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Line Positions and Intensities for the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ Bands of $H_2{}^{18}O$

C. CAMY-PEYRET, J.-M. FLAUD, AND J.-Y. MANDIN

Laboratoire de Physique Moléculaire et d'Optique Atmosphérique C.N.R.S., Bâtiment 221, Campus d'Orsay, 91405 Orsay Cedex, France

AND

R. A. TOTH

Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, California 91103

The intensities of about 90 lines of the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ bands of $H_2{}^{18}O$ have been measured using a Fourier transform spectrum of natural water vapor. The constants involved in the rotational expansion of the transformed transition moment operators corresponding to these bands have been determined through a fit of these line intensities. The constants obtained are used to compute the whole spectrum of the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ bands of $H_2{}^{18}O$ providing reliable line positions and intensities. For lines involving perturbed levels a comparison is given with the results obtained for $H_2{}^{16}O$ and it is shown that the results for one isotopic species cannot be transferred directly to another one.

INTRODUCTION

High-resolution studies demand both precise line positions and intensities. To calculate the $H_2{}^{18}O$ spectrum, in addition to the isotopic shift of the vibration-rotation lines, one has to decide how to compute their intensities. Usually, to obtain the absorption of an isotopic substituted molecule, it is assumed that the transition moment does not change very much from one isotopic species to another. Then the absorption of the less abundant isotope is derived from the absorption of the main isotope by multiplying by the isotopic ratio. For example in the case of water, one is used to multiply the absorption of $H_2{}^{16}O$ by 0.00204 (natural abundance) to get the absorption of $H_2{}^{18}O$ (*1*, *2*). However, we know from the study of the rotational energy levels of the (110) and (011) vibrational states of $H_2{}^{18}O$ (*3*) that the influence of the resonances is very sensitive to the isotopic substitution. Consequently, it is quite evident that the intensities of lines involving perturbed levels cannot be correctly estimated by the method described above. Under these conditions, we have decided to calculate directly the $H_2{}^{18}O$ spectrum in the 1.9-μm region using realistic vibration-rotation wavefunctions and an appropriate transition moment operator expansion.

The line positions have been derived from a new set of energy levels (*4*) and line

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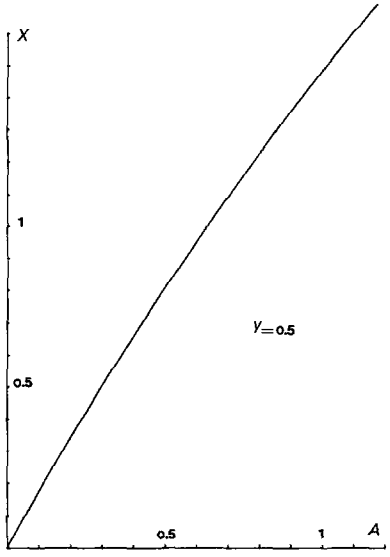

FIG. 1. Curve of growth for a Voigt profile.

TABLE I

Agreement between Observed and Calculated Line Intensities for the 1.9-μm Bands of $H_2{}^{18}O$[a]

N°	$\sigma(cm^{-1})$	$J'K'_aK'_c$	$J\ K_a\ K_c$	k^P_σ(obs)	k^P_σ(calc)	%
				($cm^{-2}\ atm^{-1}$)		
70	5121.903	8 0 8	9 0 9	0.6618×10^{-4}	0.7060×10^{-4}	6.7
70	5136.380	6 2 4	7 2 5	0.1040×10^{-3}	0.9661×10^{-4}	7.2
70	5143.603	7 0 7	8 0 8	0.5143×10^{-4}	0.4849×10^{-4}	5.7
70	5143.773	7 1 7	8 1 8	0.1540×10^{-3}	0.1454×10^{-3}	5.6
70	5156.158	6 2 5	7 2 6	0.4472×10^{-4}	0.4482×10^{-4}	0.2
70	5164.744	6 0 6	7 0 7	0.2823×10^{-3}	0.2699×10^{-3}	4.4
70	5165.141	6 1 6	7 1 7	0.8919×10^{-4}	0.9300×10^{-4}	4.3
60	5165.145	5 2 3	5 3 2			
70	5168.794	5 1 4	6 1 5	0.8225×10^{-4}	0.8880×10^{-4}	8.0
70	5185.570	5 4 2	6 4 3	0.5716×10^{-4}	0.5816×10^{-4}	1.7
70	5185.722	4 2 2	5 2 3	0.3164×10^{-3}	0.3154×10^{-3}	0.3
70	5186.115	5 1 5	6 1 6	0.4392×10^{-3}	0.4449×10^{-3}	1.3
70	5188.377	4 1 3	5 1 4	0.4200×10^{-3}	0.4439×10^{-3}	5.7
70	5197.934	4 3 1	5 3 2	0.1571×10^{-3}	0.1814×10^{-3}	15.5
70	5198.472	4 2 3	5 2 4	0.1028×10^{-3}	0.1023×10^{-3}	0.4
70	5201.675	4 3 2	5 3 3	0.7344×10^{-4}	0.6204×10^{-4}	15.5
70	5205.040	4 0 4	5 0 5	0.6312×10^{-3}	0.6620×10^{-3}	4.9
70	5210.178	3 1 2	4 1 3	0.2144×10^{-3}	0.2134×10^{-3}	0.4
70	5210.943	4 4 0	5 4 1	0.6997×10^{-4}	0.6393×10^{-4}	8.6
70	5213.265	3 2 1	4 2 2	0.1399×10^{-3}	0.1306×10^{-3}	6.6
70	5220.917	3 2 2	4 2 3	0.3346×10^{-3}	0.3182×10^{-3}	4.9
70	5224.184	3 0 3	4 0 4	0.2970×10^{-3}	0.2876×10^{-3}	3.2
70	5226.690	3 3 1	4 3 2	0.1571×10^{-3}	0.1846×10^{-3}	17.5
70	5227.851	3 1 3	4 1 4	0.7677×10^{-3}	0.8238×10^{-3}	7.3
70	5233.100	5 1 5	5 1 4	0.3495×10^{-4}	0.4041×10^{-4}	15.7
70	5243.431	2 0 2	3 0 3	0.9839×10^{-3}	0.9784×10^{-3}	0.6
70	5245.345	2 2 1	3 2 2	0.1448×10^{-3}	0.1354×10^{-3}	6.6
70	5259.412	1 1 0	2 1 1	0.2177×10^{-3}	0.2062×10^{-3}	5.3
70	5269.578	1 1 1	2 1 2	0.6375×10^{-3}	0.6689×10^{-3}	4.9
70	5295.314	2 1 2	2 1 1	0.1116×10^{-3}	0.1135×10^{-3}	1.7
70	5298.181	4 2 3	4 2 2	0.5198×10^{-4}	0.5424×10^{-4}	4.4
70	5306.544	1 1 1	1 1 0	0.7634×10^{-3}	0.7872×10^{-3}	3.1
60	5313.017	3 3 0	3 2 1	0.1842×10^{-3}	0.1768×10^{-3}	4.0
70	5315.318	2 2 1	2 2 0	0.3694×10^{-3}	0.3648×10^{-3}	1.3
70	5317.965	2 2 0	2 2 1	0.1042×10^{-2}	0.1103×10^{-2}	5.8
70	5321.569	4 3 2	4 3 1	0.1212×10^{-3}	0.1301×10^{-3}	7.3
70	5322.968	3 2 1	3 2 2	0.1420×10^{-3}	0.1588×10^{-3}	11.8

TABLE I—*Continued*

N°	σ(cm^{-1})	J' $K_a'K_c'$	J $K_a K_c$	k_σ^P(obs)	k_σ^P(calc)	%
				(cm^{-2}atm^{-1})		
70	5323.675	3 3 1	3 3 0	0.8131 x 10^{-3}	0.8525 x 10^{-3}	4.8
70	5324.373	4 3 1	4 3 2	0.3852 x 10^{-3}	0.3935 x 10^{-3}	2.2
70	5325.621	7 4 4	7 4 3	0.3543 x 10^{-4}	0.2734 x 10^{-4}	22.9
70	5327.964	2 1 1	2 1 2	0.3727 x 10^{-3}	0.3678 x 10^{-3}	1.3
70	5334.023	1 0 1	0 0 0	0.2293 x 10^{-3}	0.2126 x 10^{-3}	7.3
70	5340.780	7 5 3	7 5 2	0.2793 x 10^{-4}	0.2526 x 10^{-4}	9.5
70	5356.013	2 0 2	1 0 1	0.1050 x 10^{-2}	0.1105 x 10^{-2}	5.2
60	5360.267	3 2 1	2 1 2	0.3529 x 10^{-4}	0.3654 x 10^{-4}	3.5
70	5366.383	6 2 4	6 2 5	0.4692 x 10^{-4}	0.4337 x 10^{-4}	7.6
70	5372.690	3 1 3	2 1 2	0.1026 x 10^{-2}	0.1101 x 10^{-2}	7.3
70	5375.490	3 0 3	2 0 2	0.4274 x 10^{-3}	0.4286 x 10^{-3}	0.3
60	5386.896	3 3 1	2 2 0	0.3027 x 10^{-4}	0.3435 x 10^{-4}	13.5
70	5390.192	3 1 2	2 1 1	0.3517 x 10^{-3}	0.3478 x 10^{-3}	1.1
70	5392.749	4 0 4	3 0 3	0.1142 x 10^{-2}	0.1220 x 10^{-2}	6.9
70	5403.460	5 2 4	5 0 5	0.4349 x 10^{-4}	0.4863 x 10^{-4}	11.8
60	5406.715	4 3 2	3 2 1	0.5783 x 10^{-4}	0.5492 x 10^{-4}	5.0
70	5407.884	4 2 3	3 2 2	0.2023 x 10^{-3}	0.2064 x 10^{-3}	2.0
70	5408.871	5 0 5	4 0 4	0.3164 x 10^{-3}	0.3339 x 10^{-3}	5.5
70	5420.081	4 2 2	3 2 1	0.6195 x 10^{-3}	0.6318 x 10^{-3}	2.0
70	5420.177	4 3 2	3 3 1	0.8682 x 10^{-4}	0.9411 x 10^{-4}	8.4
70	5421.358	4 3 1	3 3 0	0.3211 x 10^{-3}	0.2823 x 10^{-3}	12.0
70	5423.910	6 1 6	5 1 5	0.2358 x 10^{-3}	0.2401 x 10^{-3}	1.8
70	5439.426	7 1 7	6 1 6	0.4670 x 10^{-3}	0.4668 x 10^{-3}	0.0
70	5439.668	7 0 7	6 0 6	0.1586 x 10^{-3}	0.1560 x 10^{-3}	1.6
70	5443.182	5 3 3	4 3 2	0.2964 x 10^{-3}	0.3164 x 10^{-3}	6.7
70	5446.664	5 2 3	4 2 2	0.1916 x 10^{-3}	0.1840 x 10^{-3}	4.0
70	5446.813	5 3 2	4 3 1	0.1074 x 10^{-3}	0.1050 x 10^{-3}	2.2
70	5453.846	6 1 5	5 1 4	0.4743 x 10^{-3}	0.4851 x 10^{-3}	2.3
70	5453.960	5 4 2	4 4 1	0.1081 x 10^{-3}	0.1088 x 10^{-3}	0.6
70	5454.170	5 4 1	4 4 0	0.3460 x 10^{-4}	0.3625 x 10^{-4}	4.8
70	5454.379	8 0 8	7 0 7	0.2821 x 10^{-3}	0.2705 x 10^{-3}	4.1
70	5465.413	6 3 4	5 3 3	0.8694 x 10^{-4}	0.8074 x 10^{-4}	7.1
70	5466.971	7 2 6	6 2 5	0.2781 x 10^{-3}	0.2623 x 10^{-3}	5.7
70	5470.519	7 1 6	6 1 5	0.9925 x 10^{-4}	0.9325 x 10^{-4}	6.0
70	5471.677	6 2 4	5 2 3	0.3572 x 10^{-3}	0.3709 x 10^{-3}	3.9
70	5473.161	6 3 3	5 3 2	0.2536 x 10^{-3}	0.2348 x 10^{-3}	7.4
70	5477.334	6 4 3	5 4 2	0.3672 x 10^{-4}	0.3668 x 10^{-4}	0.1
70	5478.190	6 4 2	5 4 1	0.1093 x 10^{-3}	0.1100 x 10^{-3}	0.6
70	5494.480	7 2 5	6 2 4	0.7018 x 10^{-4}	0.6865 x 10^{-4}	2.2
70	5494.543	4 2 2	3 0 3	0.3490 x 10^{-4}	0.3176 x 10^{-4}	9.0
70	5495.288	11 1 11	10 1 10	0.4568 x 10^{-4}	0.3754 x 10^{-4}	17.8
70	5495.296	11 0 11	10 0 10			
70	5500.289	7 4 4	6 4 3	0.7691 x 10^{-4}	0.7538 x 10^{-4}	2.0
70	5500.628	9 2 8	8 2 7	0.5936 x 10^{-4}	0.6781 x 10^{-4}	14.2
70	5501.533	9 1 8	8 1 7	0.2740 x 10^{-4}	0.2293 x 10^{-4}	16.3
70	5506.840	8 3 6	7 3 5	0.3070 x 10^{-4}	0.2623 x 10^{-4}	14.6
70	5514.656	8 2 6	7 2 5	0.9135 x 10^{-4}	0.9814 x 10^{-4}	7.4
60	5517.630	8 4 5	7 3 4	0.2479 x 10^{-4}	0.2295 x 10^{-4}	7.4
70	5525.880	9 3 7	8 3 6	0.3403 x 10^{-4}	0.3605 x 10^{-4}	6.0
70	5528.133	8 4 4	7 4 3	0.3703 x 10^{-4}	0.4068 x 10^{-4}	9.9
70	5530.958	8 3 5	7 3 4	0.4080 x 10^{-4}	0.4910 x 10^{-4}	20.4

[a] The meaning of the differents columns is:

$N°$, vibrational assignment of the transition consisting of two numbers which correspond to the upper and lower states with the abbreviation 0 for (000), 6 for (110), and 7 for (011);

σ, computed wavenumber (cm^{-1}) of the transition;

$J'K_a'K_c'$ and JK_aK_c, rotational quantum numbers, respectively, of the upper and lower levels;

k_σ^P (obs) k_σ^P (calc), observed and calculated values of the line intensity in cm^{-2} atm^{-1};

$\% = 100 \times |k_\sigma^P \text{ (obs)} - k_\sigma^P \text{ (calc)}| / k_\sigma^P \text{ (obs)}$.

The temperature is equal to 296 K.

intensities have been deduced from a Fourier transform spectrum of water vapor where the abundance of $H_2{}^{18}O$ was the natural one. From these experimental data on line intensities, the constants appearing in the transformed transition moment operator have been deduced following the theoretical formulation proposed in Ref. (*5*). Finally, using these constants, we have calculated the whole spectrum of the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ bands of $H_2{}^{18}O$.

EXPERIMENTAL LINE INTENSITIES

The spectrum of natural water (0.204% $H_2{}^{18}O$, 0.037% $H_2{}^{17}O$) has been recorded with a Fourier transform interferometer (resolution 0.015 cm^{-1}) with a pressure[1] $P \simeq 1.77 \times 10^{-2}$ atm at 296 K. At this pressure both collisions and Doppler effects contribute to the line broadening. In these conditions, the absorption coefficient $\alpha(\sigma)$ (in cm^{-1}) at the wavenumber σ is related to the reduced Voigt profile as (*7*):

$$\frac{\alpha(\sigma)}{\alpha_0} = K(x, y) = \frac{y}{\pi} \int_{-\infty}^{+\infty} \frac{\exp(-t^2)}{y^2 + (x - t)^2}\, dt,$$

$$\alpha_0 = \frac{k_\sigma{}^P P}{\gamma_D} \left(\frac{\log 2}{\pi}\right)^{\frac{1}{2}},$$

$$y = \frac{\gamma_L}{\gamma_D} (\log 2)^{\frac{1}{2}}, \quad x = \frac{\sigma - \sigma_0}{\gamma_D} (\log 2)^{\frac{1}{2}}, \quad \gamma_L = \gamma_L{}^0 P,$$

where $k_\sigma{}^P$ is the line strength or integrated absorption coefficient at unit pressure (usually in cm^{-2} atm^{-1}), γ_D is the Doppler half-width, γ_L is the Lorentz half-width at pressure P, and σ_0 is the wavenumber at the line center.

TABLE II

Constants Involved in the Expansion of the Transformed Transition Moment Operator ${}^v\mu'_z$ for $H_2{}^{18}O$

Band	j	${}^vA_j$	${}^v\mu'_j$
v=6 ($\nu_1+\nu_2$)	1	φ_x	$-\ 0.00219_8 \pm 0.00031$
	4	$\{i\varphi_y, J_z\}$	0.119 [a] $\times 10^{-3}$
	5	$\{\varphi_z, iJ_y\}$	0.646 [a] $\times 10^{-4}$
v=7 ($\nu_2+\nu_3$)	1	φ_z	$0.01830_6 \pm 0.00022$
	4	$\frac{1}{2}[\{\varphi_x, iJ_y\} - \{i\varphi_y, J_x\}]$	$(-\ 0.116_6 \pm 0.041) \times 10^{-3}$

All the results are in D. The errors quoted are 99% statistical confidence intervals.

[a] Constrained to the $H_2{}^{16}O$ value given in Ref. [6].

[1] A slight readjustment of the measured pressure has been done to improve the absolute precision of the results using the intensities of some $H_2{}^{16}O$ lines computed in Ref. (*6*).

TABLE III

Rotational Constants for the (000), (110), and (011) States of $H_2{}^{18}O$[a]

	(000)	(110)	(011)
E_v	0.0000	$5221.250_7 \pm 0.017$	$5310.463_6 \pm 0.011$
A^v	$27.531075_8 \pm 0.000098$	$29.857_7 \pm 0.011$	$29.1757_1 \pm 0.0039$
B^v	$14.522139_8 \pm 0.000056$	$14.4818_7 \pm 0.0026$	$14.6088_7 \pm 0.0018$
C^v	$9.237985_8 \pm 0.000022$	$8.9121_3 \pm 0.0016$	$8.9577_8 \pm 0.0012$
Δ_K^v	$(0.31596_6 \pm 0.00013) \times 10^{-1}$	$(0.520_7 \pm 0.018) \times 10^{-1}$	$(0.4886_5 \pm 0.0040) \times 10^{-1}$
Δ_{JK}^v	$(-0.5692_3 \pm 0.0017) \times 10^{-2}$	$(-0.748_5 \pm 0.048) \times 10^{-2}$	$(-0.767_3 \pm 0.011) \times 10^{-2}$
Δ_J^v	$(0.12531_1 \pm 0.00015) \times 10^{-2}$	$(0.1372_3 \pm 0.0030) \times 10^{-2}$	$(0.1456_3 \pm 0.0017) \times 10^{-2}$
δ_K^v	$(0.1288_4 \pm 0.0015) \times 10^{-2}$	$(0.276_3 \pm 0.028) \times 10^{-2}$	$(0.335_0 \pm 0.011) \times 10^{-2}$
δ_J^v	$(0.51014_6 \pm 0.00044) \times 10^{-3}$	$(0.584_1 \pm 0.016) \times 10^{-3}$	$(0.606_1 \pm 0.013) \times 10^{-3}$
H_K^v	$(0.1156_0 \pm 0.0012) \times 10^{-3}$	$(0.327_5 \pm 0.089) \times 10^{-3}$	$(0.262_6 \pm 0.012) \times 10^{-3}$
H_{KJ}^v	$(-0.171_9 \pm 0.016) \times 10^{-4}$	$(-0.59_0 \pm 0.27) \times 10^{-4}$	$(-0.369_6 \pm 0.037) \times 10^{-4}$
H_{JK}^v	$(-0.128_6 \pm 0.018) \times 10^{-7}$		
H_J^v	$(0.525_7 \pm 0.013) \times 10^{-6}$		$(0.70_0 \pm 0.11) \times 10^{-6}$
h_K^v	$(0.271_0 \pm 0.016) \times 10^{-4}$		$(0.691_9 \pm 0.094) \times 10^{-4}$
h_J^v	$(0.2676_6 \pm 0.0051) \times 10^{-6}$		$(0.325_4 \pm 0.076) \times 10^{-6}$
L_K^v	$(-0.405_1 \pm 0.024) \times 10^{-6}$		$(-0.1012_7 \pm 0.0096) \times 10^{-5}$
L_{KKJ}^v	$(0.48_5 \pm 0.26) \times 10^{-7}$		
l_K^v	$(-0.108_8 \pm 0.024) \times 10^{-6}$		$(-0.42_0 \pm 0.15) \times 10^{-6}$

COUPLING CONSTANT

$h_{76} = -0.3029_2 \pm 0.0013$

[a] All the results are given in cm^{-1} and the quoted errors are 99% confidence intervals.

The curve of growth method (*8*, *9*) has been used for the computation of the line strength $k_\sigma{}^P$. For that we have calculated the function $X(A,y)$ defined as follows:

$$X(A, y) = \int_{-\infty}^{+\infty} \{1 - \exp[-AK(x, y)]\} dx,$$

where

$$A = \alpha_0 l \qquad \text{and} \qquad X = \frac{W}{\gamma_D} (\log 2)^{\frac{1}{2}}.$$

l is the absorption path and W the equivalent width (i.e., the area under the absorption line).

For H_2O self-broadening, $\gamma_L{}^0$ can appreciably vary from one line to another around the mean value of 0.3 cm^{-1} atm^{-1} and this yields to variation of y between approximatively 0.4 and 0.6. On account of the maximum value measured for W in the studied spectrum, the corresponding values of X are less than 1.7. Thus using Jansson and Korb's tables (*10*) we can see that the maximum error on A due to an uncertainty on y does not exceed 11%. Since we are close enough to the linear region of the curve of growth y is not a very sensitive parameter. We have precisely sampled the curve of growth (Fig. 1) for the mean value 0.5 of y using a program (*11*) based on Gautschi's algorithm (*12*)

TABLE IV

Calculated Rotational Energy Levels for the Vibrational States (000), (110), and (011)[a]

J	K_a	K_c	(000)	(110)	% (011)	(011)	% (110)
0	0	0	0.000	a 5221.251	0.0	a 5310.464	0.0
1	0	1	23.755	a 5244.638	0.0	a 5334.026	0.0
1	1	1	36.748	a 5259.985	0.0	a 5348.568	0.0
1	1	0	42.024	a 5265.540	0.0	a 5354.200	0.0
2	0	2	69.928	a 5290.128	0.0	a 5379.770	0.0
2	1	2	78.989	a 5301.212	0.0	a 5390.104	0.1
2	1	1	94.789	a 5317.848	0.0	a 5406.955	0.0
2	2	1	133.476	a 5363.369	0.0	a 5450.102	0.0
2	2	0	134.783	a 5364.605	0.1	a 5451.446	0.0
3	0	3	136.338	a 5355.559	0.0	a 5445.420	0.0
3	1	3	141.568	a 5362.300	0.0	a 5451.681	1.4
3	1	2	172.884	a 5395.301	0.0	a 5484.983	0.1
3	2	2	204.756	a 5433.542	0.1	a 5519.538	30.2
3	2	1	210.800	a 5439.258	1.4	a 5527.727	10.9
3	3	1	282.096	a 5521.687	10.9	a 5605.984	0.0
3	3	0	282.308	a 5523.825	30.2	a 5606.195	0.0
4	0	4	221.235	a 5439.042	0.0	a 5529.089	0.0
4	1	4	223.829	a 5442.595	0.0	a 5531.868	3.4
4	1	3	274.806	a 5496.480	0.0	a 5586.738	0.1
4	2	3	298.621	a 5525.992	0.1	a 5612.642	16.2
4	2	2	314.461	b 5541.938	3.4	a 5630.880	4.0
4	3	2	379.292	a 5617.514	4.0	a 5702.278	0.9
4	3	1	380.703	a 5620.550	16.2	a 5703.668	1.0
4	4	1	482.645	c 5736.603	0.9	a 5815.705	0.0
4	4	0	482.674	c 5736.618	0.9	a 5815.733	0.0
5	0	5	324.049	a 5539.815	0.0	a 5630.107	0.0
5	1	5	325.217	a 5541.520	0.0	a 5631.461	0.3
5	1	4	398.364	a 5619.298	0.0	a 5709.979	0.0
5	2	4	414.170	c 5639.843	0.1	a 5727.510	5.9
5	2	3	445.161	b 5670.891	0.3	a 5761.120	1.6
5	3	3	500.598	a 5737.168	1.7	a 5822.481	1.9
5	3	2	505.730	a 5743.000	6.0	a 5827.517	2.4
5	4	2	604.545	b 5856.945	2.4	a 5936.608	0.5
5	4	1	604.793	b 5857.067	1.9	a 5936.846	0.5
5	5	1	733.681	6003.525	0.5	a 6077.102	0.0
5	5	0	733.684	6003.527	0.5	a 6077.105	0.0
6	0	6	444.849	a 5657.882	0.0	a 5748.529	0.0
6	1	6	445.349	a 5658.660	0.0	a 5749.126	0.1
6	1	5	541.184	a 5761.345	0.0	a 5852.216	0.0
6	2	5	550.454	a 5774.149	0.1	a 5862.761	2.1
6	2	4	601.241	a 5825.533	0.2	a 5916.825	0.7
6	3	4	645.385	a 5880.033	0.8	a 5966.013	2.6
6	3	3	658.612	a 5892.847	2.1	a 5978.889	5.7
6	4	3	751.034	c 6001.747	5.8	a 6081.888	1.1
6	4	2	752.189	b 6002.278	2.7	a 6082.990	1.1
6	5	2	880.077	6147.797	1.1	a 6222.399	0.5
6	5	1	880.115	6147.819	1.1	a 6222.435	0.5
6	6	1	1033.199	6321.545	0.4	b 6387.488	0.1
6	6	0	1033.199	6321.545	0.4	a 6387.489	0.1

leading to a quick computation of the Voigt profile. Then the reciprocal curve of growth $A(X)$ has been obtained by a least-squares fit expanding A with respect to X as a polynomial of degree 7 for X varying from 0 to 1.7 with a rms of 0.6×10^{-7}. Using this polynomial we have then calculated the line strengths k_σ^P from the measured values of the equivalent width W. However, since the automatic determination of the equivalent width W (*13*) does not provide us with the true value of W, wings and baseline corrections are necessary (*14*). Being close to the linear region of the curve of growth, the general correction formula reduces to Eq. (12) of Ref. (*15*). The final results concerning the intensities appear in Table I. The precision on the measurements is about 10%.

CALCULATED LINE INTENSITIES

The method for calculating vibration-rotation line intensities has been described elsewhere (*5*) and used successfully for $H_2{}^{16}O$ (*6*, *16*, *17*). It takes into account simultaneously the influence of the centrifugal distortion, of the variation of the rotational constants

TABLE IV—*Continued*

J	K_a	K_c	(000)	(110)	%(011)	(011)	%(110)
7	0	7	583.781	a 5793.402	0.0	a 5884.518	0.0
7	1	7	583.990	a 5797.750	0.0	a 5884.773	0.1
7	1	6	701.698	b 5920.772	0.0	a 6011.709	0.1
7	2	6	706.601	5928.014	0.0	a 6017.430	0.8
7	2	5	780.456	6003.577	0.1	b 6095.700	0.3
7	3	5	812.765	6045.281	0.5	a 6132.055	2.8
7	3	4	839.552	c 6070.651	0.9	a 6157.371	20.0
7	4	4	921.899	b 6171.581	20.3	a 6251.334	1.7
7	4	3	925.703	c 6172.867	2.9	a 6254.961	1.8
7	5	3	1050.993	6316.269	1.9	a 6391.984	1.0
7	5	2	1051.206	6316.391	1.8	a 6392.182	1.0
7	6	2	1204.172	6489.701	0.9	a 6557.265	0.5
7	6	1	1204.178	6489.704	3.9	a 6557.270	0.5
7	7	1	1378.969			a 6744.000	0.1
7	7	0	1378.969			a 6744.000	0.1
8	0	8	740.916	5946.478	0.0	a 6038.163	0.0
8	1	8	741.002	b 5946.533	0.0	a 6038.271	0.0
8	1	7	879.498	6096.862	0.0	a 6187.927	0.1
8	2	7	881.917	6100.691	0.0	a 6190.817	0.4
8	2	6	980.225	6202.507	0.1	b 6295.089	0.2
8	3	6	1001.709	6231.921	0.3	a 6319.615	2.4
8	3	5	1047.332	6275.518	0.5	a 6370.527	25.0
8	4	5	1116.641	d 6357.323	25.2	a 6444.470	2.3
8	4	4	1126.446	6369.751	2.5	a 6453.825	2.8
8	5	4	1246.376	6508.918	3.0	a 6585.786	1.5
8	5	3	1247.214	6509.396	2.4	a 6586.564	1.5
8	6	3	1399.436			a 6751.088	1.0
8	6	2	1399.471			a 6751.120	1.0
8	7	2	1574.658			a 6938.358	0.5
8	7	1	1574.658			a 6938.359	0.5
8	8	1	1768.562			a 7143.353	0.1
8	8	0	1768.562			a 7143.353	0.1
9	0	9	916.261	c 6117.141	0.0	a 6209.487	0.0
9	1	9	916.297	a 6117.211	0.0	a 6209.533	0.0
9	1	8	1074.765	6289.679	0.0	a 6381.031	0.1
9	2	8	1075.911	6291.629	0.0	d 6382.431	0.2
9	2	7	1198.202	6419.840	0/1	b 6512.500	0.1
9	3	7	1211.188	6438.923	0.2	a 6527.601	1.6
9	3	6	1279.803	6505.493	0.4	a 6600.185	4.6
9	4	6	1334.486	6574.291	4.8	a 6660.562	2.7
9	4	5	1355.212			b 6680.369	4.6
9	5	5	1466.032			a 6803.603	2.1
9	5	4	1468.629			b 6806.006	2.1
9	6	4	1618.914			a 6968.855	1.5
9	6	3	1619.074			a 6969.001	1.5
9	7	3	1794.362			7156.500	1.0
9	7	2	1794.368			7156.505	1.0
9	8	2	1989.108			7362.329	0.6
9	8	1	1989.108			7362.329	0.6
10	0	10	1109.789	d 6305.380	0.0	a 6398.474	0.0
10	1	10	1109.804	b 6305.411	0.0	a 6398.494	0.0
10	1	9	1287.734	6499.477	0.0	a 6591.290	0.1
10	2	9	1288.266	6500.455	0.0	b 6591.954	0.1
10	2	8	1433.032	6653.808	0.1	b 6746.365	0.1
10	3	8	1440.291	6665.331	0.2	a 6754.977	1.0
10	3	7	1534.379			d 6853.529	1.3
10	4	7	1574.458			a 6898.688	2.8
10	4	6	1611.678			c 6934.151	9.4
10	5	6	1709.561			7045.044	2.6
10	5	5	1716.232			a 7051.211	2.8
10	6	5	1862.487			a 7210.420	2.0
10	6	4	1863.055			7210.935	2.0
10	7	4	2037.939			7398.250	1.5
10	7	3	2037.967			7398.275	1.5

with the vibrational quantum numbers, and of the resonances. For that purpose, the matrix elements of the transformed dipole moment operator are taken between realistic vibration-rotation wavefunctions of the lower and upper states of the transition. More precisely, the relevant part of this operator can be expanded as:

$$\mu'_Z = \sum_{v=6,7} |0\rangle {}^v\mu'_Z \langle v| \qquad \text{with} \quad v = \begin{cases} 6 & \text{for (110),} \\ 7 & \text{for (011).} \end{cases}$$

${}^v\mu'_Z$ is the transformed transition moment operator which can be written as:

$${}^v\mu'_Z = \sum_j {}^v\mu'_j {}^vA_j,$$

where the ${}^vA_j$'s are rotational operators (see Table II) and the ${}^v\mu'_j$ are constants to be

TABLE IV—*Continued*

J	K_a	K_c	(000)	(110)	% (011)	(011)	% (110)
11	0	11	1321.452	6511.158	0.0	a 6605.089	0.0
11	1	11	1321.459	6511.173	0.0	a 6605.097	0.0
11	1	10	1518.539	6726.437	0.0	a 6818.879	0.1
11	2	10	1518.784	6726.928	0.0	b 6819.191	0.1
11	2	9	1684.446			b 6996.263	0.1
11	3	9	1688.291			b 7000.916	0.6
11	3	8	1808.385			7126.660	0.5
11	4	8	1835.500			a 7157.826	2.5
11	4	7	1894.246			7212.359	29.3
11	5	7	1976.331			7309.502	3.1
11	5	6	1990.920			7323.026	3.6
12	0	12	1551.194	6734.424	0.0	a 6829.285	0.0
12	1	12	1551.197	6734.431	0.0	a 6829.289	0.0
12	1	11	1767.219	6970.636	0.0	a 7063.873	0.1
12	2	11	1767.332	6970.886	0.0	b 7064.020	0.1
12	2	10	1952.696			7262.418	0.2
12	3	10	1954.669			7264.849	0.4
12	3	9	2099.608			7417.000	0.3
13	0	13	1798.948	6975.118	0.0	a 7071.011	0.0
13	1	13	1798.949	6975.122	0.0	a 7071.013	0.0
13	1	12	2033.761			c 7326.292	0.1
13	2	12	2033.813			a 7326.361	0.1
13	2	11	2238.075			7545.167	0.2
13	3	11	2239.070			7546.414	0.3
14	0	14	2064.641			7330.213	0.0
14	1	14	2064.642			7330.214	0.0
14	1	13	2318.118			7606.120	0.1
14	2	13	2318.142			7606.153	0.1
15	0	15	2348.196			7606.834	0.0
15	1	15	2348.196			7606.835	0.0

[a] A letter in front of an energy level means that the experimental value E^{obs} has been used in the least-squares fit. Moreover, the value of $\delta = |E^{obs} - E^{calc}|$ (in cm^{-1}) is such that: for *a*, $0 \times 10^{-3} < \delta \leqslant 20 \times 10^{-3}$ for *b*, $20 \times 10^{-3} < \delta \leqslant 40 \times 10^{-3}$ for *c*, $40 \times 10^{-3} < \delta \leqslant 80 \times 10^{-3}$ for *d*, $80 \times 10^{-3} < \delta \leqslant 140 \times 10^{-3}$. For the ground state, the levels introduced in the fit are those of Ref. (*7*) leading to a rms of 3.5×10^{-3} cm^{-1}.

determined to give the best agreement with the experimental line intensities. The wavefunctions used to calculate the matrix elements of ${}^{v}\mu'_Z$ have been taken from Ref. (*3*).

In this reference the wavefunctions were calculated using the rotational constants listed in Table III and the corresponding energy levels are gathered in Table IV.

As suggested by the Editor, these two tables are reproduced here because they have come out very badly in Ref. (*3*).

As can be seen in Table I which lists the experimental intensities, there are relatively few lines belonging to the $\nu_1 + \nu_2$ band. This should be expected since this band is weaker[2] than $\nu_2 + \nu_3$ roughly by a factor 30. Thus, practically, the only lines of $\nu_1 + \nu_2$ band actually seen in the spectrum are those whose intensity is enhanced by perturbation. Under these conditions we have been compelled to fix the value of the constants appearing in the rotational correcting terms of the expansion of ${}^{6}\mu'_Z$ to the value obtained for $H_2{}^{16}O$ (*6*). So, in addition to the constants ${}^{7}\mu'_j$ relative to the $\nu_2 + \nu_3$ band the only constant allowed to vary for the $\nu_1 + \nu_2$ band is the vibrational part ${}^{6}\mu'_1$ of the transformed transition moment operator corresponding to this band. The final values of the ${}^{v}\mu'_j$ introduced in the fit appear in Table II.

It is satisfying to see that the constants ${}^{v}\mu'_j$ for $H_2{}^{18}O$ are comparable to those of $H_2{}^{16}O$. A statistical analysis of the relative differences between observed and calculated

[2] Moreover, we may recall that the spectrum used for measuring $H_2{}^{18}O$ intensities is a spectrum of natural water vapor in which the amount of $H_2{}^{18}O$ is 0.204%.

TABLE V

Computed List of the Lines of the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ Bands of $H_2{}^{18}O$ at 296 K[a]

NO	SIGMA	J'	KA'	KC'	J	KA	KC	E	INTENSITY	NO	SIGMA	J'	KA'	KC'	J	KA	KC	E	INTENSITY
70	4976.471	5	2	4	6	4	3	751.036	0.680D-25	70	5157.280	6	4	2	7	4	3	925.704	0.142D-23
70	4986.076	5	1	5	6	3	4	645.385	0.555D-25	60	5157.540	3	1	3	3	2	2	204.758	0.849D-25
60	5002.865	4	4	1	5	5	0	733.685	0.873D-25	70	5157.823	7	6	2	8	6	3	1399.437	0.107D-24
70	5012.652	6	1	5	7	3	4	839.555	0.112D-24	70	5158.775	8	1	8	8	1	7	879.493	0.529D-25
60	5012.721	4	3	2	5	4	1	604.794	0.158D-24	70	5159.887	5	2	3	6	2	4	601.238	0.258D-23
60	5020.264	4	2	3	5	3	2	505.730	0.121D-24	70	5159.981	6	4	3	7	4	4	921.900	0.481D-24
60	5025.490	5	2	3	6	3	4	645.385	0.583D-25	60	5162.231	6	4	3	7	3	4	839.555	0.170D-24
70	5030.347	12	0	12	13	0	13	1798.948	0.586D-25	60	5164.022	7	2	5	7	3	4	839.555	0.503D-25
70	5036.892	3	2	2	4	4	1	482.646	0.181D-24	60	5164.240	4	0	4	4	1	3	274.803	0.101D-24
60	5039.005	3	3	1	4	4	0	482.676	0.855D-25	70	5164.744	6	0	6	7	0	7	583.782	0.109D-22
60	5041.171	3	3	0	4	4	1	482.646	0.750D-25	60	5164.879	2	1	2	3	0	3	136.338	0.203D-24
70	5051.364	5	1	4	6	3	3	658.609	0.821D-25	70	5165.141	6	1	6	7	1	7	583.985	0.362D-23
70	5051.839	11	2	10	12	2	11	1767.335	0.599D-25	60	5165.145	5	2	3	5	3	2	505.730	0.132D-24
60	5052.848	3	2	2	4	3	1	380.703	0.746D-25	60	5165.650	1	0	1	2	1	2	78.990	0.365D-24
60	5053.886	11	0	11	12	0	12	1551.195	0.595D-25	70	5165.800	6	2	4	6	4	3	751.036	0.527D-25
70	5053.894	11	1	11	12	1	12	1551.195	0.179D-24	60	5167.740	2	1	2	2	2	1	133.477	0.212D-24
60	5059.966	3	2	1	4	3	2	379.291	0.254D-24	70	5168.794	5	1	4	6	1	5	541.179	0.358D-23
70	5061.956	10	2	8	11	2	9	1684.437	0.779D-25	70	5168.907	5	3	2	6	3	3	658.609	0.162D-23
60	5068.843	5	1	4	6	2	5	550.453	0.733D-25	70	5166.969	2	0	2	3	2	1	210.800	0.956D-24
70	5072.389	3	1	3	4	3	2	379.291	0.808D-25	70	5171.230	6	5	1	7	5	2	1051.207	0.565D-24
70	5072.742	10	1	9	11	1	10	1518.541	0.182D-24	70	5171.407	6	5	2	7	5	3	1050.994	0.189D-24
70	5073.132	10	2	9	11	2	10	1518.798	0.604D-25	60	5172.356	4	3	2	5	2	3	445.159	0.421D-24
70	5077.019	10	0	10	11	0	11	1321.457	0.496D-24	60	5174.137	5	1	4	5	2	3	445.159	0.244D-24
70	5077.024	10	1	10	11	1	11	1321.464	0.165D-24	70	5177.054	5	2	4	6	2	5	550.453	0.917D-23
60	5077.385	8	4	5	9	3	6	1279.800	0.102D-24	70	5177.088	5	3	3	6	3	4	645.385	0.518D-23
70	5079.494	9	2	7	10	2	8	1433.030	0.792D-25	70	5177.922	7	0	7	7	2	6	706.599	0.119D-24
70	5081.008	4	1	3	5	3	2	505.730	0.338D-24	60	5182.011	4	1	3	4	2	2	314.461	0.122D-24
60	5081.064	2	2	1	3	3	0	282.306	0.348D-24	60	5182.675	3	0	3	3	1	2	172.884	0.463D-24
60	5082.511	2	2	0	3	3	1	282.095	0.118D-24	60	5183.068	2	1	1	2	2	0	134.785	0.960D-25
70	5083.928	4	0	4	5	2	3	445.159	0.329D-24	70	5183.077	7	1	7	7	1	6	701.695	0.373D-24
70	5086.098	9	4	6	10	4	7	1574.458	0.107D-24	70	5183.297	6	6	0	7	6	1	1204.177	0.146D-24
70	5087.300	9	3	7	10	3	8	1440.291	0.222D-24	70	5184.335	9	2	8	9	2	7	1198.210	0.588D-25
60	5090.417	2	1	2	3	2	1	210.800	0.186D-24	60	5184.490	0	0	0	1	1	1	36.750	0.107D-24
70	5090.713	8	3	5	9	3	6	1279.800	0.340D-24	60	5184.498	3	1	2	3	2	1	210.800	0.407D-24
70	5093.299	9	1	8	10	1	9	1267.727	0.167D-24	70	5184.655	5	4	1	6	4	2	752.191	0.777D-24
70	5094.017	9	5	5	10	5	6	1709.575	0.503D-25	70	5185.252	5	0	5	6	0	6	444.853	0.602D-23
70	5094.274	9	2	8	10	2	9	1288.271	0.498D-24	70	5185.570	5	4	2	6	4	3	751.036	0.235D-23
60	5094.471	5	0	5	6	1	6	445.346	0.105D-24	70	5185.722	4	2	3	5	2	3	445.159	0.127D-22
60	5096.677	3	1	2	4	2	3	298.621	0.204D-24	70	5186.115	5	1	5	6	1	6	445.346	0.179D-22
70	5096.902	8	2	6	9	2	7	1198.210	0.665D-24	70	5186.204	8	1	7	8	3	6	1001.711	0.128D-24
70	5098.616	8	4	4	9	4	5	1355.221	0.267D-24	70	5188.377	4	1	3	5	1	4	398.361	0.179D-22
70	5099.705	9	0	9	10	0	10	1109.785	0.416D-24	60	5192.553	5	3	2	6	2	5	550.453	0.646D-24
70	5099.735	9	1	9	10	1	10	1109.801	0.125D-23	60	5195.341	2	0	2	2	1	1	94.789	0.192D-24
70	5104.276	3	1	2	4	3	1	380.703	0.956D-25	70	5196.989	5	5	0	6	5	1	880.115	0.231D-24
60	5108.208	6	1	6	6	2	5	550.453	0.904D-25	70	5197.024	5	5	1	6	5	2	880.080	0.693D-24
70	5108.415	8	3	6	9	3	7	1211.191	0.196D-24	70	5197.934	4	3	1	5	3	2	505.730	0.732D-23
70	5109.976	8	4	5	9	4	6	1334.485	0.987D-25	70	5198.073	6	0	6	6	2	5	550.453	0.723D-24
70	5110.039	7	3	4	8	3	5	1047.331	0.307D-24	70	5198.472	4	2	3	5	2	4	414.170	0.413D-23
60	5113.095	2	1	1	3	2	2	204.758	0.949D-25	70	5198.932	7	1	6	7	3	5	812.766	0.872D-25
70	5113.152	8	1	7	9	1	8	1074.763	0.125D-23	70	5199.238	1	0	1	2	2	0	134.785	0.181D-24
60	5113.827	4	0	4	5	1	5	325.216	0.609D-25	70	5201.675	4	3	2	5	3	3	500.597	0.250D-23
70	5114.909	8	2	7	9	2	8	1075.911	0.411D-24	60	5202.616	1	0	1	1	1	0	42.024	0.503D-24
70	5115.489	7	2	5	8	2	6	980.229	0.567D-24	70	5205.040	4	0	4	5	0	5	324.047	0.267D-22
70	5117.943	8	5	3	9	5	4	1468.616	0.135D-24	60	5206.382	4	3	1	5	2	4	414.170	0.863D-24
60	5118.549	4	1	4	5	0	5	324.047	0.154D-24	70	5206.654	4	1	4	5	1	5	325.216	0.848D-23
70	5121.903	8	0	8	9	0	9	916.258	0.285D-23	70	5206.822	6	1	5	6	3	4	645.385	0.412D-24
70	5121.971	8	1	8	9	1	9	916.297	0.949D-24	60	5207.220	3	3	1	4	2	2	314.461	0.586D-24
60	5124.234	7	4	4	8	3	5	1047.331	0.847D-25	70	5207.447	4	1	3	4	3	2	379.291	0.336D-24
70	5124.648	2	1	1	3	3	0	282.306	0.143D-24	70	5207.947	6	1	6	6	1	5	541.179	0.269D-24
60	5125.200	1	1	1	2	2	0	134.785	0.106D-24	70	5209.376	5	1	4	5	3	3	500.597	0.153D-24
60	5127.344	5	1	5	5	2	4	414.170	0.501D-25	70	5210.178	3	1	2	4	1	3	274.803	0.861D-23
70	5128.515	7	4	3	8	4	4	1126.443	0.226D-24	70	5210.591	8	2	7	8	2	6	980.229	0.564D-25
60	5128.763	6	2	5	6	3	4	645.385	0.817D-25	70	5210.943	4	4	0	5	4	1	604.794	0.258D-23
70	5130.334	7	3	5	8	3	6	1001.711	0.139D-23	70	5211.165	4	4	1	5	4	2	604.547	0.861D-24
70	5130.957	3	0	3	4	2	2	314.461	0.243D-24	60	5211.708	5	4	1	6	3	4	645.385	0.113D-24
60	5131.730	3	0	3	4	1	4	223.829	0.273D-24	70	5213.265	3	2	1	4	2	2	314.461	0.527D-23
70	5132.042	8	6	2	9	6	3	1619.071	0.524D-25	60	5215.428	3	2	1	4	1	4	223.829	0.373D-24
60	5132.065	1	1	0	2	2	1	133.477	0.364D-24	70	5215.935	5	0	5	5	2	4	414.170	0.421D-24
70	5132.205	7	1	6	8	1	7	879.493	0.940D-24	60	5216.705	4	2	2	5	1	5	325.216	0.320D-24
70	5134.686	7	4	4	8	4	5	1116.639	0.711D-24	70	5220.917	3	2	2	4	2	3	298.621	0.128D-22
70	5134.773	9	1	9	9	1	8	1074.763	0.617D-25	70	5224.184	3	0	3	4	0	4	221.234	0.116D-22
60	5134.869	4	3	2	4	4	1	482.646	0.624D-25	60	5225.196	3	3	0	4	2	3	298.621	0.589D-23
70	5135.507	7	2	6	8	2	7	881.917	0.275D-23	70	5225.490	3	3	0	4	3	1	380.703	0.246D-23
70	5136.380	6	2	4	7	2	5	780.456	0.390D-23	60	5225.529	5	2	3	6	1	6	445.346	0.596D-25
70	5139.336	6	3	3	7	3	4	839.555	0.249D-23	70	5226.690	3	3	1	4	3	2	379.291	0.745D-23
60	5140.338	7	1	6	7	2	5	780.456	0.586D-25	70	5227.851	3	1	3	4	1	4	223.829	0.332D-22
60	5141.064	2	1	3	4	0	4	221.234	0.676D-25	70	5230.466	4	0	4	4	2	3	298.621	0.175D-23
60	5141.456	5	0	5	5	1	4	398.361	0.178D-24	60	5230.820	4	4	1	5	3	2	505.730	0.819D-25
70	5143.603	7	0	7	8	0	8	740.918	0.196D-23	70	5233.100	5	1	5	5	1	4	398.361	0.163D-23
70	5143.773	7	1	7	8	1	8	740.999	0.586D-23	70	5234.070	2	1	1	3	1	2	172.884	0.303D-22
60	5143.975	4	1	4	4	2	3	298.621	0.216D-24	70	5236.968	7	2	6	7	2	5	780.456	0.462D-24
70	5144.971	7	5	2	8	5	3	1247.210	0.103D-24	70	5240.642	2	2	0	3	2	1	210.800	0.160D-22
70	5145.607	7	5	3	8	5	4	1246.380	0.311D-24	70	5240.660	3	0	3	3	2	2	204.758	0.560D-24
60	5146.703	4	2	3	4	3	2	379.291	0.158D-24	60	5241.786	1	1	0	1	0	1	23.756	0.415D-24
60	5148.562	2	0	2	3	1	3	141.568	0.115D-24	70	5243.431	2	0	2	3	0	3	136.338	0.395D-22
70	5150.512	6	1	5	7	1	6	701.695	0.578D-23	70	5245.345	2	2	1	3	2	2	204.758	0.546D-23
70	5153.244	6	3	4	7	3	5	812.766	0.965D-24	70	5246.292	2	0	2	2	2	1	133.477	0.834D-24
70	5156.158	6	2	5	7	2	6	706.599	0.181D-23	70	5247.791	9	3	7	9	3	6	1279.800	0.603D-25
70	5156.244	8	0	8	8	2	7	881.917	0.155D-24	60	5247.925	2	1	1	2	0	2	69.928	0.145D-24
60	5156.951	3	2	1	3	3	0	282.306	0.148D-24	70	5248.535	2	1	2	3	1	3	141.568	0.118D-22

TABLE V—*Continued*

NO	SIGMA	J'	KA'	KC'	J	KA	KC	E	INTENSITY	NO	SIGMA	J'	KA'	KC'	J	KA	KC	E	INTENSITY
60	5253.380	2	0	2	1	1	1	36.750	0.911D-25	60	5347.189	6	1	5	5	2	4	414.170	0.591D-25
70	5257.067	4	1	4	4	1	3	274.803	0.977D-24	60	5348.066	7	0	7	6	1	6	445.346	0.483D-24
60	5258.960	3	1	2	3	0	3	136.338	0.303D-24	60	5348.895	7	1	7	6	0	6	444.853	0.163D-24
70	5259.412	1	1	0	2	1	1	94.789	0.832D-23	70	5349.776	9	6	4	9	6	3	1619.071	0.729D-25
60	5259.985	1	1	1	0	0	0	0.0	0.126D-24	60	5351.363	5	4	1	5	3	2	505.730	0.233D-24
70	5261.519	6	2	5	6	2	4	601.238	0.403D-24	70	5351.626	8	6	3	8	6	2	1399.471	0.805D-25
60	5261.821	3	1	2	2	2	1	133.477	0.636D-25	70	5351.676	8	6	2	8	6	3	1399.437	0.241D-24
70	5264.095	1	0	1	2	0	2	69.928	0.123D-22	70	5353.083	7	6	2	7	6	1	1204.177	0.717D-24
70	5267.118	4	2	2	4	1	3	274.803	0.221D-24	70	5353.090	7	6	1	7	6	2	1204.170	0.239D-24
70	5269.578	1	1	1	2	1	2	78.990	0.270D-22	60	5353.110	4	2	3	3	1	2	172.884	0.521D-24
70	5272.275	6	3	6	8	3	5	1047.331	0.722D-25	70	5353.353	2	1	2	1	1	1	36.750	0.106D-22
60	5272.514	5	2	3	5	1	4	398.361	0.202D-24	70	5354.276	6	6	1	6	6	0	1033.195	0.640D-24
60	5275.238	4	1	3	4	0	4	221.234	0.536D-25	70	5354.279	6	6	0	6	6	1	1033.195	0.192D-23
60	5276.569	3	0	3	2	1	2	78.990	0.556D-24	60	5355.862	4	4	0	4	3	1	380.703	0.836D-25
70	5277.196	6	3	3	7	1	6	701.695	0.641D-25	70	5356.013	2	0	2	1	0	1	23.756	0.446D-22
60	5277.461	2	1	2	1	0	1	23.756	0.590D-24	60	5356.366	5	4	2	5	3	3	500.597	0.967D-25
70	5278.796	3	1	3	3	1	2	172.884	0.690D-23	60	5356.401	6	4	3	6	3	4	645.385	0.253D-24
70	5282.348	5	2	4	5	2	3	445.159	0.298D-23	60	5357.259	4	4	1	4	3	2	379.291	0.266D-24
60	5284.380	2	2	1	2	1	2	78.990	0.700D-25	60	5358.799	7	4	4	7	3	5	812.766	0.871D-25
70	5286.712	0	0	0	1	0	1	23.756	0.233D-22	60	5360.267	3	2	1	2	1	2	78.990	0.147D-23
60	5290.245	7	3	4	7	2	5	780.456	0.501D-25	60	5362.493	8	0	8	7	1	7	583.985	0.105D-24
60	5292.370	3	1	3	2	0	2	69.928	0.256D-24	60	5362.828	8	1	8	7	0	7	583.782	0.316D-24
70	5292.490	7	3	5	7	3	4	839.555	0.739D-24	70	5362.909	4	1	3	4	1	4	223.829	0.441D-23
60	5295.249	5	1	4	5	0	5	324.047	0.727D-25	70	5363.712	8	7	1	8	7	2	1574.658	0.143D-24
70	5295.314	2	1	2	2	1	1	94.789	0.458D-23	70	5364.930	2	1	1	1	1	0	42.024	0.311D-22
60	5297.475	4	0	4	3	1	3	141.568	0.246D-24	60	5365.007	5	2	4	4	1	3	274.803	0.140D-24
60	5297.847	5	3	2	5	2	3	445.159	0.505D-24	70	5365.036	7	7	1	7	7	0	1378.970	0.423D-24
70	5298.181	4	2	3	4	2	2	314.461	0.219D-23	70	5365.036	7	7	0	7	7	1	1378.970	0.141D-24
60	5302.165	4	2	3	4	1	4	223.829	0.624D-25	70	5366.383	6	2	4	6	2	5	550.453	0.175D-23
70	5305.303	4	3	1	5	1	4	398.361	0.133D-24	70	5368.802	8	3	5	8	3	6	1001.711	0.255D-24
70	5305.335	9	4	6	9	4	5	1355.221	0.881D-25	60	5370.341	7	1	6	6	2	5	550.453	0.148D-24
60	5306.091	4	3	1	4	2	2	314.461	0.686D-24	70	5372.690	3	1	3	2	1	2	78.990	0.444D-22
60	5306.258	4	1	4	3	0	3	136.338	0.854D-24	70	5374.777	8	8	0	8	8	1	1768.562	0.734D-25
70	5306.492	3	2	1	4	0	4	221.234	0.947D-25	70	5375.490	3	0	3	2	0	2	69.928	0.173D-22
70	5306.544	1	1	1	1	1	0	42.024	0.317D-22	60	5375.787	6	2	5	5	1	4	398.361	0.306D-24
70	5306.834	4	2	2	5	0	5	324.047	0.167D-24	60	5376.090	9	0	9	8	1	8	740.999	0.182D-24
70	5307.401	6	3	4	6	3	3	658.609	0.773D-24	60	5376.304	9	1	9	8	0	8	740.918	0.609D-25
70	5308.738	3	2	2	3	2	1	210.800	0.130D-22	70	5380.175	2	2	1	2	0	2	69.928	0.416D-24
70	5310.633	3	0	3	2	2	0	134.785	0.600D-25	70	5383.200	3	2	2	3	0	3	136.338	0.175D-23
60	5313.017	3	3	0	3	2	1	210.800	0.713D-23	70	5384.757	5	1	4	5	1	5	325.216	0.830D-24
70	5315.104	2	2	0	3	0	3	136.338	0.258D-24	70	5386.061	3	2	2	2	2	1	133.477	0.177D-22
70	5315.318	2	2	1	2	2	0	134.785	0.147D-22	60	5386.835	7	2	6	6	1	5	541.179	0.671D-25
60	5315.988	5	0	5	4	1	4	223.829	0.762D-24	60	5386.896	3	3	1	2	2	0	134.785	0.139D-23
70	5316.743	5	3	3	5	3	2	505.730	0.646D-23	60	5387.479	3	3	0	3	0	3	136.338	0.807D-24
60	5316.923	3	3	1	3	2	2	204.758	0.539D-24	70	5389.119	7	2	5	7	2	6	706.599	0.244D-24
70	5317.451	1	1	0	1	1	1	36.750	0.109D-22	60	5389.182	10	1	10	9	0	9	916.258	0.948D-25
70	5317.965	2	2	0	2	2	1	133.477	0.445D-22	70	5390.192	3	1	2	2	1	1	94.789	0.140D-22
70	5318.018	8	4	5	8	4	4	1126.443	0.112D-24	70	5390.302	4	1	4	3	1	3	141.568	0.153D-22
70	5318.287	4	0	4	3	2	1	210.800	0.196D-24	60	5390.340	3	3	0	2	2	1	133.477	0.466D-23
60	5318.894	4	3	2	4	2	3	298.621	0.122D-24	70	5391.408	4	2	3	4	0	4	221.234	0.758D-24
60	5320.280	5	1	5	4	0	4	221.234	0.271D-24	70	5392.749	4	0	4	3	0	3	136.338	0.492D-22
60	5320.675	5	1	4	4	2	3	298.621	0.170D-24	70	5392.941	3	2	1	2	2	0	134.785	0.608D-23
60	5321.346	2	2	1	1	1	0	42.024	0.494D-24	60	5396.761	6	5	2	6	4	3	751.036	0.561D-25
70	5321.569	4	3	2	4	3	1	380.703	0.525D-23	60	5398.733	5	5	0	5	4	1	604.794	0.619D-25
70	5322.968	3	2	1	3	2	2	204.758	0.640D-23	60	5398.996	8	2	7	7	1	6	701.695	0.120D-24
70	5323.675	3	3	1	3	3	0	282.306	0.344D-22	60	5399.318	4	3	1	4	0	4	221.234	0.161D-24
70	5324.098	3	3	0	3	3	1	282.095	0.115D-22	60	5400.353	4	2	2	3	1	3	141.568	0.310D-24
70	5324.373	4	3	1	4	3	2	379.291	0.159D-22	70	5403.460	5	2	4	5	0	5	324.047	0.196D-23
70	5325.621	7	4	4	7	4	3	925.704	0.110D-23	60	5406.715	4	3	2	3	2	1	210.800	0.221D-23
70	5326.919	5	3	2	5	3	3	500.597	0.221D-23	70	5406.861	6	1	5	6	1	6	445.346	0.137D-23
60	5327.856	2	2	0	1	1	1	36.750	0.184D-24	70	5407.632	5	1	5	4	1	4	223.829	0.396D-22
70	5327.964	2	1	1	2	1	2	78.990	0.148D-22	60	5407.762	9	1	8	8	2	7	881.917	0.591D-25
70	5329.690	6	4	3	6	4	2	752.191	0.105D-23	70	5407.684	4	2	3	3	2	2	204.758	0.832D-23
70	5331.812	5	4	2	5	4	1	604.794	0.788D-23	70	5408.871	5	0	5	4	0	4	221.234	0.135D-22
70	5331.948	6	4	2	6	4	3	751.036	0.316D-23	70	5413.195	8	2	6	8	2	7	881.917	0.301D-24
70	5332.260	4	2	2	4	2	3	298.621	0.929D-23	70	5413.854	4	1	3	3	1	2	172.884	0.396D-22
70	5332.299	5	4	1	5	4	2	604.547	0.263D-23	60	5415.794	4	3	1	3	2	2	204.758	0.988D-24
60	5332.667	6	0	6	5	1	5	325.216	0.218D-24	70	5417.904	6	2	5	6	0	6	444.853	0.423D-24
70	5333.036	4	4	1	4	4	0	482.676	0.597D-23	60	5418.959	5	3	2	5	0	5	324.047	0.139D-24
70	5333.058	7	4	3	7	4	4	921.900	0.376D-24	70	5420.081	4	2	2	3	2	1	210.800	0.255D-22
70	5333.091	4	4	0	4	4	1	482.646	0.179D-22	70	5420.177	4	3	2	3	3	1	282.095	0.380D-23
60	5333.281	7	4	3	7	3	4	839.555	0.579D-25	70	5421.358	4	3	1	3	3	0	282.306	0.114D-22
70	5333.506	6	3	3	6	3	4	645.385	0.241D-23	60	5422.711	5	3	3	4	2	2	314.461	0.326D-24
70	5334.023	1	0	1	0	0	0	0.0	0.857D-23	70	5423.910	6	1	6	5	1	5	325.216	0.968D-23
60	5334.614	6	1	6	5	0	5	324.047	0.673D-24	70	5424.112	5	3	3	5	1	4	398.361	0.871D-24
70	5334.976	9	5	5	9	5	4	1468.616	0.981D-25	70	5424.479	6	0	6	5	0	5	324.047	0.293D-22
70	5337.198	8	4	4	8	4	5	1116.639	0.354D-24	70	5424.831	6	3	4	6	1	5	541.179	0.256D-24
70	5338.562	8	5	4	8	5	3	1247.210	0.112D-24	70	5427.469	4	3	2	4	1	3	274.803	0.222D-24
60	5338.762	3	2	2	2	1	1	94.789	0.187D-24	70	5427.686	2	2	0	1	0	1	23.756	0.855D-24
70	5340.179	8	5	3	8	5	4	1246.380	0.338D-24	70	5427.713	7	1	6	7	1	7	583.985	0.236D-24
70	5340.780	7	5	3	7	5	2	1051.207	0.102D-23	70	5428.886	5	2	4	4	2	3	298.621	0.236D-22
70	5341.187	7	5	2	7	5	3	1050.994	0.340D-24	70	5430.350	7	3	5	7	1	6	701.695	0.496D-24
70	5342.286	6	5	2	6	5	1	880.115	0.920D-24	70	5433.097	3	3	1	3	1	2	172.884	0.287D-24
70	5342.357	6	5	1	6	5	2	880.080	0.276D-23	70	5433.642	7	2	6	7	0	7	583.782	0.692D-24
70	5343.413	3	1	2	3	1	3	141.568	0.263D-23	60	5434.881	6	3	4	5	2	3	445.159	0.422D-24
70	5343.419	5	5	1	5	5	0	733.685	0.675D-23	70	5435.170	5	1	4	4	1	3	274.803	0.100D-22
70	5343.423	5	5	0	5	5	1	733.681	0.225D-23	70	5439.426	7	1	7	6	1	6	445.346	0.188D-22
70	5344.604	7	3	4	7	3	5	812.766	0.222D-24	70	5439.668	7	0	7	6	0	6	444.853	0.629D-23
70	5346.477	6	1	5	5	3	2	505.730	0.780D-25	70	5440.113	8	3	6	8	1	7	879.493	0.849D-25
70	5346.955	5	2	3	5	2	4	414.170	0.137D-23	70	5443.182	5	3	3	4	3	2	379.291	0.128D-22

TABLE V—*Continued*

NO	SIGMA	J'KA'KC'	J	KA	KC	E	INTENSITY	NO	SIGMA	J'KA'KC'	J	KA	KC	E	INTENSITY
60	5444.043	7 3 5	6	2	4	601.238	0.602D-25	70	5519.812	13 1 13	12	1	12	1551.195	0.154D-24
60	5444.385	5 3 2	4	2	3	298.621	0.769D-24	70	5522.561	8 4 5	7	4	4	921.900	0.554D-24
70	5446.664	5 2 3	4	2	2	314.461	0.742D-23	70	5524.065	7 6 1	6	6	0	1033.195	0.102D-24
70	5446.813	5 3 2	4	3	1	380.703	0.424D-23	70	5524.065	7 6 2	6	6	1	1033.195	0.306D-24
70	5446.916	8 1 7	8	1	8	740.999	0.336D-24	70	5525.880	9 3 7	8	3	6	1001.711	0.145D-23
70	5448.587	6 2 5	5	2	4	414.170	0.574D-23	70	5526.991	3 3 1	2	1	2	78.990	0.226D-24
70	5449.902	8 2 7	8	0	8	740.918	0.111D-24	60	5527.451	7 4 3	6	3	4	645.385	0.601D-25
60	5451.465	8 3 6	7	2	5	780.456	0.767D-25	70	5528.133	8 4 4	7	4	3	925.704	0.164D-23
60	5451.753	3 3 1	2	0	2	69.928	0.619D-25	70	5530.780	4 3 1	3	1	2	172.884	0.665D-24
70	5452.828	9 3 7	9	1	8	1074.763	0.111D-24	70	5530.903	11 2 10	10	2	9	1288.271	0.460D-24
70	5453.846	6 1 5	5	1	4	398.361	0.196D-22	70	5530.958	8 3 5	7	3	4	839.555	0.198D-23
70	5453.960	5 4 2	4	4	1	482.646	0.439D-23	70	5531.138	11 1 10	10	1	9	1287.727	0.154D-24
70	5454.170	5 4 1	4	4	0	482.676	0.146D-23	70	5532.295	9 2 7	8	2	6	980.229	0.556D-24
70	5454.283	8 1 8	7	1	7	583.985	0.363D-23	70	5532.531	6 4 2	6	2	5	550.453	0.833D-25
70	5454.379	8 0 8	7	0	7	583.782	0.109D-22	70	5534.778	8 5 4	7	5	3	1050.994	0.243D-24
70	5457.798	3 2 1	2	0	2	69.928	0.472D-24	70	5535.352	8 5 3	7	5	2	1051.207	0.727D-24
70	5465.413	6 3 4	5	3	3	500.597	0.326D-23	70	5539.891	5 2 3	4	0	4	221.234	0.226D-24
70	5466.287	9 2 8	9	0	9	916.258	0.145D-24	70	5543.783	10 3 8	9	3	7	1211.191	0.196D-24
70	5466.971	7 2 6	6	2	5	550.453	0.106D-22	70	5543.917	9 4 6	8	4	5	1116.639	0.765D-24
70	5468.537	9 1 9	8	1	8	740.999	0.567D-23	70	5545.193	12 2 11	11	2	10	1518.798	0.543D-25
70	5468.572	9 0 9	8	0	8	740.918	0.189D-23	70	5545.345	12 1 11	11	1	10	1518.541	0.163D-24
70	5470.519	7 1 6	6	1	5	541.179	0.376D-23	70	5546.927	8 6 3	7	6	2	1204.170	0.829D-25
70	5470.869	7 4 4	7	2	5	780.456	0.137D-24	70	5546.936	8 6 2	7	6	1	1204.177	0.249D-24
70	5471.677	6 2 4	5	2	3	445.159	0.150D-22	70	5548.183	10 2 8	9	2	7	1198.210	0.637D-24
70	5473.161	6 3 3	5	3	2	505.730	0.947D-23	70	5552.713	5 3 2	4	1	3	274.803	0.260D-24
70	5477.334	6 4 3	5	4	2	604.547	0.148D-23	70	5552.856	9 3 6	8	3	5	1047.331	0.370D-24
70	5478.190	6 4 2	5	4	1	604.794	0.444D-23	70	5553.954	9 4 5	8	4	4	1126.443	0.244D-24
70	5479.835	4 3 1	4	1	4	223.829	0.167D-24	70	5557.212	9 5 5	8	5	4	1246.380	0.355D-24
70	5480.643	6 4 3	6	2	4	601.238	0.521D-25	70	5558.775	9 5 4	8	5	3	1247.210	0.118D-24
60	5481.177	4 3 2	3	0	3	136.338	0.669D-25	70	5559.012	13 2 12	12	2	11	1767.335	0.523D-25
70	5481.482	10 1 9	10	1	10	1109.801	0.573D-25	70	5559.400	8 7 1	7	7	0	1378.970	0.571D-25
70	5482.191	10 1 10	9	1	9	916.297	0.889D-24	70	5560.608	11 3 9	10	3	8	1440.291	0.213D-24
70	5482.218	10 0 10	9	0	9	916.258	0.267D-23	70	5560.704	4 3 2	3	1	3	141.568	0.103D-24
70	5484.221	8 2 7	7	2	6	706.599	0.190D-23	70	5563.253	11 2 9	10	2	8	1433.030	0.740D-25
70	5486.220	8 1 7	7	1	6	701.695	0.588D-23	70	5564.210	10 4 7	9	4	6	1334.485	0.101D-24
70	5486.660	7 3 5	6	3	4	645.385	0.604D-23	70	5569.410	9 6 4	8	6	3	1399.437	0.136D-24
70	5488.720	6 5 2	5	5	1	733.681	0.436D-24	70	5573.638	10 3 7	9	3	6	1279.800	0.418D-24
70	5488.752	6 5 1	5	5	0	733.685	0.131D-23	70	5577.981	12 2 10	11	2	9	1684.437	0.710D-25
70	5491.447	5 4 2	5	2	3	445.159	0.133D-24	70	5578.983	10 4 6	9	4	5	1355.221	0.270D-24
70	5494.480	7 2 5	6	2	4	601.238	0.277D-23	70	5580.530	6 3 3	5	1	4	398.361	0.580D-24
70	5494.543	4 2 2	3	0	3	136.338	0.128D-23	70	5582.595	10 5 5	9	5	4	1468.616	0.144D-24
70	5495.288	11 1 11	10	1	10	1109.801	0.114D-23	70	5583.369	11 4 8	10	4	7	1574.458	0.106D-24
70	5495.296	11 0 11	10	0	10	1109.785	0.378D-24	70	5591.864	10 6 4	9	6	3	1619.071	0.592D-25
60	5496.056	6 4 3	5	3	2	505.730	0.262D-24	70	5592.789	6 2 4	5	0	5	324.047	0.283D-24
70	5498.761	7 3 4	6	3	3	658.609	0.167D-23	70	5598.644	5 3 3	4	1	4	223.829	0.259D-24
70	5500.289	7 4 4	6	4	3	751.036	0.304D-23	70	5599.927	11 5 7	10	5	6	1709.575	0.511D-25
70	5500.628	9 2 8	8	2	7	881.917	0.273D-23	70	5604.937	4 4 0	3	2	1	210.800	0.151D-24
70	5501.533	9 1 8	8	1	7	879.493	0.925D-24	70	5616.191	7 3 4	6	1	5	541.179	0.855D-25
70	5502.767	7 4 3	6	4	2	752.191	0.101D-23	70	5622.385	5 4 1	4	2	2	314.461	0.723D-25
70	5506.840	8 3 6	7	3	5	812.766	0.106D-23	70	5637.825	6 4 2	5	2	3	445.159	0.214D-24
70	5507.831	12 1 12	11	1	11	1321.464	0.146D-24	70	5637.985	5 4 2	4	2	3	298.621	0.194D-24
70	5507.838	12 0 12	11	0	11	1321.457	0.438D-24	70	5640.794	6 3 4	5	1	5	325.216	0.543D-25
70	5511.404	3 3 0	2	1	1	94.789	0.113D-24	70	5653.720	7 4 3	6	2	4	601.238	0.557D-25
70	5511.907	7 5 3	6	5	2	880.080	0.119D-23	70	5667.711	6 4 3	5	2	4	414.170	0.542D-25
70	5512.066	7 5 2	6	5	1	880.115	0.396D-24	70	5668.818	8 3 5	7	1	6	701.695	0.695D-25
60	5512.956	7 4 4	6	3	3	658.609	0.285D-24	70	5673.381	8 4 4	7	2	5	780.456	0.101D-24
70	5514.656	8 2 6	7	2	5	780.456	0.396D-23	70	5686.699	7 3 5	6	1	6	445.346	0.839D-25
70	5516.019	10 2 9	9	2	8	1075.911	0.393D-24	70	5697.813	5 5 1	4	3	2	379.291	0.642D-25
70	5516.520	10 1 9	9	1	8	1074.763	0.119D-23	70	5700.872	7 4 4	6	2	5	550.453	0.102D-24
70	5517.116	4 4 0	4	2	3	298.621	0.628D-25	70	5716.707	6 5 1	5	3	2	505.730	0.748D-25
60	5517.630	8 4 5	7	3	4	839.555	0.926D-24	70	5746.602	7 5 3	6	3	4	645.385	0.570D-25
70	5519.812	13 0 13	12	0	12	1551.195	0.513D-25								

[a] The meaning of the different columns is:
*N*0, Vibrational assignment of the line with 0 = (000), 6 = (110), 7 = (011);
SIGMA, wavenumber of the line in cm^{-1};
$J'K'_aK'_c$ and JK_aK_c, rotational quantum numbers of the upper and lower levels respectively;
E, lower level energy in cm^{-1};
INTENSITY, computed line intensity $k_\sigma{}^N$ in $cm^{-1}/(molecule\ cm^{-2})$.

intensities for 88 lines of $H_2{}^{18}O$ introduced in the fit is as follows:

$$0 \leqslant \% < 10, \quad 83.0\% \text{ of the lines,}$$
$$10 \leqslant \% < 16, \quad 10.2\% \text{ of the lines,}$$
$$16 \leqslant \% \leqslant 23, \quad 6.8\% \text{ of the lines,}$$

where $\% = 100 \times |k_\sigma{}^P(\text{obs}) - k_\sigma{}^P(\text{calc})|/k_\sigma{}^P(\text{obs})$.

Using the set of constants listed in Table II we have computed the whole spectrum

TABLE VI

Comparison of the Intensities of $H_2{}^{16}O$ and $H_2{}^{18}O$ Lines in the Case of Resonance

			$H_2{}^{16}O$			$H_2{}^{18}O$		
$(v_1'v_2'v_3')[J'K_a'K_c']$		$(v_1v_2v_3)[J\ K_aK_c]$	σ (cm^{-1})	k_σ^N (cm^{-1}/molecule.cm^{-2})	ratio	σ (cm^{-1})	k_σ^N[a] (cm^{-1}/molecule.cm^{-2})	ratio
(110) [330]	←	(000) [221]	5403.900	$0.361\ 10^{-20}$	0.414	5390.340	$0.228\ 10^{-20}$	0.263
(011) [322]	←	(000) [221]	5409.349	$0.873\ 10^{-20}$		5386.061	$0.868\ 10^{-20}$	
(110) [330]	←	(000) [423]	5238.440	$0.185\ 10^{-20}$	0.222	5225.196	$0.289\ 10^{-20}$	0.461
(011) [322]	←	(000) [423]	5243.889	$0.835\ 10^{-20}$		5220.917	$0.627\ 10^{-20}$	
(110) [431]	←	(000) [322]	5427.089	$0.309\ 10^{-20}$	1.507	5415.794	$0.484\ 10^{-21}$	0.119
(011) [423]	←	(000) [322]	5433.433	$0.205\ 10^{-20}$		5407.884	$0.408\ 10^{-20}$	
(110) [431]	←	(000) [524]	5217.182	$0.135\ 10^{-20}$	0.993	5206.382	$0.423\ 10^{-21}$	0.209
(011) [423]	←	(000) [524]	5223.526	$0.136\ 10^{-20}$		5198.472	$0.202\ 10^{-20}$	

[a] Converted to pure $H_2{}^{18}O$

of the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ bands of $H_2{}^{18}O$ for the normal abundance of this isotope in natural water at a temperature of 296 K for lines having an intensity larger than 0.5×10^{-25} cm^{-1}/molecule cm^{-2} and the results are listed in Table V. The total band intensities (i.e., the sum of the individual line strengths) for the natural abundance at 296 K are $S_v(\nu_1 + \nu_2) = 0.53 \times 10^{-22}$ and $S_v(\nu_2 + \nu_3) = 0.15 \times 10^{-20}$ (in cm^{-1}/molecule cm^{-2}).

It is interesting to make a comparison of line intensities for $H_2{}^{16}O$ and $H_2{}^{18}O$ when there is resonance. Table VI shows clearly that, for the pairs of resonating levels {(110)[330], (011)[322]} and {(110)[431], (011)[423]}, the ratio of intensities of the two perturbed lines originating from the same lower level can actually be very different from one isotopic species to another and this is a result of the differences of the mixing coefficients of the resonating levels for the two isotopic varieties.

CONCLUSION

Using a Fourier transform spectrum of water in the 1.9-μm region, we have measured about 90 lines intensities of $H_2{}^{18}O$ in natural abundance. From these data and realistic wavefunctions for the vibration-rotation energy levels of $H_2{}^{18}O$, we have determined the constants involved in the expansion of the transformed transition operators corresponding to the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ bands of this isotopic species. The whole spectrum of these two bands has been computed giving accurate positions and intensities for the vibration-rotation lines of $H_2{}^{18}O$ in the region 4900 to 5800 cm^{-1}.

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