqsrtCRDS absorption spectrum of ^{17}O enriched water vapor in the 12,277–12,894 cm^{-1} rangeYan Tan^{a,b}, Semen N. Mikhailenko^{c,d}, Jin Wang^a, An-Wen Liu^{a,e,*}, Xiao-Qin Zhao^a, Gu-Liang Liu^a, Shui-Ming Hu^{a,e}^a Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei 230026 China^b Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge, MA, USA^c Laboratory of Theoretical Spectroscopy, V.E. Zuev Institute of Atmospheric Optics SB RAS, 1, Akademician Zuev square, Tomsk 634021, Russia^d Climate and Environmental Physics Laboratory, Ural Federal University, 19, Mira av., Yekaterinburg 620002, Russia^e CAS Center for Excellence in Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei 230026, China

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ABSTRACT

The absorption spectrum of water vapor enriched in oxygen-17 has been recorded by a continuous-wave cavity ring-down spectrometer (CW-CRDS) at room temperature in the 12,277–12,894 cm^{-1} region. The typical sensitivity of $2 \times 10^{-10} \text{ cm}^{-1}$ allowed the detection of water vapor transitions with intensities larger than $1 \times 10^{-28} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$. In total, more than 3400 lines were observed in the recorded spectra with a typical frequency accuracy of 0.002 cm^{-1} . In which more than 3400 transitions were rotationally assigned to five water isotopic species (H_2^{17}O , H_2^{16}O , H_2^{18}O , HD^{16}O , and HD^{17}O) using the known empirical energy levels combined with the calculated variational line lists based on the results of Partridge and Schwenke. About 1300 transitions of H_2^{17}O were assigned, leading to the determination of new energy levels of 17 vibration states. Those assigned H_2^{17}O transitions are involved with the upper vibration states of (013), (023), (032), (051), (061), (070), (080), (090), (112), (131), (150), (160), (211), (230), (301), (310), and (320). The maximum values of the rotational numbers J and K_a were 16 and 9, respectively. The $5\nu_1$ band of HD^{17}O was assigned for the first time as well. The line positions and energy levels determined in this work were compared with literature, and it shows a significant improvement of the line positions of H_2^{17}O and HD^{17}O in the 12,277–12,894 cm^{-1} region.

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1. Introduction

The present work is a subsequent part of the systematic study regarding the absorption spectrum of some important atmospheric molecules below $1 \mu\text{m}$ by continuous-wave cavity ring-down spectroscopy [1–8]. In this paper, we focus on the absorption of ^{17}O -substituted water vapor between 12,277 and 12,894 cm^{-1} . An IUPAC task group (IUPAC-TG) has performed an exhaustive review for the nine isotopologues of water [9–11]. The spectra of the main isotopic species H_2^{16}O have been recorded by Fourier-transform spectroscopy (FTS) [12–16] and intra-cavity laser absorption spectroscopy (ICLAS) [17]. In total, about 1400 transitions of H_2^{16}O in this region have been reported in the literature. Note that more

than 60 of them have been classified as “wrong” transitions by the IUPAC task group [9].

As for the isotopic species H_2^{18}O , transitions in the 12,277–12,894 cm^{-1} region were observed from the absorption spectra of ^{18}O enriched water vapor by FTS [18,19] and ICLAS [20,21]. Some of those transitions were observed by Tolchenov et al. from FTS analysis of “natural” water vapor as well [14]. Overall, more than 820 H_2^{18}O transitions have been reported by previous work in this region so far. The absorption spectrum of water vapor enriched by ^{17}O was reported by Tanaka et al. [19] in the region of interest. The ^{17}O enrichment was about 5% in their sample. Few additional H_2^{17}O lines were reported in ICLAS studies of ^{18}O -enriched samples [20,21] and FTS spectrum of “natural” water samples [14] as well. In conclusion, More than 1810 H_2^{17}O transitions have been obtained from various experimental measurements up to 12,740 cm^{-1} but most of them were reported in the 7443–7921 cm^{-1} region by Mondelain et al. [22]. Fig. 1 shows an overview spectrum of the H_2^{17}O transitions in the investigated region of this work. As shown in this figure, the H_2^{17}O line positions from current HITRAN2016 in this region were mostly calcu-

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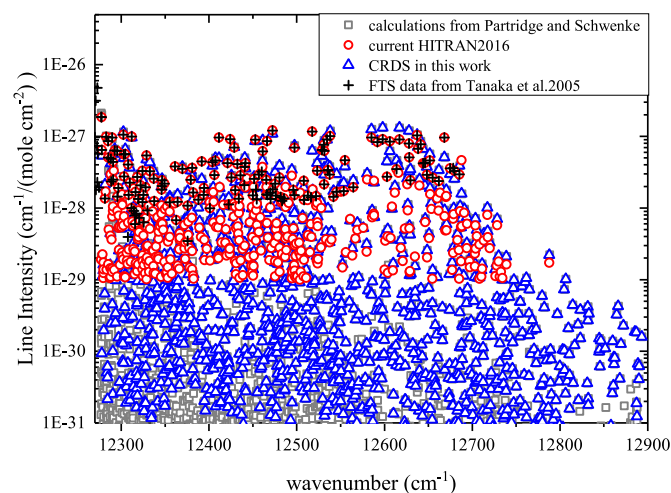


Fig. 1. Overview of the H_2^{17}O transitions in the 12,277–12,894 cm^{-1} region for line intensities in the natural abundance at 296 K. The grey squares are corresponding to the calculations by Partridge and Schwenke [31,32] while the red circles are the current HITRAN2016 [24]. The blue triangles represent the experimental observations in this work, and black cross for the FTS results from Ref. [19].

lated from the IUPAC energy levels [10,23,24]. The HD^{16}O absorption spectra between 12,200 and 12,900 cm^{-1} were studied by different techniques: photo-acoustic [25], Fourier-transform intra-cavity laser absorption spectroscopy [26], ICLAS [27,28], and FTS [29]. More than 900 transitions have been reported in these studies. As for the HD^{17}O species, there are no experimental results for transitions above 12,000 cm^{-1} to the best of our knowledge.

In the present work, we report the spectra of ^{17}O enriched water vapor absorption using CW-CRDS covering the spectral region from 12,277 to 12,894 cm^{-1} . The description of the experimental set up will be presented in Section 2 and the rotation-vibrational analysis of the recorded spectra will be presented in Section 3. In final conclusion, the obtained results for line positions related to the isotopic species H_2^{17}O and HD^{17}O will be provided and compared to the energy levels from literature.

2. Experimental details and line list preparation

The detail configuration of the continuous-wave cavity ring-down spectrometer based on a Ti:Sapphire laser has been described in Refs. [1–5]. Briefly, the structure of the setup is as follows: a beam from a CW tunable Ti:Sapphire laser (Coherent MBR 110) is coupled into a 65.5-cm-long resonance cavity. The high reflectivity of 99.995% cavity mirrors (Layertec GmbH) are installed in a high-vacuum chamber and can be precisely adjusted by a set of step motors (New Focus) using a controller outside the chamber. The ring-down signal is detected by a photodiode and recorded by an analog-digital converter (ADLink PCI 9228) installed on a personal computer. A nonlinear least-square fitting program is applied to derive the ring-down time τ . The sample absorption coefficient α at the frequency ν is obtained using the following equation:

$$\alpha(\nu) = \frac{1}{c\tau(\nu)} - \frac{1}{c\tau_0} \quad (1)$$

where c is the speed of light and τ_0 is the ring-down time of the empty cavity. The achieved sensitivity without averaging varies from 0.5 to $5 \times 10^{-10} \text{ cm}^{-1}$ depending on the reflectivity of the mirrors.

The enriched ^{17}O water vapor sample with a pressure of 7.5 Torr was filled into the CRDS cell without further purification. The enriched ^{17}O water sample was purchased from Icon Services, and the stated isotopic concentration for the oxygen atom is 60.8% of

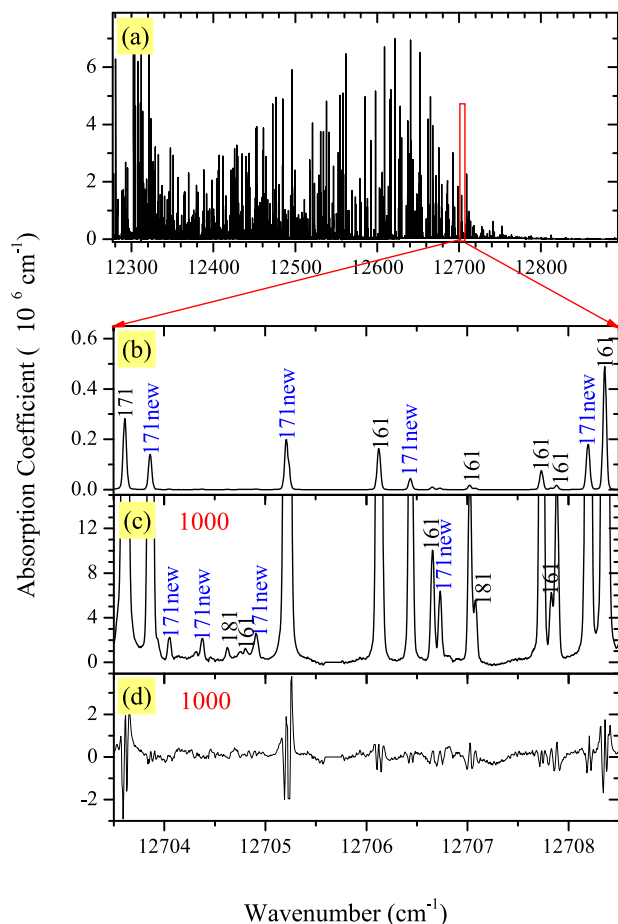


Fig. 2. (a) The overview of the recorded spectrum between 12,277 and 12,894 cm^{-1} in the upper panel; (b) and (c) an example of the H_2^{17}O line assignments around 12,700 cm^{-1} as shown in the lower panel. The marks “171 new” correspond to the lines due to transitions with previously unknown upper energy levels of H_2^{17}O transitions, while the regular H_2^{16}O , H_2^{18}O and H_2^{17}O transitions are marked as “161”, “181” and “171”; (d) the residuals between the calculated and observed spectra in the range of 12,703–12,709 cm^{-1} .

^{17}O . The spectra were recorded at room temperature ($296 \pm 1 \text{ K}$). Since there was a continuous exchange between water molecules in the gas phase and those absorbed on the walls of the sample cell, the sample pressure was continuously monitored with a capacitance gauge (full range 100 kPa, 0.5% accuracy) during the measurement. H_2^{16}O , H_2^{17}O , H_2^{18}O , HD^{16}O and HD^{17}O water isotopologues were found in the sample with the assignment of the recorded spectrum. The concentrations of three main species were estimated and listed in Table 1 together with the respective natural abundances of water isotopologues. The spectrum calibration was based on the reading given by a calibrated lambda-meter (Burleigh WA-1500) with 60 MHz accuracy.

An overview of the CW-CRDS spectra is presented in Fig. 2(a). A small part of the recorded spectrum around 12,706 cm^{-1} is given in Fig. 2(b) and (c). These pictures illustrate the transition assignments and demonstrate the detective capability of transitions with 4–5 orders of dynamic range on the absorption.

3. Spectrum analysis and the line assignments

The complete line list was obtained using the computer code SpectraPlot [30]. The high quality of the recorded spectrum allows the determination of more than 3400 absorption lines in the intensity range of 4×10^{-29} to $1.5 \times 10^{-24} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$. The line parameters were determined through the multi-line fit-

Table 1
Overview information of assigned transitions and isotopologue abundances of studied water sample.

Isotopologue	Number of transitions	Range (cm ⁻¹)	Estimated abundance	Natural abundance [24]
H ₂ ¹⁶ O	1590	12,278–12,891	0.540	0.997317
H ₂ ¹⁷ O	1283	12,277–12,893	0.454	0.371884E-3
H ₂ ¹⁸ O	411	12,277–12,794	0.006	0.199983E-2
HD ¹⁶ O	93	12,559–12,877		0.310693E-3
HD ¹⁷ O	51	12,570–12,853		0.115853E-6
Unassigned	191 (lines)	12,279–12,850		
Total	3428			

ting procedure provided by SpectraPlot. The Voigt profile was applied in the fitting procedure of each line. The Gaussian width was fixed at the Doppler width. The pressure-broadening line width as well as the line position and intensity were obtained by the fitting for each transition. For instance, Fig. 2(d) gives the residuals between the observed and simulated spectra around 12,706 cm⁻¹.

In total, 262 H₂¹⁶O line positions from Ref. [12] were used for the calibration of the recorded spectrum which yields a standard deviation of 0.0013 cm⁻¹. The absolute accuracy of the line position in this work is better than 2×10^{-3} cm⁻¹ for those not very weak and isolated lines.

The complete line list of all 3412 lines is given as Supplementary Material I to this paper. The list includes experimental lines parameters (position, intensity and line width) of all recorded lines. Empirical line positions (if possible) as well as variational line intensities are given for all assigned lines.

The transitions of five water isotopologues (H₂¹⁷O, H₂¹⁶O, H₂¹⁸O, HD¹⁶O, and HD¹⁷O) were assigned from the recorded spectrum. General information about all assigned transitions is given in Table 1. The assignment procedure was based on the variational line lists of five isotopologues mentioned above calculated by Tashkun (Tomsk, Russia) using the results of Partridge and Schwenke [31,32]. These line lists are available online at the system “Spectroscopy of Atmospheric Gases”, <http://spectra.iao.ru> [33]. During the first step of the so-called “trivial assignment”, variational line positions of H₂¹⁷O, H₂¹⁶O and H₂¹⁸O molecules were replaced by data calculated from previously reported empirical energy levels [9,10]. This allows us to assign the lines by directly comparing experimental line list with the obtained line transitions. In the next step, variational line positions and intensities were compared with the left unassigned lines after “trivial assignment”. Table 2 contains band-by-band information about assigned lines of non-deuterated species. The second step of the line assignments was to compare the experimental line list with variational calculations [33] for molecules H₂¹⁷O, H₂¹⁶O and H₂¹⁸O. This procedure allows us to assign about 800 transitions of H₂¹⁶O and H₂¹⁷O corresponding to previously unknown upper energy levels.

The comparison of previously reported H₂¹⁷O transitions to those assigned in this study is shown in Fig. 1. The line positions and intensities of the transitions reported in Refs. [14,19–21,24] are given by red open circles (current HITRAN database) and dark crosses (FTS data from Tanaka et al. [19]). As shown in Fig. 1, only a few transitions weaker than 1×10^{-28} cm⁻¹/(molecule cm⁻²) which is equivalent to 1×10^{-25} cm⁻¹/(molecule cm⁻²) in pure H₂¹⁷O were observed in the published work [14, 19–21].

The lines for isotopic species HD¹⁶O were identified by “trivial assignment” using the results of Campargue et al. [27]. Ninety-four transitions mainly of the 5ν₁ band were observed between 12,559 and 12,877 cm⁻¹. The line positions of assigned transitions are in very good agreement with the previous work [27].

Because a water sample with more than 45% ¹⁷O enrichment was used in the measurement in this work, fifty-one transitions of the strongest band (5ν₁) with maximum values of rotational numbers $J=8$ and $K_a=4$ were assigned for the HD¹⁷O isotopologue in

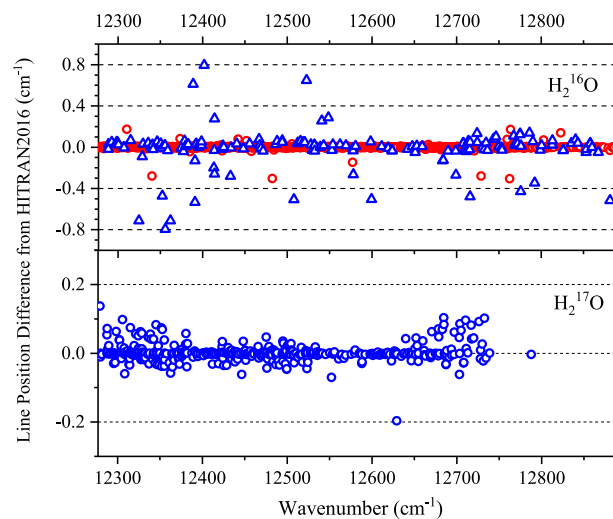


Fig. 3. H₂¹⁶O and H₂¹⁷O line position differences between HITRAN2016 and new data obtained in this work.

this region. Note that this is the first assignment of HD¹⁷O absorption lines above 8710 cm⁻¹.

In total, 3221 lines were assigned to 3428 transitions of five isotopic water species as mentioned above. The 5ν₁ band of HD¹⁷O was observed for the first time. There were still about two hundred lines with the intensity values between 4×10^{-29} and 4.5×10^{-27} cm/molecule left unassigned as shown in Table 1. In this work, a total of 1792 ro-vibrational energy levels of five different water isotopologues were determined, in which 613 levels were new or corrected. The complete list of the energy levels is given in Supplementary Material II attached to this paper.

4. Results and discussions

4.1. H₂¹⁶O

About 1600 transitions of 16 cold and 4 hot bands were assigned in this work for H₂¹⁶O. In general, the comparison of the observed data against the HITRAN2016 line list [24] shows good agreement. The line position differences are below 0.005 cm⁻¹ for 1157 transitions and less than 0.01 cm⁻¹ for 1307 ones. While there were still about 160 transitions which showed a significant difference between our results and the HITRAN2016 database. The $|\nu^{\text{HITRAN2016}} - \nu^{\text{TW}}|$ values for these transitions are between 0.01 cm⁻¹ and 0.79 cm⁻¹. Note that there are two types of H₂¹⁶O line positions included in the HITRAN2016 database for the spectral range of 12,277–12,894 cm⁻¹. The first type is the so-called “empirical line positions” (2840 of 4103 transitions). These values were calculated from empirical energy levels recommended by the IUPAC task group [9]. A general overview of the comparison between our results and HITRAN2016 “empirical” line positions is shown on the upper panel of Fig. 3 (red open circles). The average dif-

Table 2
Band by band statistic information of H₂¹⁶O, H₂¹⁶O and H₂¹⁸O assigned transitions.

Band	H ₂ ¹⁶ O			H ₂ ¹⁷ O			H ₂ ¹⁸ O					
	NT	J _{max}	K _{a max}	Region (cm ⁻¹)	NT	J _{max}	K _{a max}	Region (cm ⁻¹)	NT	J _{max}	K _{a max}	Region (cm ⁻¹)
2ν ₁ + ν ₂ + ν ₃	232	16	8	12,278–12,855	176	14	8	12,287–12,858	49	13	6	12,284–12,678
3ν ₁ + ν ₂	156	13	9	12,279–12,868	171	13	9	12,284–12,863	31	10	6	12,279–12,667
3ν ₂ + 2ν ₃	110	14	8	12,280–12,858	66	14	7	12,279–12,705	9	9	6	12,297–12,681
ν ₁ + 3ν ₂ + ν ₃	80	12	8	12,283–12,882	41	12	7	12,281–12,759	7	9	5	12,307–12,489
ν ₂ + 3ν ₃	432	16	8	12,280–12,891	390	16	7	12,277–12,893	170	12	6	12,277–12,783
ν ₁ + 6ν ₂	14	12	1	12,287–12,716	6	12	2	12,317–12,719				
ν ₁ + ν ₂ + 2ν ₃	345	14	9	12,288–12,885	283	13	8	12,278–12,889	143	10	7	12,279–12,794
4ν ₁ + ν ₂					1	6	2	12,325				
8ν ₂	12	12	4	12,298–12,823	7	10	3	12,309–12,630	1	10	2	12,284
3ν ₁ + ν ₃	17	8	4	12,281–12,392	15	8	3	12,283–12,427				
2ν ₁ + 3ν ₂	57	12	9	12,283–12,817	43	12	8	12,294–12,852				
4ν ₁	4	8	4	12,304–12,340								
2ν ₂ + 3ν ₃ - ν ₂	50	9	5	12,311–12,659	30	8	3	12,317–12,613				
2ν ₁ + 2ν ₂ + ν ₃ - ν ₂	1	6	3	12,323								
9ν ₂	6	12	1	12,324–12,891	3	5	0	12,408–12,631				
7ν ₂	5	12	8	12,332–12,761	6	12	8	12,332–12,700				
5ν ₂ + ν ₃	18	12	8	12,334–12,733	9	12	8	12,333–12,796				
3ν ₁ + 2ν ₂					3	6	2	12,341–12,438				
ν ₁ + 2ν ₂ + 2ν ₃ - ν ₂	14	6	5	12,284–12,614								
ν ₁ + 5ν ₂	7	12	8	12,455–12,772	5	11	8	12,589–12,735				
6ν ₂ + ν ₃	7	9	2	12,551–12,860	7	8	2	12,536–12,762	1	8	1	12,336
ν ₁ + 3ν ₃ - ν ₂	23	6	3	12,619–12,826	21	7	3	12,579–12,804				
Total	1590	16	9	12,278–12,891	1283	14	9	12,277–12,893	411	12	7	12,277–12,783

NT – Ro-vibrational transition number of given band.

J_{max} K_{a max} – maximum value of rotational numbers J and K_a.

ference between our line positions (ν^{TW}) and this part of the HITRAN2016 data (ν^{HITRAN} (Empirical)) is -0.00094 cm^{-1} with a root mean square (RMS) difference of 0.00048 cm^{-1} . The biggest differences are corresponding to the transitions with upper levels (211) 12_{66} (ν^{HITRAN} (Empirical) - $\nu^{\text{TW}} = 0.1743; 0.1716; 0.1714 \text{ cm}^{-1}$). Note that the (V_1, V_2, V_3) J K_a K_c is according to the domination fraction relative to the vibrational and rotational numbers. The second part of the HITRAN2016 line list came from the variational calculation by Bubukina et al. [34] (1263 transitions). The general overview of the differences between our line positions and the variational values of HITRAN2016 is shown on the lower panel of Fig. 3 (blue open triangles) as well. The average difference between our line positions (ν^{TW}) and this part of the HITRAN2016 data (ν^{HITRAN} (Variational)) is -0.021 cm^{-1} with the RMS difference of 0.017 cm^{-1} . The biggest differences are corresponding to the (160) $2_{02}-(000) 2_{11}$ (ν^{HITRAN} (Variational) - $\nu^{\text{TW}} = -0.7942 \text{ cm}^{-1}$) and (090) $1_{01}-(000) 2_{12}$ (ν^{HITRAN} (Variational) - $\nu^{\text{TW}} = -0.7116 \text{ cm}^{-1}$) transitions. Note that 162 transitions with the discrepancies larger than 0.01 cm^{-1} were provided in the Supplementary Material III.

Some examples of significant discrepancies between H₂¹⁶O observed line positions and those of the HITRAN2016 database are shown in Fig. 4. The empirical line position of the (131) $11_{38}-(000) 10_{19}$ transitions in the HITRAN database is shifted by -0.0204 cm^{-1} compared to the observed position at $12,375.8826 \text{ cm}^{-1}$ (upper panel of Fig. 4). The second line observed at $12,377.3308 \text{ cm}^{-1}$ corresponds to the (310) $6_{60}-(000) 7_{35}$ transition. The variational line position in the HITRAN list is shifted by -0.0410 cm^{-1} compared to their position in our recorded spectrum. The line intensities of these two lines are 1.24×10^{-27} and $1.78 \times 10^{-27} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$, respectively. As shown in the lower panel of Fig. 4, the line positions of two transitions in the (013) band from the HITRAN database between $12,715$ and $12,716 \text{ cm}^{-1}$ are considered to be incorrect. The HITRAN's positions of the $8_{54}-(000) 7_{53}$ ($12,714.9394 \text{ cm}^{-1}$) and $8_{53}-(000) 7_{52}$ ($12,715.8754 \text{ cm}^{-1}$) transitions are from variational calculation [34]. The corresponding lines are shifted by about 0.050 cm^{-1} comparing to the observation.

We also made the comparison of the energy levels determined from the H₂¹⁶O line list given in this work against those reported

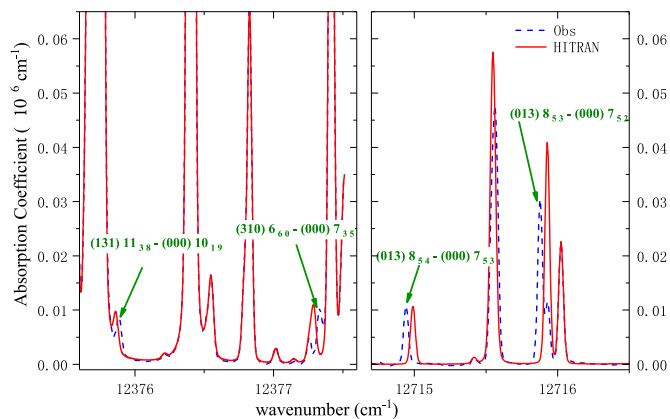


Fig. 4. Examples of H₂¹⁶O line position deviated from HITRAN2016 around $12,376 \text{ cm}^{-1}$ (left panel) and $12,715 \text{ cm}^{-1}$ (right panel). Observed and calculated spectra are given with blue dotted lines and red full lines, respectively.

by IUPAC-TG [9] and Ref. [34]. The average difference between our energies and the data from literature [9] is -0.0004 cm^{-1} with the RMS difference of 0.0006 cm^{-1} . The maximum difference is 0.408 cm^{-1} corresponding to the (230) 9_{54} energy level (see Table 3).

Based on the assigned H₂¹⁶O transitions, we are able to obtain 73 new rotational energy levels of twelve vibrational states. These energies are listed in Table 3. In addition, Table 3 contains 72 rotation-vibration energies which differ more than 0.010 cm^{-1} from the values published by IUPAC-TG [9] and Ref. [34].

4.2. H₂¹⁸O

Four hundred and eleven transitions of H₂¹⁸O were assigned in the recorded spectrum. In general, we found a very good agreement between our observations and the HITRAN2016 data. According to Ref. [24], the H₂¹⁸O transitions of the HITRAN2016 database were mainly from calculations using empirical energy levels of IUPAC-TG [10] with few updates by Kyuberis recently

[40] and the variational calculation of Bubukina et al. [34]. Average difference between 395 our line positions and those from HITRAN is -0.0001 cm^{-1} with the RMS difference of 0.0002 cm^{-1} . The differences ($\nu^{\text{HITRAN}} - \nu^{\text{TW}}$) are bigger than 0.0 cm^{-1} only for eleven transitions. The maximum difference is 0.0269 cm^{-1} for the $(013) 10_{110-9} 1_9$ transition. The line position of this transition ($12,657.0674 \text{ cm}^{-1}$) yields the upper energy level $E_{(013) 10_{110}} = 13,573.3605 \text{ cm}^{-1}$ instead of $13,573.38763 \text{ cm}^{-1}$ in Ref. [24]. Note that the $(013) 10_{110}$ level was obtained in Ref. [10] from two transitions, and it has a poor accuracy (grade B+) according to the IUPAC-TG ranking. Only one new energy $E = 13,534.0028 \text{ cm}^{-1}$ of the $(013) 7_{53}$ level has been derived from previously observed $(013) 7_{53-6} 5_2$ transition at $12,653.9266 \text{ cm}^{-1}$.

4.3. H_2^{17}O

More than 1280 transitions of H_2^{17}O were assigned in the recorded spectrum (see Tables 1 and 2). More than 1050 transitions were observed for the first time. Graphical comparison of new data against those published in Ref. [19] is shown on the lower panel of Fig. 3 (blue open circle). The line position differences are from -0.062 cm^{-1} for the transitions of the $(310) 7_{25}$ upper energy level up to 0.410 cm^{-1} for the transitions of the $(080) 5_{33}$ upper energy level. Mean difference between 458 our line positions and the data of Ref. [24] is 0.0051 cm^{-1} with the root mean square difference of 0.0019 cm^{-1} . It is interesting to note that only four experimental line positions of Ref. [19] are included in the HITRAN2016 database. In addition, the discrepancy between our line position of the $(131) 7_{52-6} 6_{33}$ transition and the value from Ref. [19] is over 0.05 cm^{-1} . There are about five hundred transitions in the HITRAN2016 database from Lodi and Tennyson [23]. This last paper is a compilation of partly “empirical” line positions calculated from energy levels [10], partly from the variational calculation of Shirin et al. [35].

Three of four line positions labeled in HITRAN2016 as the data of Ref. [19] differ from our observations by more than 0.01 cm^{-1} . These lines are shown in Fig. 5. The lines $(112) 2_{02-2} 1_1$ at $12,361.190 \text{ cm}^{-1}$ and $(131) 7_{52-6} 6_{33}$ at $12,362.708 \text{ cm}^{-1}$ (right panel) and $(112) 3_{21-3} 1_2$ at $12,424.192 \text{ cm}^{-1}$ (left panel) are shifted comparing to our results by -0.028 , -0.058 and -0.014 cm^{-1} , respectively. Once again, all three line positions in HITRAN2016 labeled as observations from Ref. [19]. Two calculated lines located at $12,423.498$ and $12,423.674 \text{ cm}^{-1}$ correspond to the $(112) 8_{54-7} 4_3$ and $(013) 6_{16-6} 1_5$ transitions from Ref. [23]. They are shifted by 0.020 and 0.033 cm^{-1} , respectively.

Only 499 of 1283 assigned H_2^{17}O transitions can be derived using energy levels given by IUPAC-TG [10]. The differences between observed line positions and calculated values using the empirical energy levels [10] are within 0.005 cm^{-1} for 345 transitions. Maximum discrepancy of 0.062 cm^{-1} is found for the transitions of the $(310) 7_{25}$ upper level.

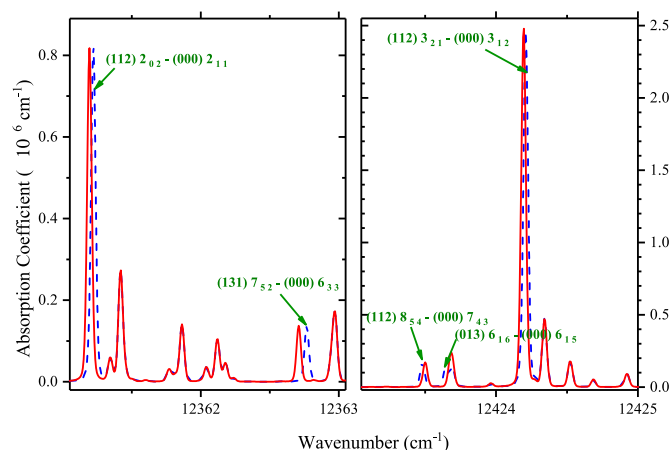


Fig. 5. Examples of H_2^{17}O line position deviated from HITRAN2016 around $12,362 \text{ cm}^{-1}$ (left panel) and $12,424 \text{ cm}^{-1}$ (right panel). Observed and calculated spectra are given in blue dotted lines and red full lines, respectively.

Based on the assigned H_2^{17}O transitions, we were able to obtain 467 new and corrected rotational energy levels of 17 vibrational states. These energies are listed in Table 4. As for H_2^{16}O energies (see Table 3), Table 4 contains 121 rotation-vibration energies which differ by more than 0.010 cm^{-1} from the values published by IUPAC-TG [10] and Ref. [23]. Corrected energy levels are given in *italic*.

4.4. Unambiguous ro-vibrational assignments

The difficulties of unambiguous assignment of vibration-rotation energy levels of the water molecule have been discussed in numerous studies on the absorption spectrum analysis of water in the near infrared range (see, for example, Refs. [36–39]). Therefore, as given in Ref. [10], for instance, some levels of the (310) state were re-assigned to the (112) and (230) states (see Table 4 and table footnotes). Our labeling gives more consistent sets of the energy levels for each of these states. The energies increase smoothly with the increasing of the rotational numbers J and K_a . Due to the small number of assigned energy levels for the (051) , (150) , (061) , (160) , (070) , (080) , and (090) states (see Table 4), the identification of these states should be considered as preliminary assignments. Their vibrational labels could be verified in future studies.

As mentioned before, the variational line list [33] based on the results of Partridge and Schwenke [31,32] was used in the spectrum assignment procedure. In some cases, two or more of the different frequency values given in this list were assigned to the same transition of highly excited upper levels. The reason is that the procedure of domination fraction relative to the vibrational and rotational numbers may not work properly

Table 3
Corrected and new energy levels of H_2^{16}O .

Vib	$J K_a K_c$	E	ΔE	Vib	$J K_a K_c$	E	ΔE
013	7 7 0	13,900.4575	-0.0307	112	10 7 4	14,444.0991	0.1718
013	7 7 1	13,900.4574	-0.0310	112	11 6 6	14,530.1983	0.0104
013	8 6 3	13,924.0045	-0.0569	131	8 8 1	14,042.0550	0.0271
013	8 7 1	14,090.6844	0.0129	131	8 8 0	14,042.0597	0.0317
013	8 7 2	14,090.6830	0.0112	131	9 7 2	13,985.9298	-0.0763
013	8 8 0	14,275.3371	0.0188	131	9 8 2	14,264.8177	0.0195
013	8 8 1	14,275.3373	0.0171	131	9 8 1	14,264.8482	0.0498
013	9 5 4	13,990.7161	-0.0119	131	11 3 8	13,668.9012	0.0217
013	9 6 3	14,206.6816	0.0154	131	11 6 6	14,174.8601	0.0308

(continued on next page)

Table 3 (continued)

Vib	$J K_a K_c$	E	ΔE	Vib	$J K_a K_c$	E	ΔE
013	10 2 8	13,959.0555	0.0103	131	12 2 10	13,819.7335	0.0267
013	10 3 8	13,959.9420	-0.0199	160	2 0 2	12,451.1602	0.0370
013	10 5 6	14,222.7949	0.0139	211	10 6 4	14,004.8612	-0.0682
013	11 4 8	14,341.1244	-0.0761	211	10 7 4	14,135.1942	-0.0156
013	11 6 6	14,634.9649	0.0142	211	11 6 5	14,264.5049	0.0116
013	12 1 12	14,042.6584	-0.0159	211	12 6 6	14,454.5671	-0.1719
013	12 2 11	14,266.0266	0.0162	211	14 3 11	14,800.1394	0.0146
013	13 0 13	14,275.2042	0.0261	211	16 1 15	14,964.3214	0.0194
013	14 1 14	14,527.7918	0.0370	230	6 5 1	12,856.8443	-0.0169
023	5 3 2	14,587.1213	0.0110	230	7 4 4	12,826.4054	0.0134
023	7 3 4	14,916.4463	-0.0108	230	8 6 2	13,439.8219	0.3723
032	9 3 6	13,343.3215	0.0388	230	8 6 3	13,439.8022	0.3418
032	9 4 5	13,459.9914	0.0171	230	9 5 4	13,428.6727	-0.4082
032	9 7 2	14,075.1198	0.0220	230	9 6 4	13,653.6622	-0.0174
032	9 7 3	14,075.1161	0.0193	230	9 9 0	14,368.8595	0.0144
032	13 2 11	14,301.2304	-0.0348	230	9 9 1	14,368.8597	0.0146
051	9 7 3	13,800.9975	0.0101	230	10 4 7	13,462.7160	-0.0186
061	0 0 0	12,586.2299	-0.0251	230	11 2 9	13,499.3326	0.0455
061	5 1 4	13,065.2492	0.0241	301	4 2 2	14,123.5240	-0.0182
061	9 1 8	13,819.5725	-0.0385	310	6 6 0	13,194.0261	-0.0629
070	11 4 7	13,778.6369	0.0111	310	10 6 5	13,999.5313	-0.0128
080	5 3 2	12,877.7365	0.1482	310	10 9 1	14,789.6155	0.0124
080	9 2 7	13,074.2001	0.3581	310	10 9 2	14,789.6158	0.0131
080	9 3 6	13,587.8400	0.0375	310	11 2 9	13,773.8357	0.1634
090	5 0 5	12,880.1436	-0.1288	310	11 3 8	13,896.2910	-0.0139
112	10 1 9	13,647.2372	0.0157	310	11 4 8	13,929.0993	0.0115
112	10 7 3	14,444.0778	0.1509	310	11 7 4	14,704.2776	0.0114
013	10 4 7	14,083.0981	new	131	11 7 5	14,488.1742	new
013	10 6 5	14,374.8268	new	131	12 6 7	14,544.3937	new
013	10 7 4	14,542.2188	new	150	9 7 2	13,657.5607	new
013	10 7 3	14,542.2560	new	150	10 7 3	14,227.2902	new
013	12 4 9	14,618.1022	new	150	11 7 5	14,490.6470	new
013	13 4 10	14,911.1967	new	150	12 6 7	14,269.9478	new
013	14 2 12	15,021.7203	new	211	10 8 3	14,384.2162	new
013	14 3 12	15,023.8963	new	211	11 7 4	14,395.2518	new
013	16 0 16	15,082.5187	new	211	12 4 8	14,289.0323	new
032	7 5 3	13,225.2783	new	211	13 3 10	14,488.8723	new
032	10 5 5	14,083.0999	new	211	13 4 9	14,604.4466	new
032	10 7 4	14,314.9461	new	230	10 5 5	13,668.9738	new
032	10 8 3	14,668.3462	new	230	10 6 5	13,890.6045	new
032	10 8 2	14,668.3415	new	230	10 8 3	14,429.8106	new
032	11 3 9	13,752.9477	new	230	10 8 2	14,429.8059	new
032	11 5 6	14,397.8638	new	230	10 9 2	14,608.2577	new
032	13 3 11	14,306.5068	new	230	10 9 1	14,608.2581	new
051	10 5 5	13,458.4487	new	230	11 4 8	13,716.8708	new
051	11 8 4	14,646.6417	new	230	11 5 6	13,932.0577	new
051	11 8 3	14,646.7035	new	230	11 7 4	14,398.5027	new
070	12 4 8	14,065.1252	new	230	12 4 8	14,050.2814	new
080	10 3 8	13,801.0016	new	230	12 5 7	14,221.7456	new
080	12 4 9	14,822.0585	new	230	12 6 7	14,539.7546	new
090	1 0 1	12,404.4517	new	310	10 2 8	13,531.6531	new
090	5 1 5	13,337.6642	new	310	10 3 7	13,629.5498	new
090	12 1 12	14,287.8202	new	310	10 4 6	13,718.3963	new
112	9 9 1	14,426.3376	new	310	10 7 4	14,137.5711	new
112	9 9 0	14,426.3381	new	310	11 7 5	14,704.3657	new
112	11 4 8	14,195.1471	new	310	11 8 4	14,586.5261	new
112	11 4 7	14,246.4807	new	310	11 8 3	14,586.5306	new
112	11 5 7	14,343.6825	new	310	11 9 3	15,053.2043	new
112	11 5 6	14,371.4599	new	310	11 9 2	15,053.2036	new
112	12 4 8	14,530.7872	new	310	12 7 6	14,987.3372	new
112	12 5 7	14,656.3786	new	310	13 2 11	14,318.1639	new
131	8 8 1	14,042.0550	new	310	13 3 10	14,460.7870	new
131	11 5 6	13,963.0297	new	310	13 6 7	15,115.9713	new
131	11 6 5	14,170.4470	new				

Notes: Vib $J K_a K_c$ - vibration and rotation assignment of the energy level; E - energy values obtained in this study (cm^{-1}); ΔE - energy difference between this work and the literature values from IUPAC [9] and Ref. [34] (cm^{-1}).

for strongly perturbed levels. As a consequence, two (or more) strongly interacting energy levels are attributed to the same quantum numbers. For instance, two sets of frequencies and intensities ($12,689.1548 \text{ cm}^{-1}$, $2.712 \times 10^{-27} \text{ cm}^{-1}/(\text{moleculecm}^{-2})$) and ($12,693.8815 \text{ cm}^{-1}$, $2.994 \times 10^{-27} \text{ cm}^{-1}/(\text{moleculecm}^{-2})$) are as-

signed for the transition (013) $12_1 12 - (000) 11_1 11$ in the calculation [33]. In this case, one of them was assigned to the transition mentioned above, and the rest needs to be re-assigned. It also means that the second transition remains uncertain in the vibrational numbers (V_1, V_2, V_3) and possibly for the rotational numbers

K_a and K_c as well. It is similar for the transition (013) $12_1 11-(000) 11_1 10 - 12,716.2038 \text{ cm}^{-1}$, $2.931 \times 10^{-27} \text{ cm}^{-1}/(\text{moleculecm}^{-2})$ and $12,719.2580 \text{ cm}^{-1}$, $2.747 \times 10^{-27} \text{ cm}^{-1}/(\text{moleculecm}^{-2})$. As can be seen from Table 4, this problem is not resolved yet for 45 levels.

Please notice here the problem of ambiguous identification of the variational lists is not a specific problem of the SP lists of Ref.

[33]. This is a common issue for variational calculations of polyatomic molecules. Regarding the list of water molecules, the predictions from UCL (including recent lists [40]) prefer not to give the complete vibrational and rotational numbers for many transitions. Since then, 174 of 493 H_2^{17}O HITRAN2016 transitions came from Ref. [23] still remain incomplete vibration-rotation assignment.

Table 4
New and corrected energy levels of H_2^{17}O .

Vib	$J K_a K_c$	Term value	Vib	$J K_a K_c$	Term value	Vib	$J K_a K_c$	Term value
013	4 3 2	12,910.1443	051	8 8 0	14,005.2276	211	9 6 4	13,741.6260
013	5 3 2	13,035.5408	051	9 8 2	14,111.8630	211	9 6 3	13,741.7825
013	5 4 1	13,131.6372	051	9 8 1	14,111.8979	211	9 7 3	13,868.4890
013	5 5 0	13,250.3432	051	10 5 5	13,429.0726	211	9 7 2	13,868.5439
013	6 1 6	12,965.6374	051	12 6 6	14,268.9936	211	10 4 7	13,666.1685
013	6 2 5	13,075.0392	061	2 2 0	12,895.9398	211	10 4 6	13,703.5819
013	6 4 3	13,276.4175	061	5 1 4	13,038.6745	211	10 5 6	13,809.0832
013	6 4 2	13,277.5624	061	6 1 5	13,193.9789	211	10 5 5	13,815.2518
013	6 5 2	13,392.3102	061	7 1 6	13,372.1051	211	10 6 5	13,977.3995
013	6 5 1	13,392.3734	061	8 1 7	13,572.1936	211	10 6 4	13,977.8366
013	6 6 1	13,538.1966	070	8 8 1	13,934.0333	211	10 7 4	14,105.6197
013	6 6 0	13,538.1989	070	8 8 0	13,934.0335	211	10 7 3	14,105.6362
013	7 0 7	13,097.7199	070	9 8 2	14,152.8366	211	11 1 10	13,587.3321
013	7 1 6	13,220.7965	070	9 8 1	14,152.8365	211	11 2 9	13,759.9917
013	7 3 4	13,365.1943	070	12 6 6	14,023.7719	211	11 3 9	13,764.7181
013	7 4 4	13,444.6627	080	4 3 2	12,732.3341	211	11 3 8	13,881.6545
013	7 4 3	13,448.5002	080	5 3 3	12,850.7892	211	11 4 7	13,975.2421
013	7 5 3	13,558.1037	080	7 3 4	13,155.6245	211	11 5 7	14,065.7315
013	7 5 2	13,558.4318	080	10 2 9	13,385.7607	211	11 5 6	14,079.3573
013	7 6 2	13,704.8293	090	5 0 5	12,854.6668	211	11 6 6	14,236.1432
013	7 6 1	13,704.8269	103	3 0 3	14,424.4111	211	11 6 5	14,237.3018
013	7 7 1	13,869.7096	112	0 0 0	12,389.0982	211	12 1 11	13,824.0075
013	7 7 0	13,869.7098	112	1 1 1	12,425.3523	211	12 2 11	13,823.9559
013	8 2 7	13,391.1882	112	2 0 2	12,456.1885	211	12 3 9	14,159.8274
013	8 2 6	13,498.4842	112	2 1 2	12,465.4581	211	12 5 8	14,343.7127
013	8 3 6	13,517.6054	112	2 1 1	12,482.1374	211	12 5 7	14,369.6720
013	8 4 5	13,635.8799	112	2 2 0	12,523.7783	211	12 6 6	14,520.2780
013	8 4 4	13,645.9383	112	3 2 1	12,597.3163	211	12 7 6	14,647.6944
013	8 5 4	13,747.5917	112	4 1 3	12,656.4227	211	13 2 11	14,292.5280
013	8 5 3	13,748.7996	112	4 3 1	12,766.3773 ^a	211	13 3 11	14,291.7728
013	8 6 3	13,894.3227	112	4 4 1	12,871.8545	211	13 3 10	14,465.3710
013	8 6 2	13,894.3506	112	4 4 0	12,871.8553	211	13 4 9	14,584.6735
013	8 7 2	14,059.8794	112	5 1 5	12,698.5162	211	14 3 11	14,774.9798
013	8 7 1	14,059.8793	112	5 2 4	12,791.8746	211	14 4 10	14,915.1957
013	9 0 9	13,412.9724	112	5 3 3	12,881.9022	230	5 5 0	12,689.6183
013	9 1 8	13,578.3877	112	5 5 1	13,120.0065	230	6 4 2	12,637.0821
013	9 2 7	13,707.7747	112	5 5 0	13,119.8881	230	6 5 1	12,832.2488
013	9 3 7	13,723.7340	112	6 1 6	12,811.9659	230	6 6 1	13,054.9417
013	9 3 6	13,796.1451	112	6 2 5	12,922.4329	230	6 6 0	13,054.9380
013	9 4 6	13,849.6136	112	6 2 4	12,976.6054	230	7 4 3	13,297.6905 ^a
013	9 4 5	13,871.3425	112	6 3 4	13,021.6023	230	7 5 3	12,998.7548
013	9 5 5	13,960.5051	112	6 3 3	13,035.2924	230	7 5 2	12,998.9286
013	9 5 4	13,963.9208	112	6 4 3	13,130.4071	230	7 6 2	13,221.9353
013	9 6 4	14,108.4659	112	6 5 1	13,259.7445	230	7 6 1	13,221.9400
013	9 6 3	14,108.7150	112	6 6 1	13,425.0044	230	7 7 1	13,543.7650
013	9 7 3	14,273.7493	112	6 6 0	13,424.9994	230	7 7 0	13,543.7652
013	9 7 2	14,273.7594	112	7 2 5	13,149.4985 ^a	230	8 5 4	13,188.7802
013	10 1 10	13,596.4001	112	7 3 4	13,209.5239 ^a	230	8 5 3	13,189.4620
013	10 1 9	13,780.6601	112	7 4 4	13,295.0249	230	8 6 3	13,412.5491
013	10 2 9	13,780.9301	112	7 5 3	13,425.1928	230	8 6 2	13,412.5741
013	10 2 8	13,932.6650	112	7 5 2	13,423.7712	230	8 7 2	13,737.2494
013	10 3 8	13,934.4728	112	7 6 2	13,592.2851	230	8 7 1	13,737.2448
013	10 3 7	14,042.7902	112	7 6 1	13,592.2634	230	8 8 1	14,075.0817
013	10 4 7	14,085.7348	112	7 7 1	13,773.2519	230	8 8 0	14,075.0819
013	10 4 6	14,122.6118	112	7 7 0	13,773.2565	230	9 5 4	13,404.0162
013	10 5 6	14,196.4166	112	8 2 6	13,073.6352	230	9 6 3	13,626.3939
013	10 5 5	14,204.1651	112	8 3 6	13,099.6240 ^a	230	9 7 2	13,954.2475
013	10 6 5	14,345.5452	112	8 3 5	13,142.5327	230	10 2 8	13,222.1291
013	10 6 4	14,346.4382	112	8 4 5	13,221.7778	230	10 4 7	13,438.6147
013	10 7 3	14,510.9924	112	8 4 4	13,229.5617	230	10 5 6	13,638.0210
013	11 0 11	13,797.0816	112	8 5 4	13,351.7746	230	10 5 5	13,644.7059
013	11 1 11	13,796.7472	112	8 5 3	13,355.2241	230	10 6 5	13,972.6397
013	11 1 10	14,001.1183	112	8 6 2	13,524.6673	230	10 7 4	14,194.3666

(continued on next page)

Table 4 (continued)

Vib	$J K_a K_c$	Term value	Vib	$J K_a K_c$	Term value	Vib	$J K_a K_c$	Term value
013	11 2 10	14,001.2429	112	8 7 2	13,654.9494	230	10 7 3	14,194.3979
013	11 2 9	14,173.3546	112	8 7 1	13,654.9448	230	10 8 3	14,394.4022
013	11 3 9	14,174.7398	112	8 8 1	13,846.3029	230	11 2 9	13,478.4030
013	11 3 8	14,306.4902	112	8 8 0	13,846.3031	230	11 3 8	13,596.8133
013	11 4 8	14,316.0702	112	9 2 7	13,285.0776	230	11 4 8	13,693.0144
013	11 4 7	14,398.6690	112	9 4 5	13,449.0326	230	11 5 6	13,908.6228
013	11 5 6	14,501.8885	112	9 5 5	13,573.5747	230	12 5 7	14,197.3815
013	12 0 12	14,014.4246	112	9 5 4	13,567.8762	310	4 3 1	12,501.1754
013	12 1 12	14,017.7220	112	9 6 3	13,738.6028	310	5 2 3	12,557.0953
013	12 1 11	14,237.4463	112	9 7 3	13,869.2758	310	5 4 2	12,726.5996
013	12 2 11	14,238.7048	112	9 7 2	13,869.7983	310	6 2 4	12,707.9009
013	12 2 10	14,430.6443	112	9 8 2	14,060.1030	310	6 3 3	12,768.5133
013	12 3 10	14,431.0632	112	9 8 1	14,060.1029	310	6 4 2	12,868.9496
013	12 3 9	14,585.6370	112	10 1 9	13,358.1987	310	6 5 1	13,001.9964
013	12 4 8	14,696.2065	112	10 2 8	13,511.4812	310	7 3 5	12,916.3286
013	12 5 7	14,793.8583	112	10 3 8	13,517.8719	310	7 3 4	12,942.6388
013	13 1 13	14,247.9783	112	10 4 7	13,662.0118	310	7 4 4	13,032.9191
013	13 1 12	14,492.2750	112	10 4 6	13,700.1557	310	7 4 3	13,036.2446
013	13 2 12	14,493.6606	112	10 5 6	13,805.2033	310	7 6 2	13,334.4951
013	13 3 11	14,704.1405	112	10 5 5	13,805.2109	310	7 6 1	13,334.1878
013	14 0 14	14,499.9287	112	10 6 4	13,978.2343	310	7 7 1	13,463.4491
013	14 1 14	14,499.9659	112	10 7 3	14,107.4283	310	7 7 0	13,463.4493
013	14 1 13	14,759.2145	112	10 8 3	14,296.6101	310	8 1 8	13,089.5121
013	14 2 13	14,761.0111	112	10 8 2	14,296.6052	310	8 1 7	13,236.8084
013	15 1 15	14,768.3668	112	11 2 9	13,755.0959	310	8 2 7	13,240.0704
013	16 0 16	15,053.5327	112	11 3 9	13,746.1355	310	8 2 6	13,342.3347
023	1 0 1	14,062.5460	112	11 4 8	13,905.5702	310	8 3 6	13,366.9024
023	1 1 1	14,077.5312	112	11 4 7	14,222.1738	310	8 3 5	13,414.4384
023	2 0 2	14,107.4037	112	11 7 4	14,367.6347	310	8 4 5	13,482.4090
023	2 1 1	14,135.9807	112	11 8 3	14,555.5513	310	8 4 4	13,489.9219
023	2 2 1	14,180.2653	112	12 2 11	13,812.0145	310	8 5 4	13,614.4032
023	2 2 0	14,181.7524	112	12 2 10	14,012.9422	310	8 5 3	13,611.7311
023	3 0 3	14,171.4394	112	12 3 10	14,005.4680	310	8 6 3	13,783.2448
023	3 1 2	14,213.3712	112	12 4 9	14,176.2383	310	8 6 2	13,783.1209
023	3 2 2	14,250.0033	112	12 5 8	14,337.7970	310	8 7 2	13,963.9670
023	3 3 0	14,337.7281	112	13 4 10	14,453.8447	310	8 7 1	13,963.9624
023	4 1 3	14,314.0216	131	5 4 1	12,521.9155	310	8 8 1	14,175.5434
023	4 2 2	14,359.4724	131	5 5 0	12,711.0583	310	8 8 0	14,175.5436
023	5 1 5	14,352.3014	131	6 4 2	12,665.2303	310	9 1 9	13,252.9844
023	5 1 4	14,435.4494	131	6 5 2	12,855.2955	310	9 1 8	13,422.5818
023	5 2 4	14,454.2088	131	6 5 1	12,855.1645	310	9 2 8	13,431.1750
023	5 3 3	14,553.5952	131	6 6 1	13,067.7143	310	9 2 7	13,552.1868
023	6 0 6	14,464.8871	131	6 6 0	13,067.7209	310	9 3 7	13,557.4993
023	6 1 5	14,575.0068	131	7 4 3	12,832.9951	310	9 3 6	13,638.4798
023	6 2 4	14,643.3381	131	7 5 3	13,023.4806	310	9 4 6	13,691.7157
023	6 3 3	14,709.5615	131	7 5 2	13,022.7544	310	9 4 5	13,705.7840
023	7 1 7	14,596.3898	131	7 6 2	13,235.8002	310	9 5 5	13,827.1263
023	7 2 6	14,742.3701	131	7 6 1	13,235.7962	310	9 5 4	13,823.5385
023	7 2 5	14,820.1109	131	8 4 5	13,023.2156	310	9 6 4	13,998.0490
023	8 0 8	14,744.3129	131	8 5 3	13,212.9771	310	9 6 3	13,997.5102
023	8 1 8	14,744.5861	131	8 6 3	13,427.4009	310	9 7 3	14,177.9134
032	5 4 1	12,700.6302	131	8 6 2	13,427.3664	310	9 7 2	14,177.9079
032	5 5 1	12,884.5978	131	8 7 2	13,738.1580	310	9 8 2	14,393.2515
032	5 5 0	12,884.2926	131	8 7 1	13,738.1619	310	9 8 1	14,393.2514
032	6 3 3	12,705.0766	131	9 2 7	13,029.9664	310	9 9 1	14,514.1374
032	6 4 3	12,843.7340	131	9 4 6	13,236.3497	310	9 9 0	14,514.1374
032	6 4 2	12,844.3443	131	9 5 5	13,421.7749	310	10 0 10	13,436.5247
032	6 5 2	13,029.0329	131	9 5 4	13,422.2579	310	10 1 10	13,436.8854
032	6 5 1	13,028.5674	131	9 6 4	13,642.7339	310	10 1 9	13,625.5693
032	6 6 1	13,235.5217	131	10 2 8	13,266.9745	310	10 2 9	13,623.7259
032	6 6 0	13,235.5180	131	10 4 7	13,471.5419	310	10 2 8	13,777.9427
032	7 2 5	12,793.9487	131	10 6 5	13,879.5412	310	10 3 8	13,779.6750
032	7 4 4	13,010.8320	131	11 3 9	13,535.2669	310	10 3 7	13,886.1255
032	7 5 2	13,196.8493	131	11 3 8	13,645.1719	310	10 4 7	13,922.0005
032	7 6 2	13,404.4220	131	11 4 8	13,727.8601	310	10 4 6	13,959.7291
032	7 6 1	13,404.4398	131	11 4 7	13,776.5673	310	10 5 6	14,062.4649
032	7 7 1	13,632.2362	131	11 5 7	13,920.6223	310	10 5 5	14,058.8641
032	7 7 0	13,632.2386	131	11 7 5	14,455.6488	310	10 6 5	14,237.1919

(continued on next page)

Table 4 (continued)

Vib	<i>J K_a K_c</i>	Term value	Vib	<i>J K_a K_c</i>	Term value	Vib	<i>J K_a K_c</i>	Term value
032	8 2 6	13,002.6834	131	12 5 7	14,221.7103	310	10 7 4	14,414.8877
032	8 3 6	13,048.5739	131	12 6 7	14,517.4420	310	10 7 3	14,414.8699
032	8 4 5	13,201.2690	131	12 6 6	14,425.8768	310	10 8 3	14,634.2104
032	8 4 4	13,216.2475	150	9 8 2	14,294.5736	310	10 8 2	14,634.2055
032	8 5 3	13,389.0166	150	9 8 1	14,294.5735	310	10 9 2	14,755.7875
032	8 6 3	13,596.9427	150	10 8 3	14,536.6212	310	10 9 1	14,755.7875
032	8 6 2	13,596.9579	150	10 8 2	14,536.6163	310	11 1 10	13,837.6346
032	8 7 2	13,826.6696	150	11 7 4	14,457.3056	310	11 2 10	13,842.6968
032	8 7 1	13,826.6684	160	4 0 4	12,593.0429	310	11 2 9	14,019.9026
032	9 3 6	13,318.0300	160	5 0 5	12,710.7098	310	11 3 9	14,018.3035
032	9 4 6	13,412.0763	160	6 1 6	12,934.8835	310	11 3 8	14,151.4816
032	9 5 4	13,605.2537	160	11 0 11	13,798.0690	310	11 4 8	14,172.3122
032	9 6 3	13,813.3222	160	12 2 11	14,240.5007	310	11 4 7	14,245.7451
032	9 7 2	14,043.5606	211	5 3 2	12,630.5888	310	11 5 6	14,345.5455
032	10 3 8	13,479.2969	211	8 4 5	13,225.7343	310	11 6 5	14,496.2902
032	10 4 7	13,672.8565	211	8 5 4	13,362.9598	310	11 7 4	14,674.6264
032	10 4 6	13,681.1811	211	8 6 3	13,529.1005	310	12 2 11	14,079.1811
032	10 7 4	14,283.1184	211	8 7 2	13,654.2506	310	12 3 10	14,275.7107
032	11 3 8	13,852.5076	211	8 7 1	13,654.2505	310	12 5 7	14,631.3305
032	11 4 8	13,919.4432	211	8 8 1	13,895.6291	310	12 6 6	14,780.1871
032	11 4 7	13,955.6084	211	8 8 0	13,895.6374	310	13 1 12	14,332.2084
032	12 3 10	13,989.3529	211	9 3 6	13,376.2645	310	13 3 10	14,438.1281
032	12 4 9	14,198.0829	211	9 4 5	13,456.5804	320	3 2 1	14,110.6224
032	14 3 12	14,585.8217	211	9 4 6	13,435.9009	320	4 2 3	14,194.9757
051	8 8 1	14,005.2230	211	9 5 4	13,575.7981			

Notes: Vib *J K_a K_c* – vibration and rotation assignment of the energy level; term value – energy level obtained in this study (cm⁻¹).

Energy term values corrected compare to corresponding value given by IUPAC-TG (10) and Ref. [23] are given in *italic*.

^a In Ref. [10], this levels assigned to the (310) vibration state (see text).

5. Conclusion

Absorption spectrum of ¹⁷O enriched water vapor was recorded and analyzed between 12,277 and 12,894 cm⁻¹. More than 3400 transitions, corresponding to five water isotopologues (H₂¹⁷O, H₂¹⁶O, H₂¹⁸O, HD¹⁶O, and HD¹⁷O), were observed in this work. About 3000 of them were assigned using the calculations of Partridge and Schwenke [31,32] in combination with the known empirical energy levels [9–11]. In which more than 1100 transitions of H₂¹⁶O and H₂¹⁷O as well as 51 lines of the 5ν₁ band of HD¹⁷O were observed for the first time. Quite a few disagreements between recorded spectrum and the HITRAN2016 data for the H₂¹⁶O and H₂¹⁷O molecules were observed.

About 420 highly excited vibration-rotation energy levels were newly obtained through this work which could make significant improvements of 193 energies reported by IUPAC-TG [9–11] and Refs. [23,34] in the studied region. Rotational energies of the (023) and (230) states of H₂¹⁷O have been assigned for the first time.

The reported data could be useful for the future improvements of the spectroscopic databases HITRAN [24] and GEISA [41] as well as for the updates of the energy level sets [9–11].

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.jqsrt.2018.10.009.

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