# The Interacting States (020), (100), and (001) of $H_2^{17}O$ and $H_2^{18}O$

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A fit of about 350 rotational levels of the (020), (100), and (001) vibrational states has been performed for  $H_2^{17}O$  as well as for  $H_2^{18}O$  leading to the determination of 51 rotational and coupling constants for each isotopic species. The Fermi-type interaction and the two Coriolis-type interactions have been taken into account by appropriate rotation-vibration operators and the v-diagonal part of the Hamiltonian is, for each vibrational state, a Watsontype Hamiltonian. The results are very satisfactory since 87% of the experimental levels are reproduced within  $15 \times 10^{-3}$  cm<sup>-1</sup>.

### INTRODUCTION

This paper is a continuation of our effort to understand precisely the vibrationrotation energy levels of water (1-3). In particular we report here a study of the triad of interacting states {(020), (100), (001)} of the isotopic species H<sub>2</sub><sup>17</sup>O and H<sub>2</sub><sup>18</sup>O. This work has two motivations. First, since the resonances affecting the vibrorotational levels are strongly isotopically dependent it is necessary to study the <sup>17</sup>O and <sup>18</sup>O species for their own and this may eventually lead to an improvement of the potential function. Second, since in high-resolution atmospheric spectra many lines of these two isotopic species contribute to the absorption, a good knowledge of energy levels and wavefunctions is necessary to calculate reliable line positions and intensities.

## THEORETICAL CONSIDERATIONS

According to the approximate relation  $2\omega_2 \simeq \omega_1 \simeq \omega_3$ , the vibrational states of water group into polyads of interacting states corresponding to a given value of  $2v_1 + v_2 + 2v_3$ ; between these states the interactions to be considered are:

-- the Fermi-type interaction  $\langle v_1 v_2 v_3 | H | v_1 - 1 v_2 + 2 v_3 \rangle$ , -- the Coriolis-type interactions  $\langle v_1 v_2 v_3 | H | v_1 - 1 v_2 v_3 + 1 \rangle$ 

	(020)			(100)		(001)	
Ev	3148.5844 ± 0.74		3649+5399	± 0.74	3748.3193	± 0.0034	
AV	35.3409 ± 0.003	33	26.9349	± 0.0016	26.4819 <sub>0</sub>	± 0.0012	
₿ <sup>V</sup>	14.8394 <sub>4</sub> ± 0.001	2	14.30515 <sub>7</sub>	± 0.00082	14.428722	± 0.0004	9
c <sup>v</sup>	8.960254 ± 0.000	08.3	9.08041 <sub>5</sub>	± 0.00063	9.11857 <sub>0</sub>	± 0.0002	6
$\Delta_{K}^{v}$	0.11062 ± 0.000	011	(0.29066	$\pm$ 0.00073) x 10 <sup>-1</sup>	(0.28436	± 0.0011	) x 10 <sup>-1</sup>
$\Delta^{v}_{IK}$	(-0.10562 <sub>7</sub> ± 0.000	) x 10 <sup>-1</sup>	(-0.5331 <sub>0</sub>	± 0.0039 ) × 10 <sup>-2</sup>	(-0.5607g	± 0.0024	) x 10 <sup>-2</sup>
Δ <sup>V</sup> I	(0.156g ± 0.016	5) x 10 <sup>-2</sup>	(0.1241 <sub>9</sub>	$\pm 0.0011$ ) x $10^{-2}$	(0.12909,	± 0.0004	9) x 10 <sup>~2</sup>
8 <sup>v</sup> <sub>K</sub>	(0.789 ± 0.016	5) x 10 <sup>-2</sup>	(0.12564	$\pm 0.0027$ ) x $10^{-2}$	(0.1199	± 0.0027	) x 10 <sup>-2</sup>
8 T	(0.666 <sub>6</sub> ± 0.012	2) x 10 <sup>-3</sup>	(0.5041 <sub>5</sub>	$\pm$ 0.0071 ) x 10 <sup>-3</sup>	(0.52895	± 0.0029	) x 10 <sup>-3</sup>
н <sup>v</sup>	(0.1111 <sub>6</sub> ± 0.002	25) x 10 <sup>-2</sup>	(0.738 <sub>5</sub>	±0.014 ) x 10 <sup>-4</sup>	(0.890,	± 0.030	) x 10 <sup>4</sup>
HKI	(-0.654g ± 0.046	5 ) x 10 <sup>-4</sup>	(-0.1402	± 0.0093 ) x 10 <sup>-4</sup>	(-0.1511 <sub>6</sub>	± 0.0054	) x 10 <sup>-4</sup>
н <sup>V</sup> I	(0.75 ± 0.16	) x 10 <sup>-6</sup>	(0.478 <sub>6</sub>	$\pm 0.072$ ) x $10^{-6}$	(0.522	± 0.027	) x 10 <sup>~6</sup>
hr	(0.1767 ± 0.018	) x 10 <sup>-3</sup>	(0.222	$\pm 0.014$ ) x 10 <sup>-4</sup>	(0.2126	± 0.0060	) x 10 <sup>-4</sup>
h <sup>V</sup> TK	,				(0.39	± 0.19	) x 10 <sup>-6</sup>
h <sup>v</sup> <sub>T</sub>	(0.327 <sub>3</sub> ± 0.099	) x 10 <sup>-6</sup>	(0.241,	$\pm 0.046$ ) x 10 <sup>-6</sup>	(0.267,	± 0.014	) x 10 <sup>-6</sup>
LV	(-0.931, ± 0.035	) x 10 <sup>-5</sup>	2		(-0.209,	± 0.025	) x 10 <sup>-6</sup>
iv	(-0.133, ± 0.026	) x 10 <sup>-5</sup>			4		
Pr	$0.3077 \times 10^{-7} a$						
ĸ			COUPL	ING CONSTANTS			
			$h_{32} = 42.6_{60}$	± 4.2			
			$h_{32}^1 = -0.160_5$	± 0.047			
			h <sub>43</sub> = - 0.3096	9 <sub>0</sub> ± 0,00070			
			$h_{AO} = (-0.696)$	$\pm 0.040$ x $10^{-1}$			

TABLE I

Constants for the Triad of Interacting States (020), (100) and (001) of  $H_2^{17}O$ 

Note. All the results are given in  $cm^{-1}$ . The quoted errors are 2 standard deviations.

<sup>a</sup> Fixed to the  $H_2^{16}O$  value taken from Ref. (1).

and  $\langle v_1 v_2 v_3 | H | v_1 v_2 - 2 v_3 + 1 \rangle$ ,

-- the Darling-Dennisson-type interaction  $\langle v_1 v_2 v_3 | H | v_1 - 2 v_2 v_3 + 2 \rangle$ .

In the triad  $\{(020), (100), (001)\}$  considered here, this last interaction does not occur.

The same Hamiltonian matrix as for  $H_2^{16}O(1)$  has been used to calculate the energy levels. We recall that the *v*-diagonal part<sup>1</sup> of this matrix is for each vibrational state a Watson-type Hamiltonian  $H_{vv}$  and that the interaction terms retained in the case of this triad are:

$$H_{32} = h_{32} + h'_{32}J_z^2,$$
  

$$H_{43} = h_{43}(J_xJ_z + J_zJ_x),$$
  

$$H_{42} = h_{42}(J_yJ_z + J_zJ_y).$$

This Hamiltonian matrix has been diagonalized in a symmetry adapted basis (1) providing us with the wavefunction of a level  $(v_1v_2v_3)(JK_aK_c)$ 

<sup>&</sup>lt;sup>1</sup> The shortened notation  $|v\rangle$  stands for  $|v_1v_2v_3\rangle_0$ , which is the eigenfunction of the zero-order vibrational Hamiltonian with the correspondence v = 0 for (000), 1 for (010), 2 for (020), 3 for (100), 4 for (001) and so on.

### TABLE II

Constants for the Triad of Interacting States (020), (100) and (001) of H<sub>2</sub><sup>18</sup>O

	(020)		(100)	(001)			
Ev	3142.43 <sub>35</sub> ± 0.49	3646.3061	± 0.49	3741.5673 ± 0.0039			
AV	35•1197 <sub>0</sub> ± 0•0031	26.7690 <sub>6</sub>	± 0.0016	26.3332 <sub>4</sub> ± 0.0014			
в <sup>v</sup>	14.8347 <sub>2</sub> ± 0.0011	14 <b>.</b> 30747 <sub>1</sub>	± 0.00074	14.42773 <sub>1</sub> ± 0.00051			
cv	8.94309 <sub>6</sub> ± 0.00088	9.06104 <sub>9</sub>	± 0.00063	9.10058 <sub>8</sub> ± 0.00028			
$\Delta_{K}^{v}$	$0.10925_1 \pm 0.00043$	(0.28785 <sub>9</sub>	± 0,00065) x 10 <sup>-1</sup>	(0•2814 <sub>3</sub> ±0•0013 ) x 10 <sup>−1</sup>			
<b>∆</b> <sup>V</sup> <sub>IK</sub>	(-0.1049 <sub>4</sub> ± 0.0011 ) x 10 <sup>-1</sup>	(-0.5314 <sub>6</sub>	$\pm 0.0038$ ) x 10 <sup>-2</sup>	$(-0.5579_1 \pm 0.0025) \times 10^{-2}$			
Δ <sub>v</sub>	$(0.1542_8 \pm 0.0014) \times 10^{-2}$	(0.12394 <sub>2</sub>	± 0.00092) x 10 <sup>-2</sup>	$(0.12914_5 \pm 0.00051) \times 10^{-2}$			
δ <sub>K</sub>	$(0.779_6 \pm 0.018) \times 10^{-2}$	(0.1234 <sub>1</sub>	$\pm$ 0.0023 ) x 10 <sup>-2</sup>	$(0.1182_4 \pm 0.0028) \times 10^{-2}$			
ð,	$(0.654_7 \pm 0.010) \times 10^{-3}$	(0•5114 <sub>9</sub>	± 0.0070 ) x 10 <sup>-3</sup>	$(0.5301_{1} \pm 0.0030) \times 10^{+3}$			
н <sup>v</sup>	$(0.1101_7 \pm 0.0020) \times 10^{-2}$	(0.728 <sub>6</sub>	$\pm 0.013$ ) x 10 <sup>-4</sup>	$(0.885_9 \pm 0.038) \times 10^{-4}$			
н <sub>кЈ</sub>	$(-0.650_3 \pm 0.045) \times 10^{-4}$	(-0.1412 <sub>6</sub>	± 0.0099 ) x 10 <sup>-4</sup>	$(-0.15015_8 \pm 0.0057) \times 10^{-4}$			
нv	$(0.72_3 \pm 0.12) \times 10^{-6}$	(0.465 <sub>9</sub>	±0.054 ) x 10 <sup>-6</sup>	$(0.5295_2 \pm 0.028) \times 10^{-6}$			
nK	$(0.175_9 \pm 0.021) \times 10^{-3}$	(0,2224	± 0.012 ) x 10 <sup>-4</sup>	$(0.2063_5 \pm 0.0062) \times 10^{-4}$			
$h_{KJ}^V$				$(0.49_2 \pm 0.19) \times 10^{-6}$			
hŗ	$(0.321_3 \pm 0.080) \times 10^{-6}$	(0.286 <sub>7</sub>	±0.043 ) x 10 <sup>-6</sup>	$(0.270_8 \pm 0.015) \times 10^{-6}$			
LKV	$(-0.934_7 \pm 0.028) \times 10^{-5}$			(-0.215 <sub>0</sub> ± 0.032 ) x 10 <sup>-6</sup>			
$\iota_{\kappa}^{\vee}$	$(-0.111_2 \pm 0.037) \times 10^{-5}$						
PK	$0.3077 \times 10^{-7}$ a						
		COUPI	ING CONSTANTS				
		$h_{32} = 41.4$	20 ± 3.0				
		$h_{32}^{I} = -0.13$	37 <sub>5</sub> ± 0.033				
		$h_{43} = -0.29$	9869 <sub>2</sub> ± 0.00051				
		$h_{ro} = (-0.713 + 0.046) \times 10^{-1}$					

Note. All the results are given in  $cm^{-1}$ . The quoted errors are 2 standard deviations.

<sup>a</sup> Fixed to the  $H_2^{16}O$  value taken from Ref. (1).

$$|v_1v_2v_3JK_aK_c\rangle = \sum_{v=2,3,4} \sum_{K} C_K^v |v\rangle |JK\gamma\rangle,$$

where the  $|JK\gamma\rangle$  are the usual Wang functions.

# RESULTS

Using the experimental data of Ref. (4) for the three vibrational states (020), (100), and (001), we performed for each isotopic species a nonlinear least-squares fit which provided us with the rotational and coupling constants quoted in Table I for  $H_2^{17}O$  and in Table II for  $H_2^{18}O$ . The agreement between the calculation and the experiment is quite satisfactory since a statistical analysis of the differences  $\delta = |E^{obs} - E^{calc}|$  (in cm<sup>-1</sup>) between the calculated and the observed energy levels gives:

	$H_2^{17}O$ (346 levels)	$H_2^{18}O$ (352 levels)
$0 \times 10^{-3} < \delta \le 15 \times 10^{-3}$	87%	87% (of the levels)
$15 \times 10^{-3} < \delta \le 40 \times 10^{-3}$	10%	11%
$40 \times 10^{-3} < \delta \le 75 \times 10^{-3}$	3%	2%

## TABLE III

Calculated Rotational Energy Levels for the Vibrational States (020), (100), and (001) of  $\rm H_2{}^{17}O$ 

J	ĸa	ĸ <sub>c</sub>	(020)	%(2)	%(3)	%(4)	(100)	%(2)	%(3)	%(4)	(001)	%(2)	%(3)	%(4)
0	0	0	3144.978	99.3	0.7	0.0	3653,147	0.7	99.3	0.0	3748,319	0.0	0.0	100.0
ł	0 1		3168.768 3189.170 3195.008	99.3 99.3 99.3	0.7 0.7 0.7		3676.529 3689.174 3594.396	0.7 0.7	99.3 99.3 99.3	0 • 0 0 • 0 0 • 0	3771.863 3783.903 3789.203		0.0	
NNNNN	Sheer	22-10	3215+229 3230+933 3248+416 3308+495 3309+578	999999 999999 999999	0.7 0.7 0.8 0.8		3721.955 3730.717 3746.356 3784.013 3785.314	0.7 0.7 0.8 0.8	99.3 999.3 999.2 999.2 999.2	0.0 0.0 0.0 0.1	3817.516 3825.716 3841.563 3877.438 3878.839	0.0000	0.0 0.0 0.0	
		MMNN	3282.389 3292.646 3379.963 3385.108 3491.699 3491.830	999.33 999.22 999.22 999.21 999.11	0.7 0.7 0.8 0.8 0.9 0.9		37823. 38543 38540. 38540. 38540. 3929. 3920. 39200. 3920. 39200. 39200. 39200. 3920	0.7 0.7 0.8 0.9 0.9	999.3 999.2 999.2 999.2 998.5 998.5 998.5 998.5 998.5 997.9	0001 0001 0001	3882 • 995 3887 • 625 3919 • 004 3948 • 313 3954 • 653 4020 • 953 4021 • 197		0300000	10000 997 10000 987 9954 10000
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ຑຑຑຑຨຨຨຨຨຨຨຨ	0	5544mmNN0	34758.5455 3558.2055 3558.2055 3519.25457 371.28.5352 371.58.5352 371.58.5352 371.58.5352 371.58.5352 371.58.5352 371.58.5352 371.58.5352 371.58.5352 371.58.5552 371.58.5552 371.58.5552 371.58.5552 371.58.5552 371.58.5552 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.58.5555 371.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.5555 375.55555 375.55555 375.55555 375.55555 375.55555 375.55555 375.55555 375.55555 375.55555 375.555555 375.555555 375.555555 375.55555555 375.5555555555	33222119966 999999998888 88888888888888888888			39772 40450 40450 40450 4094 4094 4094 4094 4	00000000000000000000000000000000000000	33212590901 99998874277 99999976899	00010643466 200010643466	4067 866 404 7253 4141 7253 4235 650 4235 337 4235 337 43357 328 4457 033	00000000000000000000000000000000000000	2 13 1901 2 13	91075883399 99089348899 990798699999
<b>~~~~</b>	0	6655443322-1-0	5155538866408 + 1559538866408 + 1559588864 + 1559588864 + 155958886 + 155958886 + 1559588 + 15595888 +	332221-994247 99999999888170 99999999888170			572-1584508655 5986930487086555 48654877846508 99804487787468575 9980548911456 000-44474444444	7728898343388 008000181111	3381968190%2V 99899987155577		244680 244680 260580370 960580370 960580370 9605847999 1180847999 1180847999 1180847999 1180847999 1180847999 118084794 4466746 4466777	00010040000000	10-10-1-100	9998921668899 9998921668899 9998921668899
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Note.  $\mathscr{H}(v)$  is the mixing coefficient of a given level  $(v_1v_2v_3)[JK_aK_c]$  on the vibrational state  $|v\rangle$  with v = 2 for (020), 3 for (100), and 4 for (001).

	к <sub>а</sub>	ĸ	(020)	%(2)	%(3)	%(4)	(100)	%(2)	%(3)	%(4)	(001)	%(2)	%(3)	%(4)
~~~~~~~~~~~~~~~~~~~~~	0	99887766554433001++0	4000.056 4254 40554.224 40559.020 40559.020 40559.000 40559.000 40559.000 40559.000 40559.000 40559.000 40559.000 40559.000 40555 4000 4000 4000 4000 4000 4000	33211008845	778990000 • • • • • • • • • •	000000000000000000000000000000000000000	00.4 c 0.14 c 0.7 d 4.7 - 6 d 4 c 0 c 10.0 c 0.1 4 c 0.7 d 4.7 - 6 d 7 - 7 - 6 d 0 d 0 c 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0 - 7 0	68990106814999988 ********************************	22109759191031144	00000000000000000000000000000000000000	00111-1-800000-1-680000-66666 800.400-8000-1-680000-6666 800.400-8000-1-6800-6600 800.40000-1-800000-6000 800.40000-1-800000-6000 800.40000-1-800000-6000 800.40000-1-800000-6000 800.40000-1-800000-6000 800.40000-1-800000-6000 800.40000-1-800000-1-80000 800.40000-1-800000-1-80000 800.40000-1-80000-1-80000 800.40000-1-80000-1-80000 800.40000-1-800000-1-80000 800.40000-1-800000-1-80000 800.40000-1-80000-1-80000 800.40000-1-80000-1-80000 800.40000-1-80000-1-80000 800.40000-1-80000-1-80000 800.40000-1-80000 800.40000-1-80000 800.40000-1-80000 800.40000-1-80000 800.40000-1-80000 800.40000-1-80000 800.40000-1-80000 800.40000-1-80000 800.40000-1-80000 800.40000-1-80000 800.40000-1-80000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.40000 800.400000 800.400000 800.40000 800.40000000000000000000000000000000000		000009-4-644NN	0007888477000088888 00009668775077888888 000096687750778888899 0009969677995599599
	01110033445566778899	100998877665544337221	424747350402735 424647350402735 42474735045420735 42474735045420735 44447473593133	331109078 9999988 9999988 999998 999998 999998	7799010	000000000000000000000000000000000000000	607(8)773-4-4088047 607-10090-108000 00-10090-10800 00-10090-1080 4460-0090 4460-0090 4460-0090 100000 100000 4460-00 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000 100000000	889004130949900 •••••• 000111110401111111	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	000012387783011	95248396911732486672400 733482502531732486672400 743482502533450486572400 74364731455245857388599 848071655245747857388599 8480716552457457857388599		0019256578990772233	09918054471009118877 09949893447365777788 0996999969999999999999
	0	111009988776655443	4460.214 4460.266 4704.707 4706.152 49911.6022 5024.998	331119 999998 9999988 999999999999999999		0000000	4400-10860-071-000-070 00080-0500-070-000-070 00080-0500-070-000-070 000440-00-070-00-070-00-0 000440-00-070-00-00-00-00-00-00-00-00-00-00-0	9000	99985549652157 99988999999898999	000000000000000000000000000000000000000	70718898667 53071889667 511487888667 511487888667 5114878888667 5114878888667 51148788888667 51148788888 51148788888 511488888 511488888 511488888 511488888 511488888 51148888 511488888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 511488888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 51148888 511488888 511488888 511488888 511488888 511488888 511488888 511488888 511488888 511488888 511488888 511488888 511488888 511488888 511488888 5114888888 5114888888 5114888888 5114888888 5114888888 511488888888 51148888888 5114888888888 511488888888 511	000000000000000000000000000000000000000	00112847363904433	119998824871577698-4-177 ***********************************
งงานการการการการการการการการการการการการการก	0	11110099887766	4686.8252 4685.8852 4955.8642 4955.8642 5172.385 5183.265	9999988 999988 888	0.7 0.9 0.9 11.2		440024609 4152303334115 77790137887379539 77790137887379534 777901771887950 777901771887950 787015554 787015554 787015556 787015556 787015556 78705556 78705556 78705556 78705556 78705556 78705556 78705556 78705556 78705556 78705556 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 78705555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 7870555 78705555 78705555 78705555 78705555 78705555 78705555 78705555 787055555 787055555 787055555 7870555555 787055555 7870555555555 78705555555555	10-1-1-805+80 2-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1	5180724839218 	0000113486423	56314037546790 668437644236790 668437644236790 889914097420000 778877163420 2244668899001 2244668899001 2014465899001 2014465899001 20146555555555555555555555555555555555555	00000000000000000000000000000000000000	000000000000000000000000000000000000000	
	- 0	5332211100998	4931.088 4931.101 5224.472 5224.895	99.3 99.3 99.1 99.1	0.7 0.7 0.9 0.9	0.0 0.0 0.0 0.0 0.0	5468 56553 56553 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 56853 57755 57755 57755 577555 5775555 57755555 577555555	9959507	99.1 99.4 98.4 98.1 98.9 98.1 98.9 98.1	00 00 01 02	55557555566483 80205555566483 80205555566483 802055555566483 802055555566683 802055555566683 8020555555566683 8020555555566683 802055555555555555555555555555555555555		4 000000000000000000000000000000000000	900997652879 1009999988878 99999988378 99999988378
4444444	0NNMM	440000	5192+965 5192+973	99 <b>.</b> 3	8:7	8:8	5682.344 5682.346 5931.671 6151.997 6151.297	001141 001141	9998558 9998558	0.0000000000000000000000000000000000000	5784.752 5784.725 6032.585 6230.891 6251.132 6438.057	2510 00000 10000		999.999.9999.73
1000000	0	1554433					5961.053 5961.053 5968.603 6228.603	0.8	99.2 99.2 98.9 98.9	0.0	6064,395 6064,395 6330,367 6330,178 6565,925 6566,310	003120	0.01	99.9 99.9 99.7 93.9 94.7 99.7
166	0112	166515					6257.236 6257.236	0.8	99.2 99.2		6361.666 6361.666 6645.705 6645.705			

TABLE III—Continued

# CAMY-PEYRET, FLAUD, AND TOTH

### TABLE IV

Calculated Rotational Energy Levels for the Vibrational States (020), (100), and (001) of  $H_2^{18}O$ 

J	ĸa	к <sub>с</sub>	(020)	%(2)	%(3)	%(4)	(100)	%(2)	%(3)	%(4)	(001)	%(2)	%(3) %(4)
0	0	0	3139+051	99,3	0.7	0.0	3649,688	0.7	99,3	0.0	3741.567	0,0	0.0 100.0
1	0 1 1	1 1 0	3162.820 3183.006 3188.858	99.3 99.3 99.3	0.7 0.7 0.7	0.00	3673.054 3685.531 3690.774	0.7 0.7 0.7	99.3 99.3 99.3		3765.092 3776.984 3782.302		0.0 100.0 0.0 100.0 0.0 100.0
NNNNN	011-NN	NN	3209.224 3224.713 3242.236 3301.682 3302.779	99999 99999 9999 9999	0.7 0.7 0.7 0.7		3718 421 3727 721 3742 721 3749 880 3781 204	0.7	99.3 999.3 999.2 999.2		3810.686 3818.763 3870.077 3871.499		0.0 100.0 0.1 99.9 0.0 100.0 0.0 100.0 0.0 100.0
<b>NUUUUUU</b>	0NNMM	mmQN0	3276 - 270 3282 - 413 33778 - 845 33778 - 885 3483 - 988 3483 - 988	99999999999999999999999999999999999999	0.77 0.77 0.8		37833.588 3682 388.5654 388.5654 388.5654 388.5654 388.5654 388.5654 388.564 88.5654 88.5654 88.5654 88.5654 88.5654 39.24 88.00 39.24 88.00 39.24 88.00 39.24 88.00 39.24 88.00 39.24 88.00 39.24 88.00 39.24 88.00 39.24 80.00 39.24 80.00 39.24 80.00 39.24 80.00 39.24 80.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 30.00 39.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 30.00 300	0.77 0.77 0.77 0.88	99999999999999999999999999999999999999	000147-6	3876.042 38876.042 39812.931 3940.932 3947.8865 4012.116 4013.116		0.0 100.0 0.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0 100.0
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Note.  $\mathscr{H}(v)$  is the mixing coefficient of a given level  $(v_1v_2v_3)[JK_aK_c]$  on the vibrational state  $|v\rangle$  with v = 2 for (020), 3 for (100), and 4 for (001).

TABLE IV—Continued

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J	ĸa	ĸ <sub>c</sub>	(020)	%(2)	%(3)	%(4)	(10C)	%(2)	%(3)	%(4)	(001)	%(2)	%(3)	%(4)
,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	0	998877665564433221-10		1122 122 1222 1	778889991+554 •••••••	000000000000000000000000000000000000000		77.39909.0	331	0000-14770673887? ••••••• 0000000-1467388??		0000000031+++++00000		00978486474222209988 009978486474222209988 0099978486474222209988 009997888699
	01-WN77445566778899	1099887766554433221	4243.1753 4424.987 4494.987 4560.0987 4660.0986 4987 4660.0986 4821.0986 4824 4844.551	3322-0089	778890021	00000000	4 4 90000400000000000000000000000000000	1799030 <b>65</b> 838899 •••••	331096760-867773 99998856-4057733 99998856-40-2057733	000000000000000000000000000000000000000	59582788074050001 57782478667405701 57782478667405704568000 ••••••••••••••••••••••••••••••••••	0005000-5		19992874447632339988 99988994243667777788 1999899942436677777888
	011-1223344556677-88	11009988776655443	44514 44594 4696 4696 4698 4698 4698 4698 4698 46	33/2080 999999 9999989 9999989 9999989	000000000000000000000000000000000000000	0000000	84401-10760-400003 695540-6050-6050-60 88580-76-10-6450-90 88580-76-10-6450-90 90	899-00-67378999 • • • • • • • • • • • •	211899698732812 999988732812 99998848152		960609986638984931 02678421-1896486280755 22778421-189641407515 2478785214896372144477 247878524488772144477 247878752466688888566 24787875566688888566 24787875566688888566 2478785556668888555556 24787855566888555556	000000000000000000000000000000000000000	00112730304674400	00000000000000000000000000000000000000
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		1111110998	4921.591 4921.604 5214.385 5214.778	99,3 99,3 99,1 99,1	0.7 0.9 0.9	0.00 000 00 00	5413.915 5413.926 5645.941 5645.941 5845.983 6013.477	9901485 1010131	998-12 998-1-2 98878-12 98878-12	00000000000000000000000000000000000000	4 37 356646301 356646301 114444 444915586 555779911133 555779911133 555779911133 5666663		0000001159	10099999999999999999999999999999999999
******		44750001	5182.912 5182.919	99.3 99.3	0.7 8.7	0.0		00113105	9998 998 998 998 998 998		557000000 6600000 6600000 6600000 6600000 6600000 6600000 6600000 6600000 6600000 66000000	1000000	000000	98.7 99. 99. 99. 99. 99. 99. 99.
5555055		15					5952.309 59529.706 6219.730	0.7 0.7 1.0	99.3 99.3 99.0 99.0	0.00	605188-3740 663188-3740 65554-7248	0.0 0.4 24.5 0.0		99 99 91 75 99
1616		16655					6247.526 6247.527	8:7	99.3 99,3	0.0	6349.804 6349.804 6633.204 6633.294			100. 100. 99.

#### TABLE V

Example of the Evolution of Mixing Coefficients in an Isotopic Substitution

(v <sub>1</sub> v <sub>2</sub> v <sub>3</sub> )[JK <sub>a</sub> K <sub>c</sub> ]	E	calc	%(020)	%(100)	%(001)
	H2 <sup>16</sup> 0	4579.002	95.6	4.2	0.3
(020) [761]	H2 <sup>17</sup> 0	4563•754	67.1	28.4	4.5
	н <sub>2</sub> 180	4551•455	96.3	3•4	0.3
	н <sub>2</sub> 160	4572.425	3.2	80.1	16.7
(100) [743]	H2 <sup>17</sup> 0	4565.834	31•9	59.7	8•4
	н <sub>2</sub> 180	4558.875	2.8	87•4	9•7
	н <sub>2</sub> 160	4553•280	0.2	16.6	83.1
(001) [735]	н <sub>2</sub> 170	4544.287	0•1	12.7	87.2
	H2 <sup>18</sup> 0	4536•224	0.1	9.9	90.0

Using the constants of Table I and Table II, we computed the energy levels which are given in Table III for  $H_2^{17}O$  and in Table IV for  $H_2^{18}O$  together with their mixing coefficients defined by

 $\mathscr{H}(v) = \sum_{K} |C_{K}^{v}|^{2} \quad \text{with} \quad v = \begin{cases} 2 \text{ for (020),} \\ 3 \text{ for (100),} \\ 4 \text{ for (001).} \end{cases}$ 

These mixing coefficients are very important since they allow the easy detection of perturbed levels. These tables contain more calculated levels than observed ones because we hope that an extrapolation to higher J or  $K_a$  values than what is experimentally available can be reasonably performed and this should facilitate the assignment of new spectra recorded with larger  $P \times l$  product.

It is interesting to compare the evolution of the mixing coefficients of perturbed levels as one goes from  $H_2^{16}O$  to  $H_2^{17}O$  and to  $H_2^{18}O$ . Indeed, the magnitude of resonance is very sensitive to isotopic substitution. As an example, we have gathered in Table V the mixing coefficients of the three resonating levels (020) [761], (100) [743], (001) [735].

#### DISCUSSION

The constants obtained in this work for  $H_2^{17}O$  and  $H_2^{18}O$  compare very well together as well as with those of  $H_2^{16}O(I)$ . As the oxygen isotopic substitution does not change the equilibrium *B* value, one can expect, as has been observed, that the  $B^v$  values of the three different isotopic species are not changing very much. A relation between the constant  $h_{43}$  involved in the Coriolis resonance between (100) and (001) and the coefficient  $k_{133}$  appearing in the expansion of the potential function with respect to normal coordinates is given in Ref. (5). If one assumes that this relation, valid up to the second order of approximation, is applicable for water, then one obtains

$k_{133} = -869 \text{ cm}^{-1}$	for	$H_{2}^{16}O$ ,
$k_{133} = -855 \text{ cm}^{-1}$	for	$H_{2^{17}}O$ ,
$k_{133} = -839 \text{ cm}^{-1}$	for	H <sub>2</sub> <sup>18</sup> O.

The  $k_{133}$  value of H<sub>2</sub><sup>18</sup>O confirms the value of this constant obtained from the study of the interacting states (110) and (011) (3).

Finally the wavefunctions obtained in this work will be used in the near future to compute the line intensities for the  $2\nu_2$ ,  $\nu_1$  and  $\nu_3$  bands of  $H_2^{17}O$  and  $H_2^{18}O$ .

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