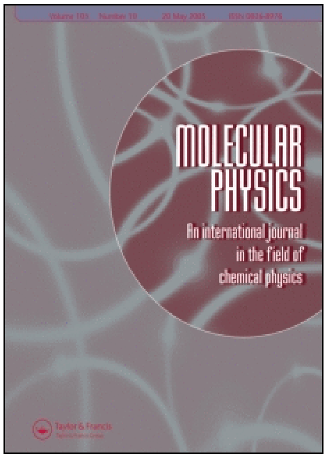

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Line positions and intensities for the $2\nu_2$, ν_1 and ν_3 bands of $H_2{}^{17}O$

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Line positions and intensities for the $2\nu_2$, ν_1 and ν_3 bands of $H_2{}^{17}O$

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The constants involved in the rotational expansion of the transformed transition moment operators of the $2\nu_2$, ν_1 and ν_3 bands of $H_2{}^{17}O$ have been determined through a fit of 280 measured line intensities. The coefficients ${}^1\mu_x$ and ${}^3\mu_z$ of the expansion of the dipole moment with respect to normal coordinates have been deduced to be ${}^1\mu_x = -0{\cdot}021500 \pm 0{\cdot}00030$ D and ${}^3\mu_z = 0{\cdot}09596 \pm 0{\cdot}0012$ D.

Moreover, the knowledge of the transition moment operators has been used to compute the whole spectrum of the $2\nu_2$, ν_1 and ν_3 bands of $H_2{}^{17}O$.

1. INTRODUCTION

In order to improve the knowledge of the water vapour spectrum in the $2{\cdot}7$ μm region we have already performed line position and intensity calculations for the $2\nu_2$, ν_1 and ν_3 bands of $H_2{}^{16}O$ [1] and $H_2{}^{18}O$ [2]. Because $H_2{}^{17}O$ is also present in natural water vapour, it is important to have at hand the line parameters for this less abundant isotope. Indeed the lines of this isotopic species are easily observed in atmospheric absorption spectra. Up to now, results concerning $H_2{}^{17}O$ were rather scanty, the only available calculation being that of [3].

We report here a greatly improved compilation of calculated line positions and intensities of the $2\nu_2$, ν_1 and ν_3 bands of this molecule.

2. INTENSITY CALCULATION

The method we have proposed to compute line intensities, when it is necessary to take into account vibrorotational resonances, has been extensively described [1] and applied to the $H_2{}^{16}O$ molecule [1, 4] and to the $H_2{}^{18}O$ molecule [2, 5].

To calculate the line intensities (the partition function was taken to be $Z(296) = 175{\cdot}4$) we have taken the matrix elements of the transformed dipole moment between the wavefunctions of the upper and lower levels of the transitions. These wavefunctions, deduced from the fit of the observed energy levels, were taken from [6] for the triad of interacting states {(020), (100), (001)} and from [7] for the ground state (000). The constants ${}^v\mu'_j$ involved in the

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expansion of the transformed transition moment operators have been determined through a fit of the experimental line intensities recently measured by Toth *et al.* [8]. The fit of the observed intensities is very satisfactory as can be seen from the following statistical analysis of the relative differences $\delta I/I$ between 280 calculated and measured line intensities (79 for $2\nu_2$, 59 for ν_1 and 142 for ν_3) :

0 per cent $\leqslant \delta I/I <$ 8 per cent	71·4 per cent (of the lines)
8 per cent $\leqslant \delta I/I <$ 15 per cent	20·4 per cent
15 per cent $\leqslant \delta I/I <$ 25 per cent	8·2 per cent.

Table 1. Constants involved in the expansion of the transformed transition moment operators ${}^v\mu'_Z$ for the $2\nu_2$, ν_1 and ν_3 bands of $H_2{}^{17}O$. All the results are in Debye, the quoted errors being twice the standard deviations. Blank entries imply that the the coefficients concerned were insignificant and constrained to zero. $\{A, B\} = AB + BA$; $J_{xy}{}^2 = J_x{}^2 - J_y{}^2$

Δv_3 even ($v = 2, 3$)

j	${}^vA_j$	${}^v\mu'_j$	
		$v = 2$ (020)	$v = 3$ (100)
1	ϕ_x	$0{\cdot}00592_2 \pm 0{\cdot}00013$	$-0{\cdot}01520_3 \pm 0{\cdot}00021$
2	$\{\phi_x, J^2\}$	$(0{\cdot}31_9 \pm 0{\cdot}17) \times 10^{-5}$	
3	$\{\phi_x, J_z{}^2\}$		
4	$\{i\phi_y, J_z\}$	$(-0{\cdot}137_4 \pm 0{\cdot}025) \times 10^{-3}$	$(0{\cdot}1311_1 \pm 0{\cdot}0037) \times 10^{-2}$
5	$\{\phi_z, iJ_y\}$	$(0{\cdot}48_5 \pm 0{\cdot}22) \times 10^{-4}$	$(-0{\cdot}559_8 \pm 0{\cdot}025) \times 10^{-3}$
6	$\{\phi_z, \{J_x, J_z\}\}$	$(-0{\cdot}80_2 \pm 0{\cdot}36) \times 10^{-5}$	
7	$\frac{1}{2}[\{\phi_x, J_{xy}{}^2\} - \{i\phi_y, i\{J_x, J_y\}\}]$	$(-0{\cdot}51_4 \pm 0{\cdot}33) \times 10^{-5}$	
8	$\frac{1}{2}[\{\phi_x, J_{xy}{}^2\} + \{i\phi_y, i\{J_x, J_y\}\}]$		

Δv_3 odd ($v = 4$)

j	${}^vA_j$	${}^v\mu'_j$ $v = 4$ (001)
1	ϕ_z	$0{\cdot}06785_5 \pm 0{\cdot}00085$
2	$\{\phi_z, J^2\}$	$(0{\cdot}201_4 \pm 0{\cdot}074) \times 10^{-4}$
3	$\{\phi_z, J_z{}^2\}$	$(-0{\cdot}85_9 \pm 0{\cdot}24) \times 10^{-4}$
4	$\frac{1}{2}[\{\phi_x, iJ_y\} - \{i\phi_y, J_x\}]$	$(-0{\cdot}1409_5 \pm 0{\cdot}0089) \times 10^{-2}$
5	$\frac{1}{2}[\{\phi_x, \{J_x, J_z\}\} - \{i\phi_y, i\{J_y, J_z\}\}]$	
6	$\frac{1}{2}[\{\phi_x, iJ_y\} + \{i\phi_y, J_x\}]$	$(0{\cdot}449_5 \pm 0{\cdot}035) \times 10^{-3}$
7	$\frac{1}{2}[\{\phi_x, \{J_x, J_z\}\} + \{i\phi_y, i\{J_y, J_z\}\}]$	$(-0{\cdot}104_7 \pm 0{\cdot}061) \times 10^{-4}$
8	$\{\phi_z, J_{xy}{}^2\}$	$(0{\cdot}137_9 \pm 0{\cdot}047) \times 10^{-4}$

The final constants ${}^v\mu'_j$ deduced from the fit are gathered in table 1 together with the corresponding rotational operators ${}^vA_j$ appearing in the expansion of the transformed transition moment operators ${}^v\mu'_Z$ of the three bands $2\nu_2$, ν_1 and ν_3. More precisely we have

$$
{}^v\mu'_Z = \sum_j {}^v\mu'_j \, {}^vA_j \text{ with } v = \left\{ \begin{array}{l} 2 \text{ for } (020) \\ 3 \text{ for } (100) \\ 4 \text{ for } (001). \end{array} \right.
$$

For B-type bands, the first term of this expansion is ${}^{v}\mu'_1\phi_x$ ($v=2$ for $2\nu_2$ and 3 for ν_1) whereas for A-type bands it is ${}^{v}\mu'_1\,\phi_z$ ($v=4$ for ν_3). The constants ${}^{v}\mu'_1$ are the so called vibrational transition moments. They are related to the coefficients involved in the expansion of the dipole moment operator with respect to normal coordinates through the following equations

$$
\begin{aligned}
{}^{2}\mu'_1 &= \langle 000|{}^{\mathrm{vib}}\mu'_x|020\rangle = \frac{1}{\sqrt{2}}\left({}^{22}\mu_x + {}^{2}\mu_x\,\frac{k_{222}}{\omega_2} - \tfrac{1}{2}\,{}^{1}\mu_x\,\frac{k_{122}}{2\omega_2+\omega_1}\right),\\
{}^{3}\mu'_1 &= \langle 000|{}^{\mathrm{vib}}\mu'_x|100\rangle = {}^{1}\mu_x/\sqrt{2},\\
{}^{4}\mu'_1 &= \langle 000|{}^{\mathrm{vib}}\mu'_z|001\rangle = {}^{3}\mu_z/\sqrt{2}.
\end{aligned}
$$

From these relations and the values of the constants ${}^{v}\mu'_1$ quoted in table 1 one derives the following values of the first derivatives of the dipole moment (D $\approx 3{\cdot}335640\times10^{-33}$ C m)

$$
\begin{aligned}
{}^{1}\mu_x &= -0{\cdot}02150_0 \pm 0{\cdot}0030\ \mathrm{D}\\
{}^{3}\mu_z &= 0{\cdot}0959_6\ \ \pm 0{\cdot}0012\ \mathrm{D}.
\end{aligned}
$$

Although slight isotopic variations must exist, these values are in good agreement with the results we have obtained for the first derivatives in the case of $H_2{}^{18}O$ [2] and $H_2{}^{16}O$ [1].

To demonstrate the influence of the isotopic substitution on line intensities in the case of resonance, we have gathered in table 2 the results for R-type transitions involving 3 resonant upper levels. It is clear that in such cases one cannot deduce the intensity for the ^{18}O or ^{17}O species from the corresponding intensity of the main ^{16}O line. This is to be related to the fact that the mixing coefficients in the case of resonance are strongly isotope dependent (see table 2 of [6] where the mixing coefficients of the resonating levels considered here are presented).

Table 2. Example of the evolution of the intensities in an isotopic substitution for the transitions $(v_1v_2v_3)$ $(JK_aK_c)\leftarrow(000)$ [634] of H_2O.

$(v_1v_2v_3)$ $[JK_aK_2]$	$\sigma_{\mathrm{cal}}/\mathrm{cm}^{-1}$	$k_\sigma{}^N/(\mathrm{cm}^{-1}/\mathrm{molecule\ cm}^{-2})$	Isotope
(020) [761]	3929·999	$0{\cdot}726\times10^{-22}$	^{16}O
	3916·705	$0{\cdot}958\times10^{-21}$	^{17}O
	3906·078	$0{\cdot}578\times10^{-22}$	^{18}O
(100) [743]	3923·467	$0{\cdot}381\times10^{-20}$	^{16}O
	3918·748	$0{\cdot}187\times10^{-20}$	^{17}O
	3913·488	$0{\cdot}214\times10^{-20}$	^{18}O
(001) [735]	3904·295	$0{\cdot}212\times10^{-19}$	^{16}O
	3897·214	$0{\cdot}203\times10^{-19}$	^{17}O
	3890·836	$0{\cdot}208\times10^{-19}$	^{18}O

Finally, using the values of the constants ${}^{v}\mu'_j$ presented in table 1, we have computed a complete spectrum of the $2\nu_2$, ν_1 and ν_3 bands for pure $H_2{}^{17}O$ at 296 K. A list containing the most intense lines appears in table 3. The

Table 3. Computed list of the lines of the $2\nu_2$, ν_1 and ν_3 bands of $H_2{}^{17}O$ at 296 K. The meaning of the different columns is as follows :
NO : vibrational assignment of the line, 2 = (020), 3 = (100), 4 = (001), 0 = (000).
SIGMA : wavenumber of the line in cm^{-1}
$J'K'_aK'_c$ JK_aK_c : rotational quantum numbers of the upper and lower levels of the transition
E : lower level energy in cm^{-1}
INTENSITY : computed line intensity in cm^{-1}/molecule cm^{-2}.

NO	SIGMA	J'	KA'	KC'	J	KA	KC	E	INTENSITY	NO	SIGMA	J'	KA'	KC'	J	KA	KC	E	INTENSITY
20	2967.069	4	2	3	5	3	2	507.175	0.300D-21	40	3450.468	4	2	2	5	4	1	607.397	0.302D-21
20	2981.586	4	3	2	5	4	1	607.397	0.350D-21	20	3452.658	4	4	1	3	3	0	283.769	0.652D-21
20	2988.208	7	0	7	8	1	8	742.492	0.365D-21	40	3453.268	10	3	7	11	3	8	1810.670	0.303D-21
20	2998.804	4	4	1	5	5	0	737.623	0.275D-21	30	3459.528	7	1	6	8	2	7	883.653	0.108D-20
20	3004.298	3	2	1	4	3	2	380.806	0.650D-21	30	3459.650	4	2	2	5	3	3	502.180	0.125D-20
20	3006.589	5	1	4	6	2	5	551.610	0.368D-21	30	3463.317	8	0	8	9	1	9	918.140	0.466D-21
20	3006.615	3	3	0	4	4	1	485.209	0.613D-21	30	3463.382	8	1	8	9	0	9	918.103	0.141D-20
20	3009.248	6	1	6	7	0	7	584.941	0.627D-21	30	3466.651	7	2	6	8	1	7	881.097	0.319D-21
20	3019.499	2	1	2	3	2	1	211.437	0.515D-21	40	3467.860	9	5	5	10	5	6	1713.853	0.281D-21
20	3024.723	2	2	1	3	3	0	283.769	0.979D-21	30	3471.967	3	2	2	4	3	1	382.177	0.164D-20
20	3025.440	5	0	5	6	1	6	446.246	0.946D-21	40	3473.445	10	2	8	11	2	9	1687.385	0.501D-21
20	3026.013	2	2	0	3	3	1	283.562	0.332D-21	40	3473.673	11	2	10	12	2	11	1770.837	0.362D-21
20	3028.211	3	1	2	4	2	3	299.440	0.732D-21	40	3475.567	12	0	12	13	0	13	1802.600	0.345D-21
20	3029.345	5	1	5	6	0	6	445.719	0.318D-21	40	3476.825	9	3	6	10	3	7	1536.155	0.338D-21
20	3042.368	4	0	4	5	1	5	325.881	0.420D-21	30	3477.179	3	1	3	4	2	2	315.079	0.656D-21
20	3042.928	2	1	1	3	2	2	205.483	0.310D-21	30	3477.556	6	1	5	7	2	6	708.016	0.529D-21
20	3049.818	4	1	4	5	0	5	324.661	0.127D-20	20	3477.754	5	4	1	4	3	2	380.806	0.386D-21
20	3053.742	1	1	1	2	2	0	135.433	0.309D-21	40	3478.983	9	4	6	10	4	7	1577.690	0.600D-21
20	3058.084	3	0	3	4	1	4	224.305	0.147D-20	30	3479.330	3	2	1	4	3	2	380.806	0.525D-20
20	3060.858	1	1	0	2	2	1	134.146	0.112D-20	40	3481.710	5	1	4	6	3	3	659.987	0.446D-21
20	3071.290	3	1	3	4	0	4	221.622	0.473D-21	30	3484.487	7	0	7	8	1	8	742.492	0.268D-20
20	3072.806	5	0	5	5	1	4	398.880	0.437D-21	30	3484.767	7	1	7	8	0	8	742.398	0.888D-21
20	3073.329	2	0	2	3	1	3	141.904	0.500D-21	30	3491.311	6	2	5	7	1	6	702.886	0.154D-20
20	3075.040	4	1	4	4	2	3	299.440	0.512D-21	40	3492.704	8	5	3	9	5	4	1472.686	0.739D-21
20	3075.364	4	2	3	5	1	4	398.880	0.380D-21	30	3493.466	5	1	4	6	2	5	551.610	0.311D-20
20	3089.548	1	0	1	2	1	2	79.227	0.136D-20	40	3494.504	8	4	4	9	4	5	1357.558	0.147D-20
20	3093.437	4	2	3	4	3	2	380.806	0.407D-21	40	3494.804	9	2	7	10	2	8	1435.366	0.509D-21
20	3094.397	2	1	2	3	0	3	136.539	0.124D-20	40	3495.427	10	1	9	11	1	10	1521.519	0.109D-20
20	3096.789	2	1	2	2	2	1	134.146	0.558D-21	40	3496.030	9	3	7	10	3	8	1443.043	0.131D-20
20	3101.336	3	2	1	3	3	0	283.769	0.376D-21	40	3497.192	11	0	11	12	0	12	1554.336	0.345D-21
20	3108.046	0	0	0	1	1	1	36.932	0.351D-21	40	3497.192	11	1	11	12	1	12	1554.339	0.103D-20
20	3109.278	3	0	3	3	1	2	173.111	0.131D-20	30	3500.251	2	2	1	3	3	0	283.769	0.711D-20
20	3112.103	5	2	3	5	3	2	507.175	0.418D-21	30	3501.760	2	2	0	3	3	1	283.562	0.239D-20
20	3112.405	5	1	4	5	2	3	445.794	0.709D-21	40	3501.982	8	3	5	9	3	6	1281.271	0.297D-20
20	3112.978	2	1	1	2	2	0	135.433	0.274D-21	40	3503.775	8	4	5	9	4	6	1337.488	0.536D-21
20	3116.214	3	1	2	3	2	1	211.437	0.118D-20	30	3505.271	6	0	6	7	1	7	585.160	0.151D-20
20	3116.419	4	1	3	4	2	2	315.079	0.357D-21	30	3505.953	6	1	6	7	0	7	584.941	0.448D-20
20	3120.262	2	0	2	2	1	1	94.971	0.554D-21	40	3506.820	3	1	3	4	3	2	380.806	0.584D-21
20	3126.588	1	0	1	1	1	0	42.187	0.146D-20	30	3508.416	4	1	3	5	2	4	415.129	0.147D-20
20	3171.230	1	1	0	1	0	1	23.774	0.150D-20	40	3510.521	7	6	2	8	6	3	1405.149	0.526D-21
20	3178.406	2	1	1	2	0	2	70.005	0.544D-21	40	3512.649	4	1	3	5	3	2	507.175	0.193D-20
20	3189.174	1	1	1	0	0	0	0.0	0.357D-21	40	3516.018	8	2	6	9	2	7	1199.964	0.426D-20
20	3191.112	3	1	2	3	0	3	136.539	0.121D-20	40	3516.934	9	1	8	10	1	9	1290.227	0.984D-21
20	3203.161	3	0	3	2	1	2	79.227	0.112D-20	40	3517.073	9	2	8	10	2	9	1290.799	0.291D-20
20	3207.162	2	1	2	1	0	1	23.774	0.138D-20	40	3518.069	8	3	6	9	3	7	1213.561	0.108D-20
20	3211.994	3	2	1	3	1	2	173.111	0.105D-20	30	3518.156	5	2	4	6	1	5	541.997	0.667D-21
20	3213.170	4	2	2	4	1	3	275.132	0.305D-21	40	3518.600	10	1	10	11	1	11	1324.131	0.942D-21
20	3220.398	5	2	3	5	1	4	398.880	0.577D-21	40	3518.605	10	0	10	11	0	11	1324.124	0.283D-20
20	3222.907	3	1	3	2	0	2	70.005	0.511D-21	30	3519.280	2	1	2	3	2	1	211.437	0.391D-20
20	3226.344	4	0	4	3	1	3	141.904	0.440D-21	40	3519.940	7	5	2	8	5	3	1251.292	0.543D-21

20	3229.264	2	2	1	2	1	2	79.227	0.594D-21	40	3520.463	7	5	3	8	5	4	1250.499	0.163D-20
20	3233.538	5	1	4	5	0	5	324.661	0.385D-21	40	3520.802	4	0	4	5	2	3	445.794	0.172D-20
20	3237.941	4	1	4	3	0	3	136.539	0.151D-20	30	3522.888	8	5	4	9	4	5	1357.558	0.300D-21
20	3247.380	5	0	5	4	1	4	224.305	0.121D-20	30	3523.800	3	1	2	4	2	3	299.440	0.564D-20
20	3249.938	4	2	3	4	1	4	224.305	0.529D-21	30	3524.094	7	0	7	7	1	6	702.886	0.550D-21
20	3253.442	5	1	5	4	0	4	221.622	0.429D-21	40	3524.199	7	4	3	8	4	4	1128.938	0.124D-20
20	3258.759	5	1	4	4	2	3	299.440	0.310D-21	30	3525.470	5	0	5	6	1	6	446.246	0.680D-20
20	3266.305	2	2	1	1	1	0	42.187	0.117D-20	30	3527.086	5	1	5	6	0	6	445.719	0.221D-20
20	3266.581	6	0	6	5	1	5	325.881	0.312D-21	40	3529.050	7	3	4	8	3	5	1048.656	0.241D-20
20	3268.060	5	3	2	5	2	3	445.794	0.326D-21	40	3529.263	7	4	4	8	4	5	1119.489	0.378D-20
20	3269.528	6	1	6	5	0	5	324.661	0.961D-21	30	3533.407	6	3	4	6	4	3	753.705	0.550D-21
20	3272.643	2	2	0	1	1	1	36.932	0.346D-21	40	3536.674	6	6	0	7	6	1	1209.818	0.695D-21
20	3280.388	3	3	0	3	2	1	211.437	0.367D-21	40	3536.826	3	1	2	4	3	1	382.177	0.579D-21
20	3284.455	7	0	7	6	1	6	446.246	0.629D-21	40	3537.782	7	2	5	8	2	6	981.494	0.358D-20
20	3284.993	3	2	2	2	1	1	94.971	0.326D-21	40	3538.131	8	1	7	9	1	8	1076.802	0.729D-20
20	3289.543	4	3	2	4	2	3	299.440	0.405D-21	40	3538.484	8	2	7	9	2	8	1078.019	0.236D-20
20	3301.133	4	2	3	3	1	2	173.111	0.776D-21	30	3539.283	6	1	6	6	2	5	551.610	0.104D-20
20	3302.022	8	1	8	7	0	7	584.941	0.377D-21	40	3539.802	9	0	9	10	0	10	1112.025	0.234D-20
20	3305.877	3	2	1	2	1	2	79.227	0.657D-21	40	3539.809	9	1	9	10	1	10	1112.042	0.701D-20
30	3308.261	6	5	2	7	6	1	1209.818	0.298D-21	30	3539.997	4	3	2	4	4	1	485.209	0.718D-21
20	3329.116	6	2	5	5	1	4	398.880	0.402D-21	40	3540.504	7	3	5	8	3	6	1003.783	0.688D-20
30	3331.918	6	4	3	7	5	2	1055.256	0.655D-21	30	3540.590	5	3	2	5	4	1	607.397	0.966D-21
30	3334.638	5	5	0	6	6	1	1038.765	0.652D-21	30	3540.866	2	1	1	3	2	2	205.483	0.221D-20
40	3351.566	5	3	3	6	5	2	884.078	0.581D-21	30	3544.803	4	0	4	5	1	5	325.881	0.298D-20
30	3353.331	6	2	5	7	3	4	840.866	0.447D-21	30	3546.308	6	4	3	7	3	4	840.866	0.342D-20
40	3356.015	5	3	2	6	5	1	884.114	0.289D-21	40	3546.634	6	5	1	7	5	2	1055.256	0.287D-20
20	3356.263	3	3	1	2	2	0	135.433	0.356D-21	40	3546.785	6	5	2	7	5	3	1055.056	0.955D-21
20	3357.679	3	3	0	2	2	1	134.146	0.107D-20	30	3547.124	6	2	5	6	3	4	647.073	0.981D-21
30	3358.816	6	3	4	7	4	3	928.297	0.777D-21	30	3547.606	4	2	3	5	1	4	398.880	0.197D-20
30	3360.043	7	3	4	8	4	5	1119.489	0.282D-21	30	3548.434	6	0	6	6	1	5	541.997	0.370D-21
30	3364.695	5	4	1	6	5	2	884.078	0.723D-21	30	3548.478	4	1	4	5	0	5	324.661	0.844D-20
20	3377.547	4	3	2	3	2	1	211.437	0.699D-21	40	3552.917	6	4	2	7	4	3	928.297	0.753D-20
40	3380.164	4	3	1	5	5	0	737.623	0.688D-21	20	3553.088	5	5	0	4	4	1	485.209	0.275D-21
30	3389.785	5	3	3	6	4	2	754.813	0.562D-21	30	3553.742	1	1	1	2	2	0	135.433	0.204D-20
30	3389.975	4	4	0	5	5	1	737.621	0.540D-21	40	3555.202	6	4	3	7	4	4	924.642	0.251D-20
30	3390.100	4	4	1	5	5	0	737.623	0.153D-20	30	3557.676	5	1	5	5	2	4	415.129	0.600D-21
30	3394.282	5	3	2	6	4	3	753.705	0.192D-20	40	3557.813	2	1	1	3	3	0	283.769	0.923D-21
30	3400.167	5	2	4	6	3	3	659.987	0.413D-21	30	3557.974	5	2	4	5	3	3	502.180	0.528D-21
40	3413.981	6	2	4	7	4	3	928.297	0.287D-21	40	3558.403	6	3	3	7	3	4	840.866	0.127D-19
20	3414.414	5	3	2	4	2	3	299.440	0.397D-21	40	3558.936	7	1	6	8	1	7	881.097	0.545D-20
30	3417.374	7	2	5	8	3	6	1003.783	0.504D-21	40	3559.690	7	2	6	8	2	7	883.653	0.153D-19
30	3417.809	4	3	2	5	4	1	607.397	0.307D-20	20	3559.995	7	6	1	8	3	6	1003.783	0.507D-21
30	3419.048	4	3	1	5	4	2	607.159	0.108D-20	30	3560.248	1	1	0	2	2	1	134.146	0.721D-20
30	3419.854	10	1	10	11	0	11	1324.124	0.286D-21	40	3560.774	8	0	8	9	0	9	918.103	0.158D-19
40	3421.557	5	1	5	6	3	4	647.073	0.508D-21	40	3560.787	8	1	8	9	1	9	918.140	0.525D-20
30	3427.344	4	1	4	5	2	3	445.794	0.840D-21	40	3560.901	6	2	4	7	2	5	781.378	0.240D-19
30	3430.219	6	2	4	7	3	5	814.611	0.332D-21	40	3561.455	5	1	5	5	3	2	507.175	0.498D-21
30	3439.312	4	2	3	5	3	2	507.175	0.277D-20	30	3561.804	7	1	6	7	2	5	781.378	0.671D-21
40	3441.356	6	1	5	7	3	4	840.866	0.598D-21	30	3562.037	7	4	3	8	3	6	1003.783	0.970D-21
30	3441.700	9	0	9	10	1	10	1112.042	0.670D-21	30	3562.940	3	0	3	4	1	4	224.305	0.102D-19
30	3443.326	8	2	7	9	1	8	1076.802	0.501D-21	40	3563.918	6	3	4	7	3	5	814.611	0.435D-20
30	3444.195	5	2	3	6	3	4	647.073	0.173D-20	30	3565.680	4	2	3	4	3	2	380.806	0.203D-20
30	3444.383	3	3	1	4	4	0	485.237	0.160D-20	30	3567.587	7	5	2	8	4	5	1119.489	0.355D-21
30	3444.540	3	3	0	4	4	1	485.209	0.485D-20	40	3567.916	3	0	3	4	2	2	315.079	0.125D-20

Table 3 (*continued*)

NO	SIGMA	J'KA'KC'			J	KA	KC	E	INTENSITY	NO	SIGMA	J'KA'KC'			J	KA	KC	E	INTENSITY
30	3570.583	3	2	2	3	3	1	283.562	0.585D-21	40	3677.512	3	0	3	3	2	2	205.483	0.356D-20
30	3570.636	3	1	3	4	0	4	221.622	0.297D-20	40	3680.976	2	0	2	3	0	3	136.539	0.202D-18
30	3572.836	5	0	5	5	1	4	398.880	0.209D-20	40	3682.973	8	3	6	8	3	5	1048.656	0.329D-21
40	3572.915	5	5	0	6	5	1	884.114	0.114D-20	40	3683.369	2	0	2	2	2	1	134.146	0.542D-20
40	3572.947	5	5	1	6	5	2	884.078	0.341D-20	40	3683.815	2	1	2	3	1	3	141.904	0.593D-19
30	3573.699	4	1	4	4	2	3	299.440	0.270D-20	30	3685.021	2	0	2	1	1	1	36.932	0.837D-21
40	3575.049	9	1	9	9	1	8	1076.802	0.450D-21	40	3686.373	6	2	5	6	2	4	601.961	0.157D-20
30	3576.368	3	2	1	3	3	0	283.769	0.185D-20	30	3686.698	4	2	2	4	1	3	275.132	0.283D-21
30	3579.013	3	2	2	4	1	3	275.132	0.471D-21	30	3686.701	3	1	2	3	0	3	136.539	0.522D-20
40	3579.336	6	1	5	7	1	6	702.886	0.333D-19	30	3687.026	3	2	1	3	1	2	173.111	0.370D-20
30	3579.652	4	2	2	4	3	1	382.177	0.859D-21	30	3689.093	3	1	2	2	2	1	134.146	0.456D-21
30	3579.957	6	4	2	7	3	5	814.611	0.116D-20	30	3689.175	1	1	1	0	0	0	0.0	0.149D-20
30	3580.049	2	0	2	3	1	3	141.904	0.330D-20	30	3690.351	2	2	0	2	1	1	94.971	0.948D-21
40	3580.142	5	3	2	6	3	3	659.987	0.561D-20	30	3692.388	5	2	3	5	1	4	398.880	0.376D-20
30	3580.292	7	2	5	7	3	4	840.866	0.639D-21	40	3692.411	8	7	1	8	7	2	1582.197	0.535D-21
40	3580.318	6	2	5	7	2	6	708.016	0.882D-20	40	3694.150	4	1	4	4	1	3	275.132	0.728D-20
40	3580.527	5	4	1	6	4	2	754.813	0.401D-20	40	3694.234	1	1	0	2	1	1	94.971	0.420D-19
40	3581.334	5	4	2	6	4	3	753.705	0.120D-19	40	3694.532	7	7	1	7	7	0	1386.419	0.156D-20
40	3581.512	7	0	7	8	0	8	742.398	0.107D-19	40	3694.532	7	7	0	7	7	1	1386.419	0.520D-21
40	3581.550	7	1	7	8	1	8	742.492	0.319D-19	30	3698.154	7	3	4	7	2	5	781.378	0.939D-21
30	3583.611	6	1	5	6	2	4	601.961	0.443D-21	40	3699.115	9	4	6	9	4	5	1357.558	0.387D-21
30	3584.093	5	2	3	5	3	2	507.175	0.169D-20	30	3700.203	6	3	3	6	2	4	601.961	0.118D-20
30	3584.843	6	2	4	6	3	3	659.987	0.403D-21	40	3701.340	9	6	4	9	6	3	1624.843	0.296D-21
40	3585.713	5	2	3	6	2	4	601.961	0.154D-19	40	3701.855	1	0	1	2	0	2	70.005	0.614D-19
30	3586.775	3	1	3	3	2	2	205.483	0.111D-20	30	3701.923	4	1	3	4	0	4	221.622	0.989D-21
40	3588.570	5	3	3	6	3	4	647.073	0.229D-19	30	3702.193	5	3	2	5	2	3	445.794	0.671D-21
40	3588.573	6	2	4	6	4	3	753.705	0.481D-21	30	3702.832	6	2	4	6	1	5	541.997	0.500D-21
30	3589.783	6	5	2	7	4	3	928.297	0.474D-21	40	3703.421	7	3	5	7	3	4	840.866	0.290D-20
30	3589.839	5	4	2	6	3	3	659.987	0.391D-20	40	3703.741	8	6	3	8	6	2	1405.182	0.324D-21
30	3594.149	6	3	3	7	2	6	708.016	0.150D-20	40	3703.819	8	6	2	8	6	3	1405.149	0.971D-21
30	3594.178	2	1	2	3	0	3	136.539	0.718D-20	40	3704.675	1	1	1	2	1	2	79.227	0.132D-18
40	3595.224	8	0	8	8	2	7	883.653	0.109D-20	30	3704.792	2	2	1	2	1	2	79.227	0.191D-20
30	3595.552	4	0	4	4	1	3	275.132	0.124D-20	40	3705.852	7	6	2	7	6	1	1209.818	0.286D-20
30	3595.878	7	3	4	8	2	7	883.653	0.459D-21	40	3705.865	7	6	1	7	6	2	1209.813	0.953D-21
30	3596.377	5	3	2	6	2	5	551.610	0.900D-20	30	3706.943	2	1	2	1	0	1	23.774	0.516D-20
40	3596.493	8	2	6	8	4	5	1119.489	0.324D-21	40	3707.727	6	6	1	6	6	0	1038.765	0.253D-20
30	3596.571	2	1	2	2	2	1	134.146	0.287D-20	40	3707.727	6	6	0	6	6	1	1038.765	0.759D-20
30	3597.297	1	0	1	2	1	2	79.227	0.829D-20	30	3708.018	3	0	3	2	1	2	79.227	0.381D-20
40	3597.830	8	1	8	8	1	7	881.097	0.364D-21	40	3709.027	9	5	5	9	5	4	1472.686	0.415D-21
30	3599.281	5	1	4	5	2	3	445.794	0.315D-20	40	3711.473	5	2	4	5	2	3	445.794	0.186D-19
40	3599.700	5	1	4	6	1	5	541.997	0.204D-19	30	3712.241	3	2	2	3	1	3	141.904	0.718D-21
30	3601.700	5	4	1	6	3	4	647.073	0.599D-20	40	3712.325	8	4	5	8	4	4	1128.938	0.478D-21
40	3601.983	6	0	6	7	0	7	584.941	0.585D-19	40	3713.032	8	5	4	8	5	3	1251.292	0.472D-21
40	3602.092	6	1	6	7	1	7	585.160	0.194D-19	40	3714.515	3	1	3	3	1	2	173.111	0.357D-19
40	3603.857	3	1	3	3	3	0	283.769	0.329D-21	40	3714.890	8	5	3	8	5	4	1250.499	0.141D-20
40	3605.657	5	2	4	6	2	5	551.610	0.446D-19	40	3715.706	7	5	3	7	5	2	1055.256	0.428D-20
40	3606.078	2	0	2	3	2	1	211.437	0.513D-20	40	3716.177	7	5	2	7	5	3	1055.056	0.142D-20
40	3607.207	4	4	0	5	4	1	607.397	0.130D-19	40	3717.727	6	5	2	6	5	1	884.114	0.385D-20
40	3607.410	4	4	1	5	4	2	607.159	0.432D-20	40	3717.812	6	5	1	6	5	2	884.078	0.116D-19
40	3607.908	9	2	8	9	2	7	1199.964	0.386D-21	30	3718.272	7	2	5	7	1	6	702.886	0.562D-21

30	3608.466	4	1	3	4	2	2	315.079	0.166D-20	40	3718.542	6	3	4	6	3	3	659.987	0.277D-20
40	3610.612	4	3	1	5	3	2	507.175	0.336D-19	40	3719.401	5	5	1	5	5	0	737.623	0.282D-19
30	3610.909	2	2	1	3	1	2	173.111	0.637D-21	40	3719.408	5	5	0	5	5	1	737.621	0.941D-20
30	3610.917	2	1	1	2	2	0	135.433	0.135D-20	30	3720.414	5	1	4	5	0	5	324.661	0.149D-20
30	3611.078	4	3	1	5	2	4	415.129	0.545D-21	40	3720.455	7	4	4	7	4	3	928.297	0.468D-20
40	3611.150	8	1	7	8	3	6	1003.783	0.891D-21	30	3722.181	4	2	3	4	1	4	224.305	0.168D-20
30	3611.803	3	1	2	3	2	1	211.437	0.565D-20	30	3722.253	3	1	3	2	0	2	70.005	0.166D-20
40	3612.070	4	2	2	5	2	3	445.794	0.746D-19	20	3722.912	7	6	1	7	3	4	840.866	0.474D-21
30	3614.135	3	0	3	3	1	2	173.111	0.607D-20	40	3724.544	0	0	0	1	0	1	23.774	0.113D-18
40	3614.154	4	3	2	5	3	3	502.180	0.116D-19	30	3724.955	7	4	3	7	3	4	840.866	0.919D-21
40	3615.894	7	0	7	7	2	6	708.016	0.792D-21	40	3725.032	6	4	3	6	4	2	754.813	0.448D-20
30	3616.211	0	0	0	1	1	1	36.932	0.195D-20	30	3725.766	4	3	2	4	2	3	299.440	0.560D-21
30	3619.170	1	1	1	2	0	2	70.005	0.123D-20	40	3726.566	4	2	3	4	2	2	315.079	0.147D-19
30	3619.698	5	5	0	6	4	3	753.705	0.340D-21	40	3727.509	6	4	2	6	4	3	753.705	0.133D-19
30	3620.548	4	4	1	5	3	2	507.175	0.619D-20	40	3727.642	5	4	2	5	4	1	607.397	0.341D-19
40	3620.944	4	1	3	5	1	4	398.880	0.100D-18	40	3728.180	5	4	1	5	4	2	607.159	0.114D-19
40	3621.157	7	1	7	7	1	6	702.886	0.242D-20	40	3728.468	5	3	3	5	3	2	507.175	0.235D-19
40	3622.147	5	0	5	6	0	6	445.719	0.320D-19	40	3728.495	7	4	3	7	4	4	924.642	0.150D-20
40	3622.384	5	1	5	6	1	6	446.246	0.939D-19	30	3728.780	4	0	4	3	1	3	141.904	0.122D-20
30	3625.416	4	4	0	5	3	3	502.180	0.165D-20	40	3729.332	4	4	1	4	4	0	485.237	0.261D-19
40	3625.421	7	1	6	7	3	5	814.611	0.612D-21	40	3729.395	4	4	0	4	4	1	485.209	0.783D-19
40	3626.517	4	2	3	5	2	4	415.129	0.260D-19	40	3730.748	2	1	2	2	1	1	94.971	0.226D-19
30	3626.982	2	0	2	2	1	1	94.971	0.267D-20	40	3732.573	8	4	4	8	4	5	1119.489	0.126D-20
30	3630.309	3	3	0	4	2	3	299.440	0.403D-21	40	3734.157	4	3	2	4	3	1	382.177	0.209D-19
30	3634.338	1	0	1	1	1	0	42.187	0.730D-20	30	3734.273	5	2	4	5	1	5	325.881	0.350D-21
40	3635.008	8	2	7	8	2	6	981.494	0.340D-21	30	3734.582	6	4	2	6	3	3	659.987	0.122D-20
40	3635.149	6	1	5	6	3	4	647.073	0.296D-20	30	3735.502	6	3	4	6	2	5	551.610	0.489D-21
40	3635.313	6	0	6	6	2	5	551.610	0.465D-20	40	3736.055	4	1	3	3	3	0	283.769	0.335D-21
40	3635.441	3	1	2	3	3	1	283.562	0.353D-21	30	3736.600	4	1	4	3	0	3	136.539	0.407D-20
30	3635.949	4	2	2	5	1	5	325.881	0.243D-20	40	3736.882	3	2	2	3	2	1	211.437	0.969D-19
40	3636.428	1	0	1	2	2	0	135.433	0.103D-20	40	3736.980	4	3	1	4	3	2	380.806	0.599D-19
40	3639.017	4	1	3	4	3	2	380.806	0.256D-20	40	3737.185	3	3	1	3	3	0	283.769	0.156D-18
40	3639.018	3	3	0	4	3	1	382.177	0.126D-19	40	3737.633	3	3	0	3	3	1	283.562	0.519D-19
40	3639.517	5	1	4	5	3	3	502.180	0.114D-20	40	3737.949	5	3	2	5	3	3	502.180	0.544D-20
40	3639.578	3	2	1	4	2	2	315.079	0.317D-19	30	3740.101	6	4	3	6	3	4	647.073	0.155D-20
40	3640.147	3	3	1	4	3	2	380.806	0.377D-19	40	3741.129	6	0	6	5	2	3	445.794	0.293D-21
40	3641.935	4	0	4	5	0	5	324.661	0.140D-18	30	3741.598	5	4	1	5	3	2	507.175	0.852D-20
40	3643.402	4	1	4	5	1	5	325.881	0.433D-19	40	3741.716	1	1	1	1	1	0	42.187	0.152D-18
40	3643.872	3	1	2	4	1	3	275.132	0.467D-19	30	3741.833	2	2	1	1	1	0	42.187	0.411D-20
30	3645.022	5	2	3	6	1	6	446.246	0.127D-20	40	3742.007	2	2	1	2	2	0	135.433	0.686D-19
40	3645.255	6	1	6	6	1	5	541.997	0.162D-20	40	3742.300	2	2	0	3	0	3	136.539	0.586D-21
40	3648.879	3	2	2	4	2	3	299.440	0.966D-19	40	3744.693	2	2	0	2	2	1	134.146	0.205D-18
40	3652.738	5	0	5	5	2	4	415.129	0.264D-20	30	3745.418	4	4	0	4	3	1	382.177	0.370D-20
40	3657.802	9	3	7	9	3	6	1281.271	0.316D-21	30	3745.636	5	1	4	4	2	3	299.440	0.613D-21
40	3661.373	3	0	3	4	0	4	221.622	0.602D-19	30	3746.916	4	4	1	4	3	2	380.806	0.136D-19
40	3661.966	7	2	6	7	2	5	781.378	0.247D-20	30	3747.411	5	0	5	4	1	4	224.305	0.266D-20
40	3663.321	3	1	3	4	1	4	224.305	0.172D-18	40	3747.563	3	0	3	2	2	0	135.433	0.478D-21
40	3667.156	4	0	4	4	2	3	299.440	0.110D-19	30	3747.646	5	4	2	5	3	3	502.180	0.505D-20
40	3667.402	2	2	0	3	2	1	211.437	0.820D-19	30	3747.951	6	2	5	6	1	6	446.246	0.557D-21
40	3668.471	2	1	1	3	1	2	173.111	0.159D-18	30	3748.390	2	2	0	1	1	1	36.932	0.126D-20
40	3669.750	5	1	5	5	1	4	398.880	0.874D-20	40	3749.174	3	2	1	3	2	2	205.483	0.319D-19
30	3670.620	1	1	0	1	0	1	23.774	0.675D-20	30	3751.183	5	1	5	4	0	4	221.622	0.930D-21
40	3671.957	2	2	1	3	2	2	205.483	0.274D-19	40	3752.196	6	3	3	6	3	4	647.073	0.103D-19
30	3676.344	2	1	1	2	0	2	70.005	0.241D-20	40	3752.273	1	1	0	1	1	1	36.932	0.506D-19

Table 3 (*continued*)

NO	SIGMA	J'KA'KC'			J	KA	KC	E	INTENSITY	NO	SIGMA	J'KA'KC'			J	KA	KC	E	INTENSITY
40	3752.788	5	0	5	4	2	2	315.079	0.281D-21	40	3877.797	7	1	7	6	1	6	446.246	0.790D-19
40	3755.159	4	0	4	3	2	1	211.437	0.166D-20	40	3878.190	7	0	7	6	0	6	445.719	0.264D-19
30	3758.241	7	1	6	7	0	7	584.941	0.291D-21	30	3879.999	6	4	3	5	3	2	507.175	0.111D-19
40	3758.425	4	2	2	4	2	3	299.440	0.424D-19	40	3883.342	6	1	5	5	1	4	398.880	0.784D-19
30	3758.779	7	5	2	7	4	3	928.297	0.637D-21	40	3884.652	3	2	1	2	0	2	70.005	0.267D-20
30	3759.174	3	2	2	2	1	1	94.971	0.108D-20	40	3886.885	7	5	3	6	5	2	884.078	0.388D-20
30	3760.957	8	5	4	8	4	5	1119.489	0.399D-21	30	3887.036	6	3	3	5	2	4	415.129	0.232D-20
40	3762.354	2	1	1	2	1	2	79.227	0.677D-19	40	3887.118	7	5	2	6	5	1	884.114	0.129D-20
40	3763.096	7	3	4	7	3	5	814.611	0.136D-20	40	3889.769	9	2	8	9	0	9	918.103	0.460D-21
30	3763.276	6	5	1	6	4	2	754.813	0.362D-21	40	3891.733	7	2	6	6	2	5	551.610	0.415D-19
30	3764.374	6	5	2	6	4	3	753.705	0.113D-20	40	3892.094	6	3	3	5	3	2	507.175	0.254D-19
30	3764.550	6	0	6	5	1	5	325.881	0.523D-21	30	3892.389	6	4	2	5	3	3	502.180	0.174D-20
30	3766.006	5	5	0	5	4	1	607.397	0.123D-20	40	3893.767	8	1	8	7	1	7	585.160	0.151D-19
30	3766.232	6	1	6	5	0	5	324.661	0.161D-20	40	3893.936	8	0	8	7	0	7	584.941	0.453D-19
30	3766.243	5	5	1	5	4	2	607.159	0.412D-21	40	3895.046	7	4	4	6	4	3	753.705	0.103D-19
40	3771.860	1	0	1	0	0	0	0.0	0.395D-19	40	3896.484	6	2	4	5	2	3	445.794	0.593D-19
40	3772.545	5	2	3	5	2	4	415.129	0.598D-20	30	3896.924	7	4	4	6	3	3	659.987	0.635D-21
30	3773.376	4	2	3	3	1	2	173.111	0.221D-20	40	3897.214	7	3	5	6	3	4	647.073	0.203D-19
40	3775.047	6	1	5	5	3	2	507.175	0.785D-21	40	3898.035	7	1	6	6	1	5	541.997	0.149D-19
40	3777.099	3	1	2	3	1	3	141.904	0.117D-19	40	3898.324	7	4	3	6	4	2	754.813	0.337D-20
40	3779.470	8	3	5	8	3	6	1003.783	0.130D-20	40	3899.150	8	6	2	7	6	1	1209.818	0.728D-21
30	3780.734	7	0	7	6	1	6	446.246	0.769D-21	30	3908.376	8	4	5	7	3	4	840.866	0.302D-21
30	3780.909	3	2	1	2	1	2	79.227	0.337D-20	40	3908.486	8	2	7	7	2	6	708.016	0.742D-20
30	3785.022	5	2	4	4	1	3	275.132	0.434D-21	40	3909.269	8	5	4	7	5	3	1055.056	0.765D-21
40	3788.787	2	1	2	1	1	1	36.932	0.479D-19	40	3909.359	9	1	9	8	1	8	742.492	0.233D-19
40	3790.668	6	2	4	6	2	5	551.610	0.732D-20	40	3909.430	9	0	9	8	0	8	742.398	0.777D-20
40	3793.741	2	0	2	1	0	1	23.774	0.200D-18	40	3910.134	8	5	3	7	5	2	1055.256	0.229D-20
30	3794.188	3	3	1	2	2	0	135.433	0.147D-20	30	3910.683	6	5	2	5	4	1	607.397	0.494D-21
30	3795.317	6	2	5	5	1	4	398.880	0.661D-21	40	3912.047	8	1	7	7	1	6	702.886	0.230D-19
40	3795.519	4	1	3	4	1	4	224.305	0.188D-19	40	3916.621	8	4	5	7	4	4	924.642	0.182D-20
30	3795.603	3	3	0	2	2	1	134.146	0.588D-20	20	3916.705	7	6	1	6	3	4	647.073	0.958D-21
30	3796.544	8	1	8	7	0	7	584.941	0.315D-21	40	3917.018	8	3	6	7	3	5	814.611	0.369D-20
40	3799.395	2	1	1	1	1	0	42.187	0.137D-18	40	3917.315	7	2	5	6	2	4	601.961	0.107D-19
40	3807.435	2	2	1	2	0	2	70.005	0.158D-20	40	3917.720	7	3	4	6	3	3	659.987	0.658D-20
40	3808.399	3	1	3	2	1	2	79.227	0.201D-18	30	3918.748	7	4	3	6	3	4	647.073	0.187D-20
40	3811.260	7	2	5	7	2	6	708.016	0.970D-21	40	3921.034	9	6	4	8	6	3	1405.149	0.386D-21
40	3811.780	3	2	2	3	0	3	136.539	0.966D-20	40	3921.326	4	2	2	3	0	3	136.539	0.696D-20
40	3812.990	3	0	3	2	0	2	70.005	0.760D-19	40	3923.765	8	4	4	7	4	3	928.297	0.501D-20
30	3813.770	4	3	2	3	2	1	211.437	0.320D-20	40	3924.219	9	2	8	8	2	7	883.653	0.106D-19
40	3814.173	3	2	2	2	2	1	134.146	0.906D-19	40	3924.591	10	1	10	9	1	9	918.140	0.361D-20
40	3815.816	5	1	4	5	1	5	325.881	0.336D-20	40	3924.626	10	0	10	9	0	9	918.103	0.108D-19
40	3819.224	3	2	1	2	2	0	135.433	0.303D-19	40	3926.065	9	1	8	8	1	7	881.097	0.358D-20
30	3819.926	4	2	2	3	1	3	141.904	0.601D-20	40	3926.224	3	3	0	2	1	1	94.971	0.480D-21
40	3820.023	4	2	3	4	0	4	221.622	0.339D-20	30	3927.921	7	3	4	6	2	5	551.610	0.724D-21
30	3820.724	4	3	1	3	2	2	205.483	0.305D-20	40	3931.214	9	5	5	8	5	4	1250.499	0.108D-20
30	3823.326	5	3	2	5	0	5	324.661	0.139D-20	30	3933.370	7	5	2	6	4	3	753.705	0.617D-21
40	3824.032	3	1	2	2	1	1	94.971	0.603D-19	40	3933.647	9	5	4	8	5	3	1251.292	0.357D-21

40	3827.378	4	1	4	3	1	3	141.904	0.623D-19
30	3829.519	5	3	3	4	2	2	315.079	0.545D-21
40	3830.057	4	0	4	3	0	3	136.539	0.213D-18
40	3832.329	8	2	6	8	2	7	883.653	0.112D-20
40	3832.606	5	2	4	5	0	5	324.661	0.638D-20
40	3832.772	4	3	2	3	3	1	283.562	0.146D-19
40	3834.018	4	3	1	3	3	0	283.769	0.428D-19
40	3835.977	6	1	5	6	1	6	446.246	0.523D-20
40	3836.162	4	2	3	3	2	2	205.483	0.360D-19
40	3836.531	6	3	4	6	1	5	541.997	0.668D-21
40	3836.763	5	3	3	5	1	4	398.880	0.224D-20
40	3841.202	4	3	2	4	1	3	275.132	0.592D-21
30	3841.318	6	3	4	5	2	3	445.794	0.661D-21
40	3841.401	7	3	5	7	1	6	702.886	0.139D-20
40	3842.615	6	2	5	6	0	6	445.719	0.135D-20
30	3843.954	4	4	1	3	3	0	283.769	0.289D-20
30	3844.033	4	4	0	3	3	1	283.562	0.658D-21
40	3844.324	5	1	5	4	1	4	224.305	0.170D-18
40	3846.245	5	0	5	4	0	4	221.622	0.578D-19
40	3846.428	4	2	2	3	2	1	211.437	0.110D-18
40	3846.713	4	1	3	3	1	2	173.111	0.166D-18
40	3847.843	3	3	1	3	1	2	173.111	0.811D-21
30	3848.548	5	3	2	4	2	3	299.440	0.253D-19
40	3849.830	5	4	2	4	4	1	485.209	0.163D-19
30	3849.893	5	4	1	5	1	4	398.880	0.538D-21
40	3850.102	5	4	1	4	4	0	485.237	0.543D-20
40	3854.837	5	3	3	4	3	2	380.806	0.442D-19
40	3854.872	7	1	6	7	1	7	585.160	0.846D-21
40	3855.065	2	2	0	1	0	1	23.774	0.405D-20
40	3857.827	5	2	4	4	2	3	299.440	0.748D-19
40	3857.952	5	3	2	4	3	1	382.177	0.116D-19
40	3858.403	7	2	6	7	0	7	584.941	0.236D-20
40	3861.371	6	1	6	5	1	5	325.881	0.411D-19
40	3862.262	6	0	6	5	0	5	324.661	0.124D-18
40	3862.271	9	3	7	9	1	8	1076.802	0.337D-21
40	3864.220	6	5	2	5	5	1	737.621	0.148D-20
40	3864.267	6	5	1	5	5	0	737.623	0.443D-20
40	3866.565	5	1	4	4	1	3	275.132	0.410D-19
30	3866.963	5	2	3	4	1	4	224.305	0.102D-20
40	3867.374	7	4	4	7	2	5	781.378	0.302D-21
30	3867.648	5	4	2	4	3	1	382.177	0.493D-20
30	3867.966	5	4	1	4	3	2	380.806	0.613D-20
40	3872.440	8	1	7	8	1	8	742.492	0.114D-20
40	3872.595	5	2	3	4	2	2	315.079	0.304D-19
40	3872.685	6	4	3	5	4	2	607.159	0.526D-20
40	3873.205	6	2	5	5	2	4	415.129	0.210D-19
40	3873.817	6	4	2	5	4	1	607.397	0.157D-19
40	3874.105	8	2	7	8	0	8	742.398	0.367D-21
40	3876.349	6	3	4	5	3	3	502.160	0.107D-19
40	3876.906	7	6	2	6	6	1	1038.765	0.928D-21
40	3876.913	7	6	1	6	6	0	1038.765	0.309D-21
40	3934.604	8	2	6	7	2	5	781.378	0.149D-19
40	3935.289	9	3	7	8	3	6	1003.783	0.518D-20
40	3937.185	9	4	6	8	4	5	1119.489	0.244D-20
20	3938.914	10	5	5	9	2	8	1078.019	0.529D-21
40	3939.430	10	2	9	9	2	8	1078.019	0.979D-21
40	3939.488	11	1	11	10	1	10	1112.042	0.457D-20
40	3939.503	11	0	11	10	0	10	1112.025	0.152D-20
40	3940.144	10	1	9	9	1	8	1076.802	0.456D-20
40	3941.726	3	3	1	2	1	2	79.227	0.869D-21
40	3942.387	8	3	5	7	3	4	840.866	0.103D-19
40	3944.676	4	3	1	3	1	2	173.111	0.299D-20
40	3948.676	9	2	7	8	2	6	981.494	0.206D-20
40	3948.785	9	4	5	8	4	4	1128.938	0.601D-21
40	3951.947	10	3	8	9	3	7	1213.561	0.701D-21
30	3952.149	8	5	4	7	4	3	928.297	0.781D-21
40	3953.710	11	2	10	10	2	9	1290.799	0.175D-20
40	3954.037	12	1	12	11	1	11	1324.131	0.582D-21
40	3954.043	12	0	12	11	0	11	1324.124	0.175D-20
40	3954.148	11	1	10	10	1	9	1290.227	0.584D-21
30	3954.612	4	4	1	3	1	2	173.111	0.336D-21
40	3956.576	10	4	7	9	4	6	1337.488	0.322D-21
40	3958.047	10	5	5	9	5	4	1472.686	0.416D-21
40	3960.866	10	2	8	9	2	7	1199.964	0.232D-20
40	3964.324	9	3	6	8	3	5	1048.656	0.144D-20
40	3964.997	5	3	2	4	1	3	275.132	0.107D-20
40	3966.052	5	2	3	4	0	4	221.622	0.125D-20
40	3967.243	11	3	9	10	3	8	1443.043	0.759D-21
40	3967.958	12	1	11	11	1	10	1521.519	0.613D-21
40	3968.249	13	1	13	12	1	12	1554.339	0.608D-21
30	3968.681	10	5	6	9	4	5	1357.558	0.304D-21
40	3974.430	4	3	2	3	1	3	141.904	0.409D-21
40	3974.641	11	4	8	10	4	7	1577.690	0.340D-21
30	3974.694	5	4	2	4	1	3	275.132	0.415D-21
40	3982.667	10	3	7	9	3	6	1281.271	0.154D-20
40	3987.739	10	4	6	9	4	5	1357.558	0.675D-21
30	3988.294	6	4	3	5	1	4	398.880	0.147D-20
40	4000.389	6	3	3	5	1	4	398.880	0.222D-20
40	4003.167	4	4	0	3	2	1	211.437	0.529D-21
40	4011.338	5	3	3	4	1	4	224.305	0.109D-20
40	4017.617	6	2	4	5	0	5	324.661	0.163D-20
40	4020.261	5	4	1	4	2	2	315.079	0.315D-21
40	4035.420	6	4	2	5	2	3	445.794	0.115D-20
40	4035.599	5	4	2	4	2	3	299.440	0.771D-21
40	4035.709	7	3	4	6	1	5	541.997	0.524D-21
40	4051.176	7	4	3	6	2	4	601.961	0.358D-21
40	4070.684	8	4	4	7	2	5	781.378	0.744D-21
40	4080.367	8	3	5	7	1	6	702.886	0.667D-21
40	4094.715	6	5	1	5	3	2	507.175	0.279D-21
40	4097.142	7	4	4	6	2	5	551.610	0.551D-21
40	4098.041	7	3	5	6	1	6	446.246	0.470D-21
40	4131.041	8	2	6	7	0	7	584.941	0.282D-21

intensity cut-off is $0{\cdot}27\times10^{-21}$ cm^{-1}/molecule cm^{-2} which corresponds to $0{\cdot}10\times10^{-24}$ cm^{-1}/molecule cm^{-2} in natural water vapour. The total band intensities (that is the sum of the individual line strengths) are $S_v(2\nu_2)=0{\cdot}717\times10^{-19}$, $S_v(\nu_1)=0{\cdot}461\times10^{-18}$ and $S_v(\nu_3)=0{\cdot}681\times10^{-17}$ cm^{-1}/molecule cm^{-2} at 296 K. A more complete list with an intensity cut-off of $0{\cdot}1\times10^{-22}$ cm^{-2}/molecule cm^{-2} has been deposited with the British Library. Copies of this table which comprises 7 pages may be obtained from the British Library, Lending Division, by quoting the number SP16040 according to the procedure described at the end of this issue.

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