Fourier Transform Absorption Spectra of $H_2^{18}O$ and $H_2^{17}O$ in the $3\nu + \delta$ and 4ν polyad region

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Abstract

Fourier transform absorption spectra of $H_2^{18}O$-enriched and $H_2^{17}O$-enriched water vapor in the $3\nu + \delta$ and 4ν polyad region have been analyzed. With the aid of theoretically calculated linelists, we have assigned 910 lines identified as belonging to $H_2^{18}O$ and 823 lines belonging to $H_2^{17}O$.

1 INTRODUCTION

A precise knowledge of line positions and strengths of water vapor is crucial for accurate atmospheric modelling. Current models of the Earth's atmosphere may underestimates the absorption of solar energy by as much as 15-30 Wm^{-2} on average [1–4]. Water vapor is considered to be the major candidate for the missing absorption, although it already accounts for about 70 % of the known absorption of incoming soalr radiation in the Earth's atmosphere [5]. Trace isotopologues of water, such as $H_2^{17}O$ and $H_2^{18}O$, have been less extensively studied than the most abundant $H_2^{16}O$, despite their significant possible contribution to the absorption of solar radiation in the atmosphere.

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In 1981, Chevillard and co-workers recorded spectra with isotopically enriched $H_2^{18}O$ and $H_2^{17}O$ samples over a wide frequency range using the Fourier transform spectrometer at the National Solar Observatory (Kitt Peak, AZ). Many studies of the spectra have been made and the detailed information of the experiment can be found elsewhere [6–16]. Tanaka et al. [12] previously analyzed the $H_2^{18}O$ spectrum in the $3\nu + \delta$ and 4ν polyad region using a variational linelist generated by Partridge and Schwenke [17]. In this work, we re-analyzed this spectrum using newly calculated linelists. This allowed us to extend the number of assignments made from 747 to 910, leaving only 15 lines unassigned. The spectra of $H_2^{17}O$ have been extensively analyzed by Toth [6–10] in the past. The highest frequency region studied is by Camy-Payret et al. [13], in which they analyzed up to 11335 cm^{-1}. In this work, again using newly calculated linelists, we extend the analysis of $H_2^{17}O$ up to 14520 cm^{-1}, covering the entire $3\nu+\delta$ and 4ν polyad.

2 EXPERIMENTAL CONDITIONS

Table 1
Experimental conditions of the spectra analyzed in this work. l is the absorption pathlength, P is the total pressure with error of $\pm1\%$, T is the temperature and R is the resolution. These spectra can be found in the digital archive at the National Solar Observatory website (http://diglib.nso.edu/) under the file names given below.

Type of spectrum (file name)	l (m)	P (hPa)	T (K)	R (cm^{-1})	Range (cm^{-1})
$H_2^{18}O$ enriched (810825R0.002)	434.0	3.62	300.5	0.0168	12400 – 14520
$H_2^{17}O$ enriched (810827R0.001)	434.0	6.32	301.2	0.0143	11500 – 12800
$H_2^{17}O$ enriched (810827R0.002)	434.0	6.32	301.4	0.0168	12900 – 14500

The spectra of two isotopically enriched samples of water vapor were recorded using the McMath-Pierce Fourier transform spectrometer. The first sample contained $H_2^{18}O$ at $73\pm1\%$ [15], referred as "^{18}O" below, and the second sample, "^{17}O" below, contained enriched $H_2^{17}O$ and $H_2^{18}O$ [16]. In both experiments, the sample was contained in a 6-m White type cell to create the absorption pathlength of 434 m. The experimental conditions of each spectrum can be found in Table 1. Lines in both spectra were fitted using the GREMLIN program of Brault (unpublished).

The ^{17}O and ^{18}O spectra contain transitions by $H_2^{16}O$, $H_2^{17}O$ and $H_2^{18}O$ and in some cases even by HDO. In order to filter the transitions due to the isotopologue of interest – $H_2^{17}O$ for ^{17}O spectrum and $H_2^{18}O$ for ^{18}O – we compared the spectra of natural abundance water, ^{17}O and ^{18}O simultaneously. In this

work, the Fourier transform spectrum of natural abundance pure water measured by Schermaul et al. [18] at Rutherford Appleton Laboratory (UK) was used instead of the one by Mandin et al. [19] recorded at the same time as the isotopically enriched spectra at Kitt Peak. The spectrum by Schermaul et al. was selected as it is known to contain many lines that were not observed previously. Three spectra were read into a spreadsheet and lines of the same frequency were aligned. The intensities of these were ratioed to look for the characteristic patterns that have been derived from the isotopic composition of each sample. For the ^{18}O spectrum, 925 lines were attributed to $H_2^{18}O$ and for the ^{17}O spectrum, 845 lines were attributed to $H_2^{17}O$ in this fashion. A complete list of these lines including absolute intensities and rotational and vibrational quantum numbers are given in the electric archive. Absolute intensities (given in cm molecule^{-1}) are scaled to the natural abundance of each isotopologue and normalized to 296 K to match the HITRAN temperature.

3 LINE ASSIGNMENTS

Two linelists were used for line assignments. One was generated at University College London using the DVR3D program suite [20] with the potential energy surface (PES) by Shirin et al. [21] and the ab initio dipole moment surface (DMS) fitted by Lynas-Gray et al. to the calculations of Polyansky and co-workers [22]. The parameters used in this calculation can be found in reference [23]. Another linelist was generated by Tashkun and Uzed (??) at the Institute of Atmospheric Optics following the method in reference [17] with the PES by Partridge and Schwenke [17] and the ab initio DMS by Schwenke and Partridge [24].

The following procedure was used for making assignments. First we made "trivial" assignments, which are ones linking upper energy levels already determined experimentally. The remaining unassigned lines were compared to the spectra synthesized from the two linelists, which contain:

(1) Line positions in cm^{-1}
(2) Line intensity in cm molecule^{-1}
(3) Upper rotational quantum numbers, J' K'$_a$ K'$_c$
(4) Lower rotational quantum numbers, J" K"$_a$ K"$_c$
(5) Upper vibrational quantum numbers, (v'$_1$ v'$_2$ v'$_3$)
(6) Lower vibrational quantum numbers, (v"$_1$ v"$_2$ v"$_3$)

Initial assignments were made for each experimental line by selecting the theoretical lines whose line positions fall within the experimental position $\pm$ 0.03 cm^{-1}. The value of error can be varied to narrow or broaden the selection window. Intensities were also taken into consideration to make initial assign-

ments. The intensities of the 100 strongest experimental lines were compared with those of the corresponding theoretical lines to give the intensity ratios. These ratios were used as a rough guide for making the initial assignments.

Upper energy levels were then determined by adding the energies of lower levels, which were taken from the earlier study by Toth [7], to the experimental frequencies. All possible combinations of transitions with those upper energy levels were generated to search for further assignments by combination differences. Upper energy levels that were not confirmed by combination differences are re-considered and any necessary changes were made. The ratios of new upper energy levels to $H_2^{16}O$ energy levels were taken to check the reliability of assignments, as these ratios are approximately constant within a vibrational band [12]. Another way to check the assignments was to look at the differences between the observed and calculated energy levels. The Obs − Calc values tend to be systematic, like the ratios, and can be used to check the validity of energy levels. Further assignments were made using a small computer program that calculates all possible combinations of upper and lower energy levels with the observed transition frequencies.

The previous analysis of the ^{18}O spectrum assigned 746 out of 926 lines in the range of $12400 - 14520$ cm^{-1} [12]. In this work, we extended the number of assigned lines to 910 including 4 lines belonging to $H_2^{16}O$ at 13563.32, 13907.03, 14136.20 and 14386.61 cm^{-1}. A comparison of the assignments between the previous analysis and this work are as follows. The same assignments were found in both works for 616 lines and different assignments for 125 lines. Previously unassigned 169 lines were newly assigned in this work and 5 previously assigned lines were not assigned in this work. Ten lines were not assigned in both works.

Table 2 gives the summary of $H_2^{18}O$ energy levels determined in the previous analysis and this work. In this work, the lines are assigned to 17 different upper vibrational bands, giving 459 new energy levels. This is a great improvement compared to the previous analysis, in which 384 new energy levels were determined. In particular, the (301) vibrational band is significantly improved as almost twice as many levels are obtained in this work. The band origin of the (112) band is newly derived at 12408.797 cm^{-1}, though that of (202), which was determined in the previous analysis, was not included since the previous assignment of this transition was incorrect. Table 3 gives the derived energy levels for (221), (400), (301), (202) and (103) vibrational bands.

Table 2
Summary of $H_2{}^{18}O$ energy levels determined in the previous analysis (a) and this work (b). Bands are labelled using normal mode (left) and local mode (right) notations. No. of levels shows the number of newly determined energy levels. No. of trans. shows the number of transitions to the vibrational bands.

Band	Origin (cm^{-1})		No. of levels		No. of trans.	
	a	b	a	b	a	b
(070) or 00 7	—	—	0	1	0	1
(230) or 20^+3	—	—	0	1	0	1
(310) or 30^+1	—	—	0	8	0	8
(112) or 21^+1	—	12408.797	42	37	57	52
(211) or 30^-1	—		7	3	12	3
(013) or 21^-1	12520.123	12520.123	62	63	95	96
(141) or 20^+4	—	—	1	1	2	1
(320) or 30^+2	—	—	0	16	0	18
(042) or 11 4	—	—	1	3	2	4
(122) or 21^+2	—	—	9	10	10	14
(221) or 30^-2	13612.710	13612.710	63	66	140	141
(023) or 21^-2	—	—	11	12	15	15
(400) or 40^+0	13793.093	13793.093	45	51	101	112
(301) or 40^-0	13795.398	13795.398	47	80	122	219
(202) or 31^+0	14188.823	—	38	46	82	92
(103) or 31^-0	14276.336	14276.336	43	60	95	127
(071) or 10^-7	—	—	0	1	0	2
		Total	**384**	**459**	**746**	**906**

J	K_a	K_c	(221) or 30^-2		(400) or 40^+0		(301) or 40^-0		(202) or 31^+0		(103) or 31^-0	
0	0	0	13612.71029	1	13793.09263	1	13795.39829	1			14276.33594	1
1	0	1	13635.47507	1	13815.59986	1	13817.70342	2	14210.32317	2	14298.91140	2
1	1	1	13651.98268	2			13828.30932	2	14221.01936	2	14308.78585	2
1	1	0	13657.84428	2			13833.44816	2	14226.20768	2	14314.08100	2
2	0	2	13679.55793	2	13858.82353	2	13860.81739	3	14253.48141	2	14342.39912	3
2	1	2	13691.79112	3	13865.89185	3	13867.80525	3	14260.48336	3	14348.71126	3
2	1	1	13709.27878	3			13883.19049	4	14276.00949	1	14364.54358	3
2	2	1	13757.79133	2	13912.95811	3	13914.90280	2	14307.88613	3	14393.96665	2
2	2	0	13759.09973	2			13916.36102	2	14309.32461	1	14395.59132	3
3	0	3	13743.82800	2	13919.95382	2	13922.46923	3	14315.15534	3	14404.30826	2
3	1	3	13750.40525	3	13924.60916	3	13926.26742	4	14318.83042	3	14407.71132	3
3	1	2	13785.36505	2	13954.59924	3	13956.63031	3	14349.54377	3	14438.85673	3
3	2	2	13826.22733	4	13980.00173	3	13981.85123	4	14374.78800	1	14462.30154	4
3	2	1	13832.33231	3	13986.48666	2	13988.46695	4	14381.30031	4	14469.35834	4
3	3	1	13920.64162	2	14046.11288	1	14047.93090	4	14440.77476	2	14524.26011	2
3	3	0	13920.17986	2	14046.38039	2	14048.20104	3	14440.79902	3	14524.59279	2
4	0	4	13824.20313	3	13999.43072	2	14001.79765	4	14393.73465	3	14483.13081	3
4	1	4	13827.77120	2	14000.37909	3	14002.83899	3	14395.37957	3	14486.10948	2
4	1	3	13884.62104	3	14050.14656	3	14052.07040	5	14445.05599	1	14535.04019	3
4	2	3	13916.52921	2	14068.12697	5	14069.83089	3	14462.74970	4	14552.07242	2
4	2	2	13932.60782	3	14084.79248	1	14086.09077	4	14478.34927	2	14569.38969	3
4	3	2	14013.56790	3	14137.08567	2	14139.53803	4	14532.19471	2	14625.15782	2
4	3	1	14014.70784	3	14139.47837	2	14141.32217	3	14532.92982	1	14625.85421	3
4	4	1	14136.83791	1	14226.98082	3	14228.72822	2	14614.41463	3	14700.01981	2
4	4	0	14137.80518	5	14227.02494	2	14228.77416	3	14612.98367	2	14700.11566	2
5	0	5	13921.24394	2	14094.85513	2	14097.01368	3	14488.92057	3	14578.70108	3
5	1	5	13922.96724	3			14097.34284	3	14489.59278	2	14578.84244	3
5	1	4	14004.81826	3	14165.41210	2	14167.13472	3	14560.10049	3	14650.39783	2
5	2	4			14176.38001	2	14177.89117	4	14570.80649	1	14663.40709	2
5	2	3	14059.51085	3	14208.15462	3	14210.13363	4	14604.02424	2	14694.45647	2
5	3	3	14130.17703	3	14252.11938	3	14253.79726	5			14742.84949	3
5	3	2	14134.65727	3	14258.18173	5	14260.08003	4	14649.28398	3	14746.06618	1
5	4	2	14254.29839	1	14342.22639	2	14343.90916	3	14729.97901	1	14814.53462	3
5	4	1	14254.58044	1	14342.56177	3	14344.25567	4	14725.98397	3	14815.00955	1
5	5	1	14403.02357	2			14461.44404	1			14920.61971	1
5	5	0			14459.52415	1						
6	0	6	14034.75914	2			14208.49623	4	14600.77549	2	14691.21013	3
6	1	6	14035.65941	2			14209.41305	3	14601.15128	2	14691.31229	2
6	1	5	14143.37873	2	14298.24448	1	14299.75424	5			14782.66823	2
6	2	5	14155.69990	2	14303.85880	5	14305.09126	4	14697.99098	2		

Table 3: Continued.

J	K_a	K_c	(221) or 30^-2		(400) or 40^+0		(301) or 40^-0		(202) or 31^+0		(103) or 31^-0	
6	2	4	14212.57896	3	14354.73609	2	14356.66563	4	14750.62614	1	14842.36805	3
6	3	4	14269.31665	2	14388.38345	3	14389.96178	5	14782.01039	1	14883.09568	1
6	3	3	14281.02374	2			14405.51508	3	14802.09627	1	14892.38763	3
6	4	3	14395.09222	2	14480.74647	4	14482.38676	3	14869.82308	2	14952.44196	2
6	4	2	14396.32699	4			14483.95878	3	14862.31441	1	14954.52556	3
6	5	2			14598.93038	2	14543.03817	1				
6	5	1	14600.90788	2			14543.06111	3			15058.80154	1
6	6	0			14699.06176	1					15185.26879	1
7	0	7	14164.98360	2	14336.00436	1	14338.16022	3	14729.68938	1	14820.77804	2
7	1	7	14166.15979	2			14338.19745	3			14821.32304	2
7	1	6	14299.34341	2	14450.08116	3	14449.58071	2			14931.11087	1
7	2	6	14305.54084	2	14445.63518	2	14451.94496	3			14931.67598	2
7	2	5					14523.75755	2	14918.21965	1		
7	3	5	14430.31292	2			14546.88825	3	14933.63752	1	15047.53278	1
7	3	4					14577.28115	3			15065.09786	1
7	4	4	14559.95017	3	14642.23213	2	14643.89424	3			15113.44632	2
7	4	3	14563.03734	1			14648.90231	2	15021.00190	1		
7	5	3	14763.80889	3			14706.28910	4				
7	5	2			14762.19471	2						
7	6	1			14861.21203	2						
7	7	1					15006.27198	1				
8	0	8	14312.78125	2					14875.28773	1	14967.27005	2
8	1	8	14310.23219	1	14484.28747	3	14484.31235	1	14875.95652	1	14967.30694	1
8	1	7	14470.93016	2	14610.56440	1	14613.41220	4			15095.98645	2
8	2	7			14611.18528	1	14613.83616	2				
8	2	6			14706.38994	1	14708.94136	3			15196.79084	1
8	3	6					14723.86310	1				
8	3	5	14656.46424	2			14773.49755	4			15261.97758	1
8	4	5	14746.52326	1	14826.16782	1	14827.79287	1				
8	4	4	14755.67830	2			14840.17578	3				
8	6	3			15046.44596	1						
8	7	1					15191.25310	1				
9	0	9	14470.24389	1			14647.38424	1			15130.93636	1
9	1	9	14474.76447	2			14647.43967	2			15130.94430	1
9	1	8	14658.71978	1			14794.39631	1				
9	2	8	14658.61047	1			14794.52476	2				
9	2	7			14909.12492	1	14910.64274	1				
9	3	7	14812.23491	1	14918.54467	1	14919.63884	2				
9	4	6	14955.62868	1			15033.55578	1				
10	0	10	14654.06973	1							15311.61809	2
10	1	10					14827.43811	1				

J	K_a	K_c	(221) or 30^-2		(400) or 40^+0	(301) or 40^-0		(202) or 31^+0	(103) or 31^-0
10	1	9				14992.29033	2		
10	2	9				14992.31379	1		
10	2	8	15028.64285	1		15132.67530	1		
10	3	7				15229.07469	1		
10	4	6				15301.95453	1		
11	0	11				15024.31130	2		

The ^{17}O spectrum was analyzed in the range of $11335 - 14520$ cm^{-1}, which covers the entire $3\nu + \delta$ and 4ν polyad. We assigned 823 lines out of 845 lines attributed to $H_2^{17}O$, leaving only 22 lines unassigned. Table 4 gives the summary of energy levels derived in this work. All the lines originate in the (000) ground vibrational level and are assigned to 15 different upper vibrational levels. Band origins of (131), (211), (013), (221), (301) and (103) are newly determined at 11792.827, 12132.993, 12541.226, 13631.500, 13812.158 and 14296.280 cm^{-1}, respectively. As was recognised in the earlier analysis of the ^{18}O spectrum [12], the ratios of $H_2^{17}O$ to $H_2^{16}O$ energy levels were constant within the vibrational bands. Also the systematic differences in observed and calculated energy levels were seen, which helped to check the validity of the energy levels derived. Many levels were confirmed by combination differences, especially those in (211) and (301) vibrational states, which makes the derived energy levels much more reliable. Table 5 gives the newly determined energy levels of the $3\nu + \delta$ polyad, (131), (310), (112), (211) and (013) and Table 6 gives the energy levels of the 4ν polyad, (221), (400), (301), (202) and (103). The number of levels assigned to each level is also given in those tables. Many lines are assigned to the (211) and (301) vibrational bands, which are the strongest bands in the $3\nu + \delta$ and 4ν polyad respectively.

Table 4
Summary of $H_2^{17}O$ energy levels determined. Bands are labelled using normal mode (left) and local mode (right) notations. "levels" shows the number of newly determined energy levels. "trans" shows the number of transitions to the vibrational bands.

Band	Origin (cm^{-1})	levels	trans
(003) or 21^-0	—	1	1
(131) or 10^-3	11792.827	31	47
(310) or 30^+1	—	25	35
(112) or 21^+1		45	45
(211) or 30^-1	12132.993	77	189
(013) or 21^-1	12541.226	38	65
(141) or 20^+4	—	1	1
(320) or 30^+2	—	3	5
(042) or $11\ 4$	—	1	1
(221) or 30^-2	13631.500	46	100
(400) or 40^+0		31	55
(301) or 40^-0	13812.158	74	192
(202) or 31^+0	—	13	19
(103) or 31^-0	14296.280	35	65
(071) or 10^-7	—	2	3
	Total	**402**	**823**

Table 5: H$_2$^{17}O energy levels determined using the newly calculated linelist (cm^{-1}). Also given are the number of transitions assigned to each level.

J	K_a	K_c	(131) or 30$^-$2		(310) or 40$^+$0		(112) or 40$^-$0		(211) or 31$^+$0		(013) or 31$^-$0	
0	0	0	11792.82700	1					12132.99260	1	12541.22550	1
1	0	1	11816.05370	1	12144.98240	1	12411.93400	2	12155.59840	1	12564.35220	1
1	1	1	11838.44175	2	12158.97125	2			12169.33615	2	12576.62510	2
1	1	0					12430.92195	2	12174.88130	2	12582.32490	1
2	0	2	11861.33315	2			12456.16010	1	12200.76697	4	12608.99765	2
2	1	2			12198.04125	2	12465.45070	2	12209.35277	3	12617.18930	1
2	1	1	11897.17285	2					12225.92685	2	12634.26443	3
2	2	1	11962.49960	1	12256.37715	2	12522.38277	3	12266.28460	2	12670.69500	1
2	2	0	11963.61530	2					12267.66577	3	12672.25635	2
3	0	3			12252.45030	1	12519.56983	3	12263.67740	3	12672.90415	2
3	1	3	11938.38175	2	12257.69180	1	12524.78763	3	12268.62667	4	12677.12280	2
3	1	2	11975.04207	3	12290.72490	1	12557.83495	2	12301.35840	3	12710.87990	1
3	2	2	12032.23413	3	12324.84210	1	12590.89930	2	12334.60165	4	12740.17557	3
3	2	1			12330.88040	1	12597.30240	1	12340.98587	4	12747.30710	2
3	3	1	12151.83090	1			12671.05745	2	12415.26155	2	12814.68590	2
3	3	0	12151.95690	1			12671.51660	2	12415.48680	2	12814.97070	1
4	0	4	12009.84515	2			12600.42505	2	12344.16707	3	12753.40925	2
4	1	4	12016.91630	1	12335.57130	1	12602.66560	2	12346.51193	3	12755.67965	2
4	1	3	12076.78425	2					12399.52863	3	12810.29705	2
4	2	3			12415.04203	3	12681.04295	2	12424.54793	4		
4	2	2	12138.65505	2			12697.78500	1	12441.17624	5	12849.68450	2
4	3	2	12246.90120	1	12499.80920	1	12765.08800	1	12508.65537	3		
4	3	1							12510.14947	4	12912.00185	2
4	4	1							12616.39270	2		
4	4	0	12402.72870	1	12609.09910	1			12616.41805	2	13008.49125	2
5	0	5			12430.27630	1	12696.99530	2	12441.42487	3	12851.19880	1
5	1	5			12431.39830	1			12442.42300	3	12852.33270	3
5	1	4					12775.58670	2	12517.88630	3	12929.91330	2
5	2	4	12237.69800	1	12526.37870	3			12535.36052	4	12943.35433	3
5	2	3					12824.44425	2	12567.59030	3		
5	3	3	12365.53960	1			12881.88360	1	12625.18173	3	13029.04557	3
5	3	2			12621.43380	1			12630.59070	2		
5	4	2	12521.62515	2					12733.62580	2	13131.38360	1
5	4	1							12733.89403	3		
5	5	1	12711.07360	1	12860.91340	1			12868.94150	1	13250.33350	1
5	5	0			12860.95640	1						
6	0	6	12226.13790	2			12811.32850	1	12555.52837	3	12965.87370	2
6	1	6			12544.74860	1			12555.96855	2		
6	1	5	12346.86740	1					12658.93855	4	13067.16485	2
6	2	5	12372.01400	1	12653.08947	3			12662.10230	1		

Table 5: Continued.

J	K_a	K_c	(131) or 30^-2		(310) or 40^+0		(112) or 40^-0		(211) or 31^+0		(013) or 31^-0	
6	2	4							12718.46697	4	13131.22100	1
6	3	4			12755.60580	1			12764.16637	3		
6	3	3	12516.28170	1					12778.04082	4	13186.71170	1
6	4	3	12668.36585	2			13130.32240	1	12874.51820	2		
6	4	2							12875.73610	5		
6	5	2			13001.73670	1			13009.99960	1		
6	5	1	12855.13170	1					13010.01190	2	13392.34550	1
6	6	0							13175.36840	1		
7	0	7					12942.50990	1	12686.64430	1		
7	1	7							12687.18183	3	13097.77805	2
7	1	6					13066.53390	1	12811.88110	2		
7	2	6			12805.93200	1			12813.56767	4	13226.43090	1
7	2	5							12891.47220	1		
7	3	5	12670.65420	2	12916.31280	1			12924.66043	3		
7	3	4							12952.60805	2		
7	4	4	12833.07180	1					13038.78660	3		
7	5	3							13174.67000	2		
7	5	2	13022.69500	1								
7	6	2							13339.97860	1		
7	7	1							13463.09680	1		
8	0	8							12835.28435	2	13246.77950	1
8	1	8							12834.24467	3		
8	1	7							12979.83160	2	13390.76430	1
8	2	7							12981.25605	2		
8	2	6							13083.84330	2		
8	3	6			13099.62000	1						
8	3	5							13152.85837	3		
8	4	4							13236.13030	1		
8	5	3							13363.62350	2		
9	0	9							12999.13090	1		
9	1	9							12999.86095	2		
9	1	8							13166.39080	1		
9	2	8							13166.45910	2		
9	3	7					13293.19310	1				
9	3	6							13376.28000	1		
9	4	6							13435.89650	1		
10	0	10							13181.62105	2		
10	1	10							13181.57620	1		
10	1	9							13365.21130	1		
10	2	9							13368.73930	1		
10	2	8							13524.27990	1		

J	K_a	K_c	(131) or 30^-2	(310) or 40^+0	(112) or 40^-0	(211) or 31^+0	(013) or 31^-0
10	3	7				13618.93760 1	
10	4	6				13703.59770 1	
11	1	11				13380.83600 1	
11	2	10				13586.32560 1	

Table 6: $H_2^{17}O$ energy levels determined in this work (in cm^{-1}). Also given are the number of transitions assigned to each level.

J	K_a	K_c	(221) or 30^-2		(400) or 40^+0		(301) or 40^-0		(202) or 31^+0		(103) or 31^-0	
0	0	0	13631.49980	1			13812.15810	1			14296.27950	1
1	0	1	13654.26415	2	13832.08220	1	13834.48680	2	14225.90410	1	14318.87850	2
1	1	1	13670.98940	2			13845.21055	2			14328.88035	2
1	1	0	13676.85125	2			13850.33605	2	14241.93080	1	14334.16110	2
2	0	2	13698.30330	2	13875.37620	1	13877.91880	3			14362.42545	2
2	1	2	13710.87750	2	13882.60000	2	13884.75020	3	14276.28470	2	14368.85827	3
2	1	1	13728.28323	3			13900.08675	4	14291.73835	2	14384.64507	3
2	2	1	13777.38650	2	13930.08735	2	13932.28335	2			14414.46010	2
2	2	0	13778.67775	2			13933.72510	3			14416.06120	2
3	0	3	13762.75575	2	13937.30000	1	13939.16153	3	14330.92273	3	14424.45170	1
3	1	3	13769.54527	3	13941.46610	3	13943.34780	4			14427.92710	3
3	1	2	13804.39640	2	13971.27700	1	13973.56427	3	14365.31405	2		
3	2	2	13845.86960	3	13997.19130	2	13999.27500	4			14482.78740	3
3	2	1	13851.88910	3			14005.79260	3	14397.46990	1	14489.79835	2
3	3	1	13940.42787	4			14066.13480	2			14545.42095	2
3	3	0	13940.69567	3			14066.39915	2				
4	0	4	13843.36830	2	14016.29675	2	14018.94880	4			14503.44410	1
4	1	4	13847.02420	2	14017.31550	1	14020.01550	3	14411.40560	2	14505.95540	2
4	1	3	13903.70945	4	14066.93010	1	14069.10837	4			14555.32065	2
4	2	3	13936.43720	1	14085.41365	2	14087.33192	4			14572.54210	1
4	2	2	13952.14760	3			14104.01343	4			14589.83377	3
4	3	2	14034.09330	3	14155.80383	3	14157.78747	3				
4	3	1	14035.20995	2			14159.51073	4			14645.59940	2
4	4	1	14158.73170	1	14246.24060	1	14248.24330	2	14633.90990	1		
4	4	0	14158.76175	2			14248.28025	2			14722.22560	1
5	0	5	13940.63310	1	14111.91690	2	14114.34920	3			14599.21695	2
5	1	5	13942.40140	3			14114.68570	2			14599.24510	2
5	1	4	14024.04630	2	14182.43810	2	14184.38260	3			14670.89625	2
5	2	4	14044.43750	1	14193.81485	2	14195.52103	4			14683.46175	2
5	2	3	14079.06155	2	14225.16210	2	14227.45197	4	14620.37150	1	14714.97440	1
5	3	3	14150.74927	3			14272.08798	4			14762.59420	1
5	3	2			14276.16632	4	14278.20683	3				
5	4	2					14363.48190	4				
5	4	1	14276.23720	1	14361.87910	1	14363.81615	2	14745.61500	1		
5	5	1					14483.46140	2				
6	0	6	14054.38970	2	14225.02390	1	14226.21417	4			14711.95080	2
6	1	6	14055.33480	2			14227.04275	2			14712.05340	1
6	1	5	14163.58460	1	14315.65310	1	14317.38415	4			14803.46030	2
6	2	5	14176.12350	1	14321.54600	4	14322.92103	3				
6	2	4	14231.94132	4			14374.09867	4			14863.05215	2

Table 6: Continued.

J	K_a	K_c	(221) or 30^-2		(400) or 40^+0		(301) or 40^-0		(202) or 31^+0		(103) or 31^-0	
6	3	4			14406.59673	6	14408.23570	2				
6	3	3	14301.24553	3	14421.32480	1	14423.55100	5	14820.10680	1		
6	4	3			14500.16210	1	14502.05627	3				
6	4	2	14417.95733	3			14503.54183	3				
6	5	2							15009.23130	1		
6	5	1	14623.13710	1			14565.42670	3				
6	6	0	14657.62010	1			14724.60100	1				
7	0	7					14356.00595	2			14841.69650	1
7	1	7	14186.28530	2			14356.01660	3			14841.55380	2
7	1	6			14460.90970	1	14467.57827	3				
7	2	6	14325.93480	1	14463.70520	1	14468.27965	2			14952.64220	1
7	2	5			14538.86750	1	14541.46063	3			15031.17270	1
7	3	5	14451.09210	1	14563.62040	1	14565.49243	3				
7	3	4					14595.29065	2				
7	4	4	14581.57820	1			14663.64290	1				
7	4	3					14668.42560	1				
7	5	3	14786.21350	1			14728.54115	2				
7	6	2					14885.76160	1				
8	0	8	14333.14800	1			14502.39173	3			14988.56840	1
8	1	8					14502.43040	1				
8	1	7	14491.38290	1			14631.79133	3				
8	2	7					14632.24545	2				
8	2	6					14727.04580	2				
8	3	6	14632.47650	1	14741.23050	1	14742.53940	2				
8	3	5					14791.55880	3				
8	4	4					14859.78790	1				
9	0	9					14665.81940	1				
9	1	9					14665.92625	2				
9	1	8					14813.17950	2				
9	2	8	14679.52800	1			14813.32640	1				
9	3	7					14938.82250	1				
9	4	6					15053.79620	1				
10	0	10					14846.20660	2				
10	1	10					14846.19650	1				
10	1	9	14887.31770	1			15011.52915	2				
10	2	9					15011.59060	1				

4 DISCUSSION AND CONCLUSION

A new version of HITRAN (HITRAN2004) has just been released [25] and all the transitions of $H_2^{18}O$ analyzed in this work are included in this edition. The previous version of HITRAN (HITRAN2000) [26] contained 51 transitions assigned to $H_2^{18}O$ by Mandin *et al.* [19] in the region studied here, which are confined to the frequency range $13608 - 13893$ cm^{-1}. These 51 common lines have been all replaced by the new lines obtained in this work.

The highest frequency listed for $H_2^{17}O$ in the HITRAN2000 is 11143 cm^{-1}, which is considerably low compared to that for $H_2^{16}O$ and $H_2^{18}O$. Unlike the $H_2^{18}O$, the $H_2^{17}O$ lines analyzed are got to be included in HITRAN. However the significance of this data to atmospheric modelling and other applications is beyond doubt.

The cavity ring-down spectra of $H_2^{18}O$ and $H_2^{17}O$ in the 5ν polyad region have been analyzed recently [23, 27]. In order to provide more complete data for water isotopologues, the missing $4\nu + \delta$ polyad region ($14500 - 16700$ cm^{-1}) need to be studied. The success of analyzing the $H_2^{18}O$ and $H_2^{17}O$ spectra in this work should encourage the measurements of isotopically enhanced spectra in the $4\nu + \delta$ and higher polyad regions.

In this work, the Fourier transform spectra of $H_2^{18}O$-enriched and $H_2^{17}O$-enriched water vapor have been analyzed using theoretically calculated linelists. We have assigned 910 out of 926 lines attributed to $H_2^{18}O$ and 823 out of 845 lines attributed to $H_2^{17}O$.

5 ACKNOWLEDGEMENTS

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