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High Resolution Infrared Spectra of Water Vapor[1]

ν_1 and ν_3 Bands of $H_2{}^{18}O$

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The ν_1 and ν_3 bands of $H_2{}^{18}O$ occurring in the region 2.5–3.0 μ were recorded with a high resolution vacuum infrared spectrograph and an analysis is presented of the rotational structure observed. A discussion is presented of the effects of perturbations between the upper states of the transitions involved. Several lines belonging to the ν_1 and ν_3 bands of $H_2{}^{17}O$ have been identified.

INTRODUCTION AND EXPERIMENTAL PROCEDURE

The interpretation of high resolution near infrared bands of the water vapor molecule offers many challenges. Apart from the complications arising out of the molecule being an asymmetric rotor with a large centrifugal distortion, the near infrared fundamental vibration rotation bands ν_1 and ν_3 (*1*)[3] of water vapor are influenced by the effects of vibrational interactions. The present article relates to the $H_2{}^{18}O$ molecule.

A sample of water vapor enriched in the ^{18}O content was used in a 1-m long absorption cell equipped with infrared transmitting windows. The observational data were recorded in the region 2.5–3.0 μ with a vacuum prism-grating spectrograph in an Ebert-type mounting. When the data reported here were measured,

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[3] For the notation used in the present paper see Ref. (*1*).

the 6-m focal length Ebert-type spectrograph at The Ohio State University was newly constructed and suitable calibration procedures were still being explored (*2*). The present set of data was obtained by using double-pen recorders. Atomic emission lines of neon were used as a source of "wave number markers." Two beams of radiation were passed through the spectrograph at the same time; one of these comprised the infrared under study and the other was from a neon emission source. At various predetermined spots, by suitably manipulating the foreprism monochromator in the infrared optics, internal standards [as, for example, the 2–0 band lines of CO (*3*)] were recorded on the infrared spectrum without stopping the rotation of the grating. Details of this method were published in an earlier paper (*4*). It is believed that, in the case of unblended lines, the wave numbers obtained in this work are accurate to ± 0.005 cm^{-1}. In fact, some impurity lines due to the CO_2 bands were also observed in the $H_2{}^{18}O$ spectra and it was later discovered that there was excellent agreement between their positions determined here as compared to the measurements of Gordon and McCubbin (*5*).

ANALYSIS AND RESULTS

Notation

Each energy level is labeled by the set of quantum numbers J, K_{-1}, K_{+1} (written also in the form $J_{K_{-1}K_{+1}}$), K_{-1} and K_{+1} being the limiting prolate and oblate symmetric top quantum numbers. The representation of the energy levels by the J_τ values, $\tau = (K_{-1} - K_{+1})$, has been found to be inadequate. In the notation *ee*, *eo*, *oe*, and *oo* the first letter refers to the parity of K_{-1} and the second one to the parity of K_{+1}, *e* standing for even and *o* for odd. The following selection rules are applicable: for the ν_1 band: $\Delta J = 0, \pm 1$ along with K_{-1} and K_{+1} both changing parity, i.e., *ee* $\leftrightarrow$ *oo* and *eo* $\leftrightarrow$ *oe*; and for the ν_3 band: $\Delta J = 0, \pm 1$ along with the parity of K_{-1} remaining unaltered and K_{+1} changing parity, i.e., *ee* $\leftrightarrow$ *eo* and *oo* $\leftrightarrow$ *oe*.

Analysis

In the analysis of the ν_1 and ν_3 bands, the initial trials involved use of iterative procedures of fitting the transitions to the expressions for term values of the energy levels of an asymmetric rotor. Since the ν_1 and ν_3 bands have a common lower vibrational level, namely the ground state of the $H_2{}^{18}O$ molecule, it has been possible to form combination differences which are purely functions of the energy levels of the ground state and thereby verify the assignments. For example:

$$[(2_{02} \leftarrow 1_{11}) - (2_{02} \leftarrow 2_{11})]_{\nu_1\,\text{band}} = [(1_{10} \leftarrow 1_{11}) - (1_{10} \leftarrow 2_{11})]_{\nu_3\,\text{band}}$$
$$= (2_{11} \leftarrow 1_{11})_{\text{ground state}}.$$

The validity of the analysis was further verified from combinations of the sum rule plots for the ground state discussed in a previous paper (*6*); Figs. 1–4 of Ref. (*6*) show that the ground state combination sums plotted for $H_2{}^{16}O$ gave rise to smooth curves. Corresponding plots were made for the ground state of $H_2{}^{18}O$ based on the data presented in this article and it was noticed (*7*) that they were very similar to the $H_2{}^{16}O$ plots. This gave further credence to the assignments. The ground state energy levels of $H_2{}^{18}O$ given in Table I are based on the final analysis of the observational data.

Molecular Constants

In attempting to derive meaningful values for the molecular constants of an asymmetric rotor like the water vapor molecule, one is confronted with some-

TABLE I

ENERGY LEVELS OF $H_2{}^{18}O$ AS DETERMINED FROM OBSERVATIONAL DATA (cm^{-1})

$J\ K_{-1}K_1$	(000)	(100)	(001)	$J\ K_{-1}K_1$	(000)	(100)	(001)
1 0 1	23.756	3673.055	3765.092	6 1 5	541.183	4181.222	4274.649
1 1 1	36.751	3685.534	3776.999	6 2 5	550.447	4189.593	4280.851
1 1 0	42.024	3690.776	3782.299	6 2 4	601.246	4240.672	4334.805
				6 3 4	645.377	4281.977	4370.671
2 0 2	69.932	3718.423	3810.691	6 3 3	658.601	4297.017	4391.671
2 1 2	78.995	3727.028	3818.743	6 4 3	751.031	4380.890	4470.772
2 1 1	94.790	3742.722	3834.652	6 4 2	752.195	4387.916	4472.200
2 2 1	133.479	3779.896	3870.084	6 5 2	880.100	4510.458	4591.520
2 2 0	134.785		3871.528	6 5 1	880.146	4510.466	4591.571
				6 6 1	1033.548	4657.792	
3 0 3	136.344	3783.609	3876.045	6 6 0	1033.548		
3 1 3	141.576	3788.473	3880.575				
3 1 2	172.887	3819.571	3912.035	7 0 7	583.767	4222.358	4315.886
3 2 2	204.762	3849.958	3940.926	7 1 7	583.972	4222.551	4316.179
3 2 1	210.800	3856.044	3947.335	7 1 6	701.697	4338.491	4432.080
3 3 1	282.093	3924.669	4012.876	7 2 6	706.608		4435.323
3 3 0	282.304	3924.781	4013.129	7 2 5	780.428	4416.800	4511.585
				7 3 5	812.753		4536.232
4 0 4	221.237	3866.837	3959.455	7 3 4	839.561	4474.706	4569.749
4 1 4	223.830	3869.209	3962.360	7 4 4	921.908		4639.662
4 1 3	274.811	3919.781	4012.741	7 4 3	925.698	4558.881	4644.246
4 2 3	298.629	3942.225	4034.211	7 5 3	1051.036		4760.605
4 2 2	314.460	3957.484	4050.544	7 5 2	1051.334	4679.357	4760.915
4 3 2	379.293	4020.218	4108.431	7 6 1		4827.142	
4 3 1	380.700	4021.191	4109.976				
4 4 1	482.632	4121.384	4205.510	8 0 8	740.940		4470.708
4 4 0	482.660	4121.318	4205.518	8 1 8	741.013		4470.745
				8 1 7	879.481		4606.627
5 0 5	324.026	3967.659	4060.525	8 2 7	881.902		4608.149
5 1 5	325.194		4061.277	8 2 6	980.230		4707.901
5 1 4	398.371	4041.102	4134.431	8 3 6	1001.718		
5 2 4	414.177	4055.754	4150.247	8 3 5	1047.317		4775.200
5 2 3	445.160	4087.163	4180.320	8 4 5	1116.635		
5 3 3	500.604	4139.556	4227.840	8 4 4	1126.433		
5 3 2	505.726	4142.464	4232.824	8 5 4	1246.319		
5 4 2	604.549	4242.990	4325.951	8 5 3	1247.234		
5 4 1	604.796	4242.299	4326.284				
5 5 1	733.708	4365.886	4446.736	9 1 8	1074.779		
5 5 0	733.712	4365.884	4446.715	9 2 8	1075.932		
				9 2 7	1198.194		
6 0 6	444.848	4086.078	4179.344	9 3 6	1279.822		
6 1 6	445.354	4086.531	4179.655				

what formidable problems because of the complex nature of the theoretical expressions involved especially when perturbations are taken into account. The combinations of sum rules given in Ref. (*6*) have been an attempt to obtain expressions combining molecular constants associated with each moment of inertia axis.

Let us multiply the sum rule combinations given in Eqs. (3)–(6) of Ref. (*6*) by $J(J+1)$ and represent the products by $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$, and $\mathcal{S}$, respectively. In other words, for vibration rotation bands arising from the ground state we define

$$\mathcal{A}_v = \nu_0 + (X_{\mathcal{A}}{}^v)J(J+1) + (Y_{\mathcal{A}}{}^v)J^2(J+1)^2, \tag{1}$$

$$\mathcal{B}_v = \nu_0 + (X_{\mathcal{B}}{}^v)J(J+1) + (Y_{\mathcal{B}}{}^v)J^2(J+1)^2, \tag{2}$$

$$\mathcal{C}_v = \nu_0 + (X_{\mathcal{C}}{}^v)J(J+1) + (Y_{\mathcal{C}}{}^v)J^2(J+1)^2, \tag{3}$$

$$\mathcal{S}_v = \nu_0 + (X_{\mathcal{S}}{}^v)J(J+1) + (Y_{\mathcal{S}}{}^v)J^2(J+1)^2, \tag{4}$$

where ν_0 is the band origin and

$$X_{\mathcal{A}}{}^v = A_v - \tfrac{1}{4}(T^v_{aaaa} + T^v_{aa}), \tag{5}$$

$$Y_{\mathcal{A}}{}^v = (\tfrac{1}{4})\, T^v_{aaaa}\,, \tag{6}$$

$$X_{\mathcal{B}}{}^v = B_v - \tfrac{1}{4}(T^v_{bbbb} + T^v_{bb}), \tag{7}$$

$$Y_{\mathcal{B}}{}^v = (\tfrac{1}{4})T^v_{bbbb}\,, \tag{8}$$

$$X_{\mathcal{C}}{}^v = C_v - (\tfrac{1}{4})(T^v_{cccc} + T^v_{cc}), \tag{9}$$

$$Y_{\mathcal{C}}{}^v = (\tfrac{1}{4})T^v_{cccc}\,, \tag{10}$$

$$X_{\mathcal{S}}{}^v = (\tfrac{1}{3})(A_v + B_v + C_v) - (\tfrac{1}{60})(T^v_{aaaa} + T^v_{aa} + T^v_{bbbb} + T^v_{bb} + T^v_{cccc} + T^v_{cc}), \tag{11}$$

$$Y_{\mathcal{S}}{}^v = (\tfrac{1}{60})(3T^v_{aaaa} + 3T^v_{bbbb} + 3T^v_{cccc} - 2T^v_{aa} - 2T^v_{bb} - 2T^v_{cc}). \tag{12}$$

From the above Eqs. (1)–(4), the following relations (13)–(17) are easily derived for the ν_3 and ν_1 bands of the water molecule. The manner in which the numerical values given in Eqs. (13a), (14a), (15a), and (16a) were arrived at is discussed below.

$$\mathcal{A}_{v=3} - \mathcal{A}_{v=1} = (\nu_3 - \nu_1) + \{(X_{\mathcal{A}})^{v=3} - (X_{\mathcal{A}})^{v=1}\}J(J+1) + \{(Y_{\mathcal{A}})^{v=3} - (Y_{\mathcal{A}})^{v=1}\}J^2(J+1)^2 \tag{13}$$

$$= 91.9010 - 0.4714\, J(J+1) + (11 \times 10^{-4})J^2(J+1)^2, \tag{13a}$$

$$\mathcal{B}_{v=3} - \mathcal{B}_{v=1} = (\nu_3 - \nu_1) + \{(X_{\mathcal{B}})^{v=3} - (X_{\mathcal{B}})^{v=1}\}J(J+1) + \{(Y_{\mathcal{B}})^{v=3} - (Y_{\mathcal{B}})^{v=1}\}J^2(J+1)^2 \tag{14}$$

$$= 91.9010 + 0.1137\, J(J+1), \tag{14a}$$

$$\mathcal{C}_{v=3} + \mathcal{C}_{v=1} = (\nu_3 + \nu_1) + \{(X_{\mathcal{C}})^{v=3} + (X_{\mathcal{C}})^{v=1}\}J(J+1) + \{(Y_{\mathcal{C}})^{v=3} + (Y_{\mathcal{C}})^{v=1}\}J^2(J+1)^2 \quad (15)$$

$$= 7391.2620 + 18.167J(J+1) - (5 \times 10^{-4})J^2(J+1)^2, \quad (15a)$$

$$\mathcal{S}_{v=3} + \mathcal{S}_{v=1} = (\nu_3 + \nu_1) + \{(X_{\mathcal{S}})^{v=3} + (X_{\mathcal{S}})^{v=1}\}J(J+1) + \{(Y_{\mathcal{S}})^{v=3} + (Y_{\mathcal{S}})^{v=1}\}J^2(J+1)^2 \quad (16)$$

$$= 7391.2620 + 33.341\, J(J+1) - (9.48 \times 10^{-3})J^2(J+1)^2. \quad (16a)$$

The molecular constants presented in this paper are the ones derived from graphical plots of some of the relations given above.

First, for the ground state the sum rule combinations given in Eqs. (3)–(6) of Ref. (*6*) have been plotted for $H_2{}^{18}O$ [see Fraley (*7*)] and the numerical values were determined for the coefficients of $J(J+1)$ and $J^2(J+1)^2$. Figure 1 shows how the coefficients so determined represent the observational data for the ground state. Since the scatter of ± 0.01 cm^{-1} of points is what one should expect from the accuracy of spectral positions, we believe that the assignments are reasonable.

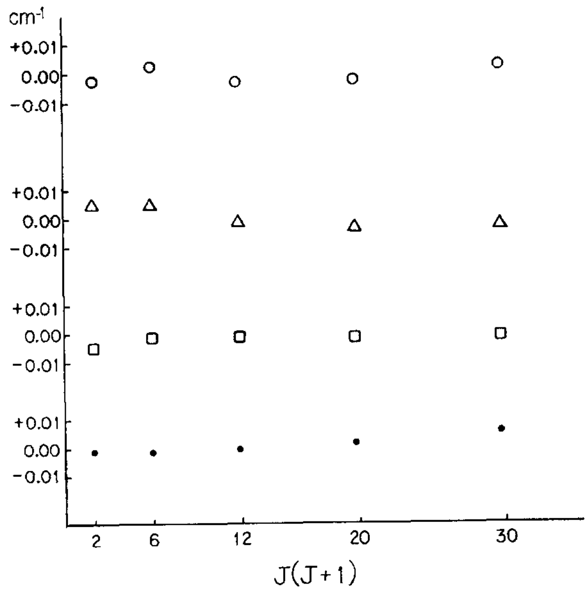


FIG. 1. Plot of the observed *minus* calculated values of the sum rule combinations $\mathcal{A}_{v=0}$, $\mathcal{B}_{v=0}$, $\mathcal{C}_{v=0}$, and $\mathcal{S}_{v=0}$ *versus* $J(J+1)$ for the ground state of $H_2{}^{18}O$, represented, respectively, by ○, △, □, ●.

The upper states of the ν_1 and ν_3 bands of the water molecule are affected by perturbations. The major contribution to the interactions is due to the operators P_y and $P_xP_z + P_zP_x$ (Γ^r representation). Attempts to derive sum rules involving these operators resulted in rather unwieldy expressions. In order to eliminate the effects of the interaction, graphical plots are made for some of the combination differences involving the upper states of the ν_1 and ν_3 bands. These particular combinations have been derived keeping in mind the selection rules for the perturbations. The plots using Eqs. (13) and (14) are displayed in Fig. 2 whereas those using Eqs. (15) and (16) are shown in Fig. 3. From these plots, numerical values are determined for the slopes and intercepts and they are given in Eqs. (13a), (14a), (15a), and (16a). How well these numerical values represent the observational data is indicated in Fig. 4 where the observed values for the sums and differences appearing on the left side of the Eqs. (13a), (14a), (15a), and (16a) have been plotted against the calculated values derived from the right sides of the same equations. Even though the ground state (Fig. 1) and upper state (Fig. 4) plots were based on the same observational data, the scatter of points in Fig. 4 (viz. ± 0.05 cm^{-1}) is somewhat larger than the scatter of points appearing in Fig. 1 (viz. ± 0.01 cm^{-1}). This small but significant scatter of

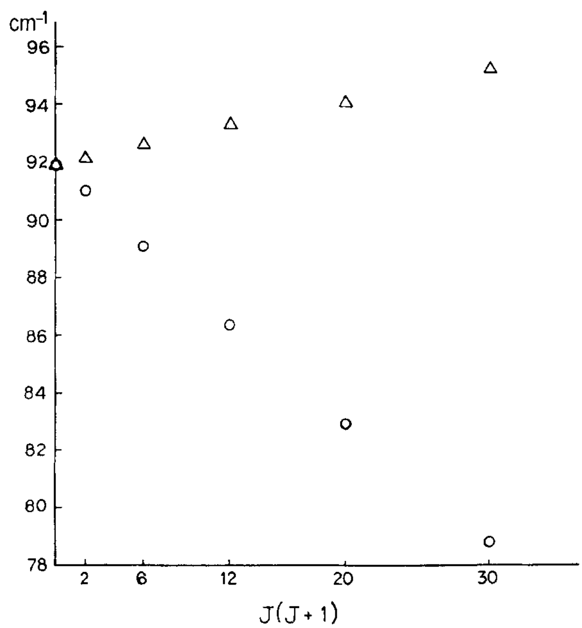


FIG. 2. Plots of the $(\mathcal{A}_{v=3} - \mathcal{A}_{v=1})$ and $(\mathcal{B}_{v=3} - \mathcal{B}_{v=1})$ versus $J(J+1)$ for $H_2^{18}O$ represented, respectively, by ○ and △. The common intercept for the plots $= (\nu_3 - \nu_1) = 91.90$ cm^{-1} [see Eqs. (13) and (14)].

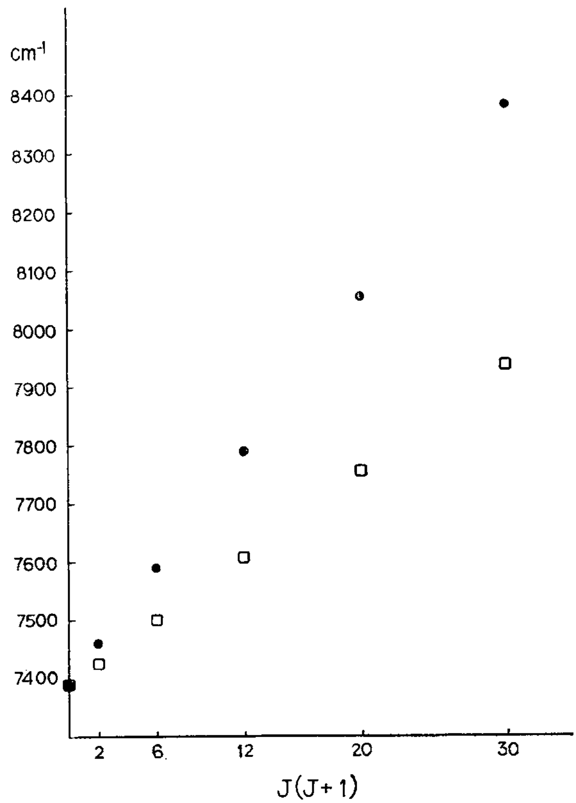


FIG. 3. Plots of the $(\mathcal{C}_{v=3} + \mathcal{C}_{v=1})$ and $(\mathcal{S}_{v=3} + \mathcal{S}_{v=1})$ *versus* $J(J + 1)$ for $H_2{}^{18}O$ represented respectively, by □ and ●. The common intercept for the plots $= (\nu_3 + \nu_1) = 7391.26$ cm^{-1} [see Eqs. (15) and (16)].

± 0.05 cm^{-1} may be the result of the effects arising out of the proximity of the rotational levels of the 020 state to the rotational levels of the 100 and 001 states. Data for the 020 level with the accuracy available for the 100 and 001 levels are not available at this time. It is interesting to note that in the analysis of some of the bands of H_2Se where complications due to Coriolis interaction were noticed, Hill (*8*) also found it necessary to couple the sum rules of the submatrices of the Hamiltonian which contain the interacting energy levels. Figure 5 shows the spectrum of the ν_1 and ν_3 bands of $H_2{}^{18}O$ and Table II gives the wave numbers and assignments for the rotational structure of these vibration rotation bands. The line numbers appearing in column 1 of Table II correspond to the serial numbers indicated in Fig. 5.

Impurity Lines Due to $H_2{}^{17}O$

Several lines have been identified as due to the $H_2{}^{17}O$ impurity. Table III gives the wave numbers and assignments of the $H_2{}^{17}O$ lines appearing in the spectrum. The following empirical relation seems to hold for the lines of the various isotopic species of water vapor:

$$\frac{\nu(H_2{}^{16}O) - \nu(H_2{}^{17}O)}{\nu(H_2{}^{16}O) - \nu(H_2{}^{18}O)} = 0.529 \tag{17}$$

where ν is the wave number for the same transition in each of the species.

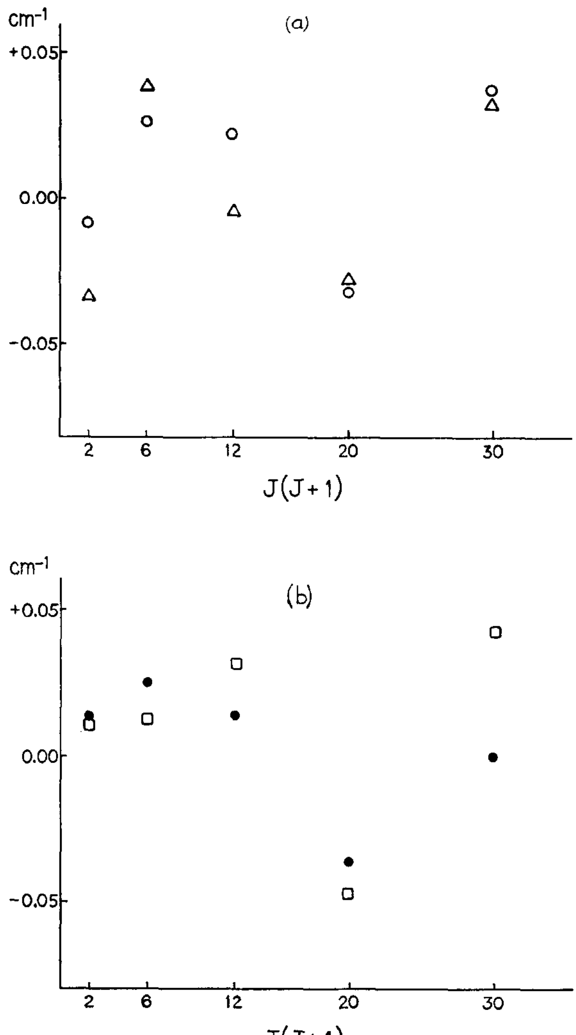


FIG. 4. Observed *minus* calculated values of the sum rule combinations *versus* $J(J + 1)$ for the upper states of the ν_3 and ν_1 bands of $H_2{}^{18}O$. (a) (○), ($\mathcal{A}_{v=3} - \mathcal{A}_{v=1}$); (△), ($\mathcal{B}_{v=3} - \mathcal{B}_{v=1}$); (b) (□), ($\mathcal{C}_{v=3} + \mathcal{C}_{v=1}$); (●), ($\mathcal{S}_{v=3} + \mathcal{S}_{v=1}$).

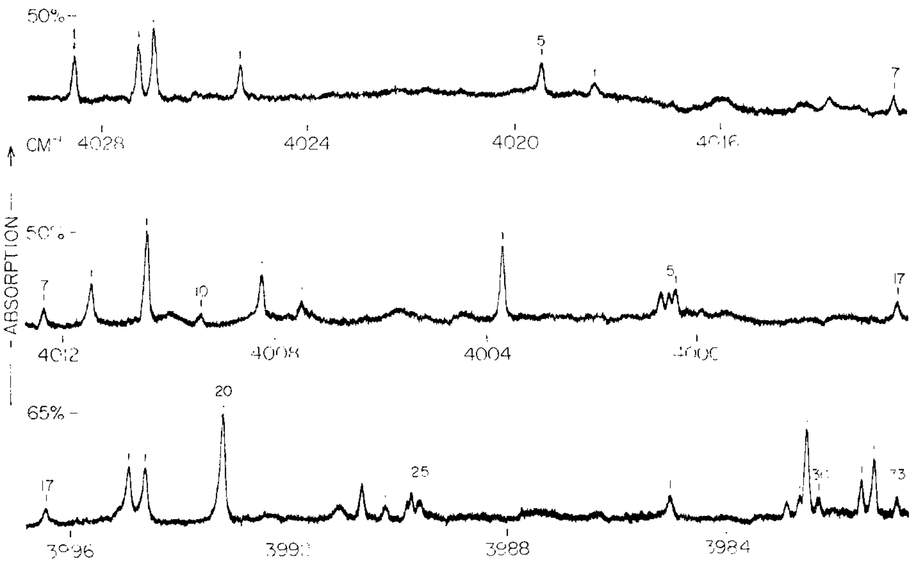


FIG. 5. (Part 1)

FIG. 5. High resolution infrared spectrum of 1m of $H_2{}^{18}O$ in the region 3–2.5 μ. Grating: plane 10 × 5 in., 73.25 grooves per mm echelle in a 6-m focal length Ebert-type spectrograph used double-passed. Detector: PbS cooled to liquid nitrogen. Source: Nernst glower operating at 1.1 A. $H_2{}^{17}O$ lines which appeared as an impurity are identified with black dots (●) in the spectrum. Lines not identified as due to either $H_2{}^{18}O$ or $H_2{}^{17}O$ (see Tables II and III belong to the $H_2{}^{16}O$ species.

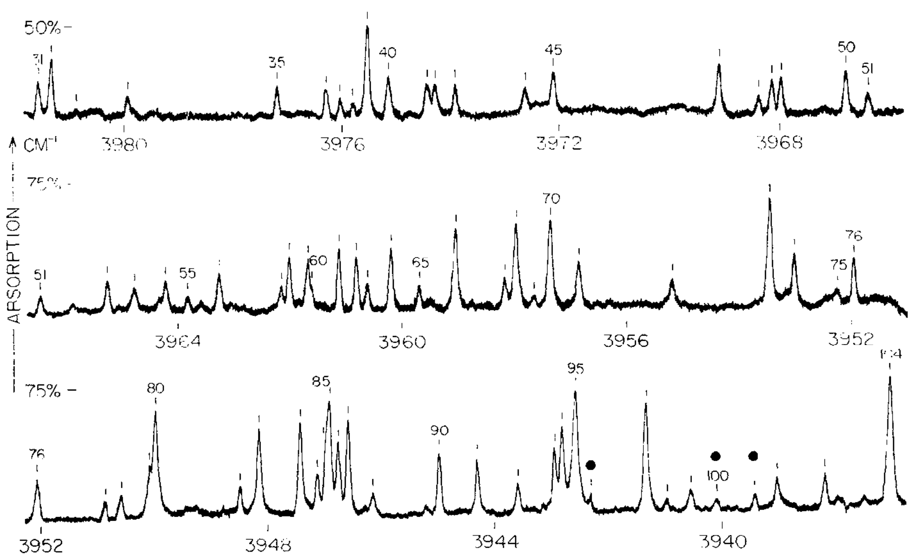


FIG. 5. (Part 2)

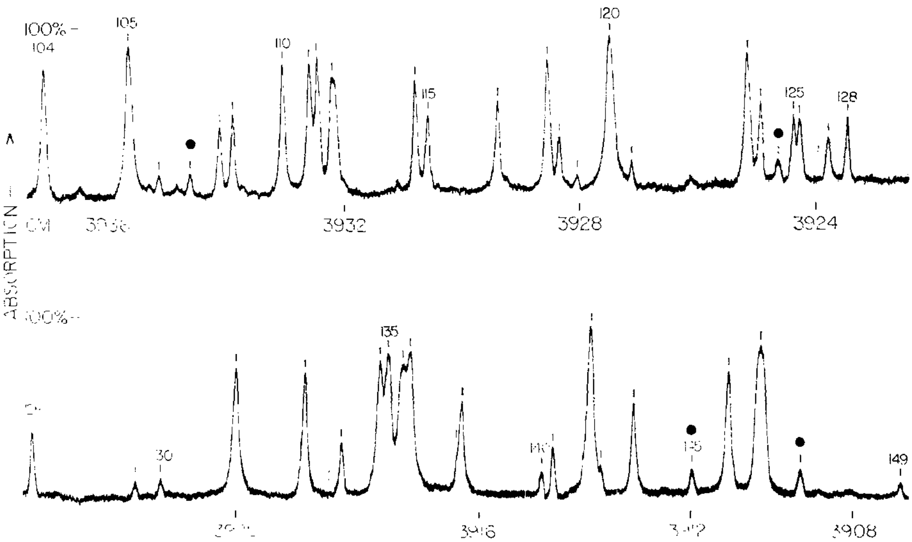


FIG. 5. (Part 3)

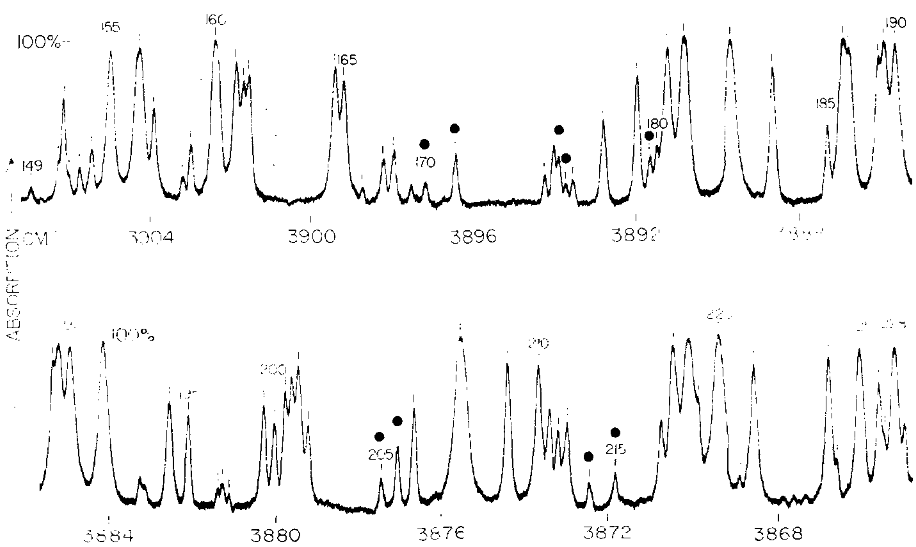


FIG. 5. (Part 4)

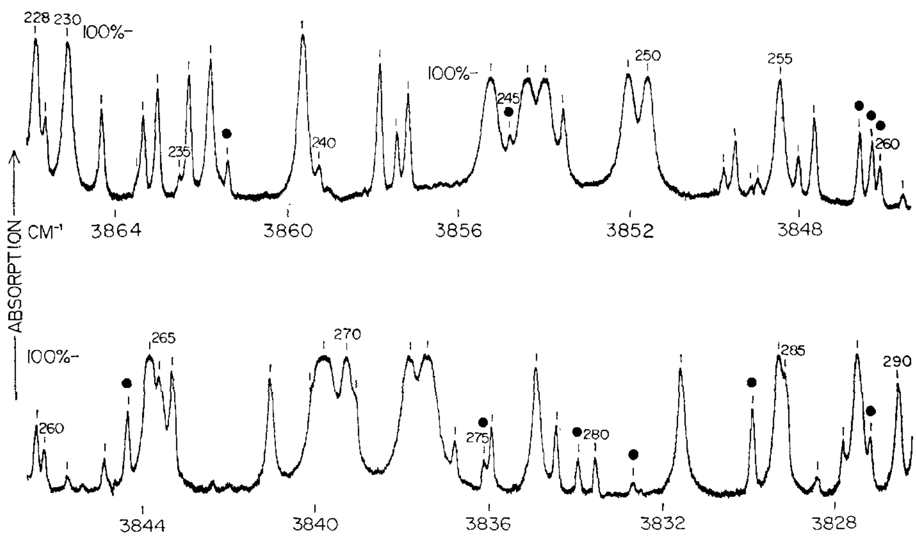


FIG. 5. (Part 5)

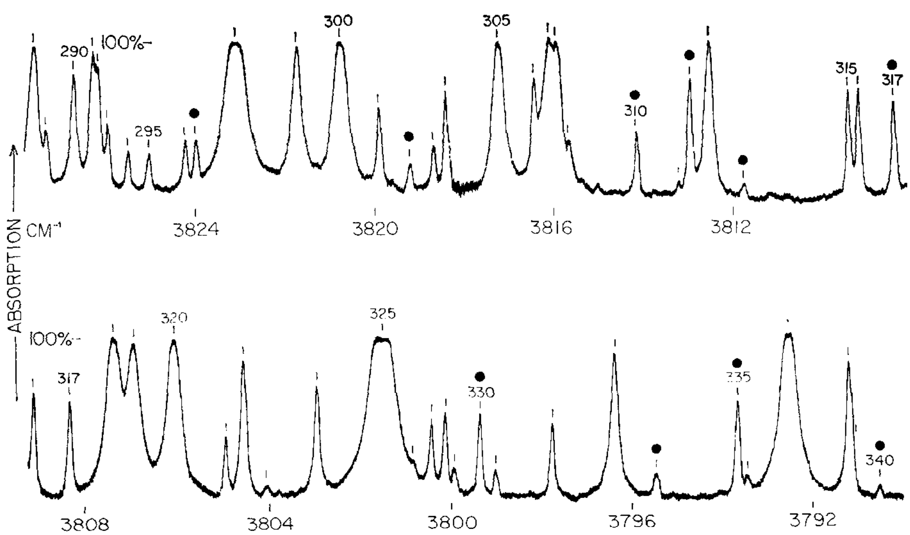
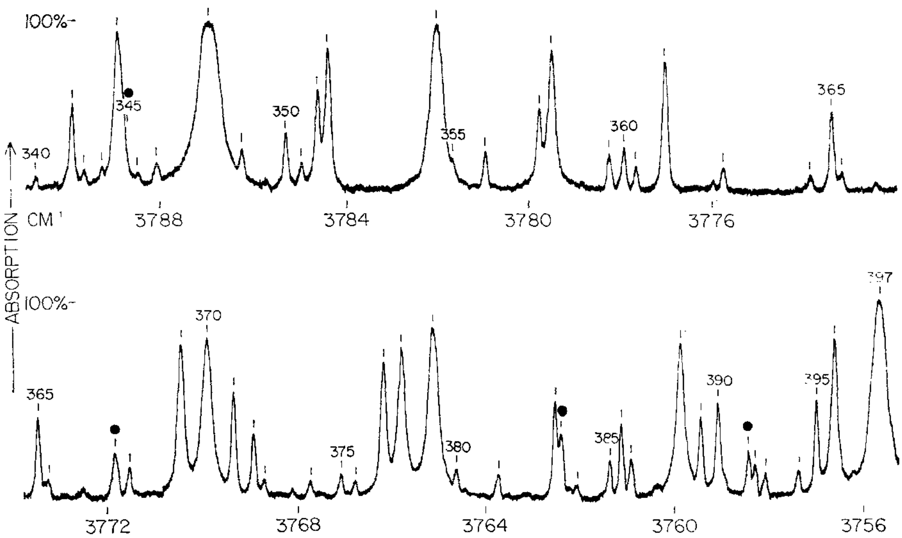


FIG. 5. (Part 6)



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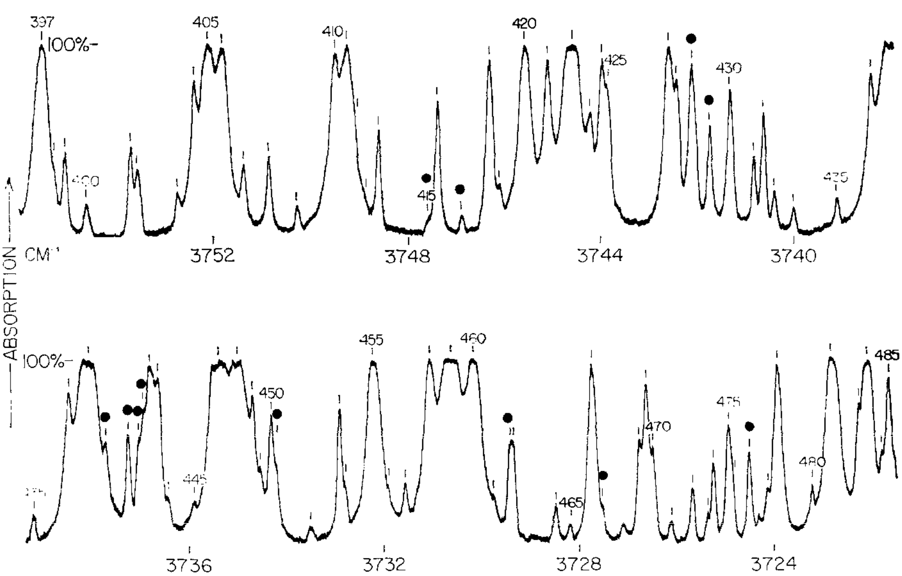


FIG. 5. (Part 8)

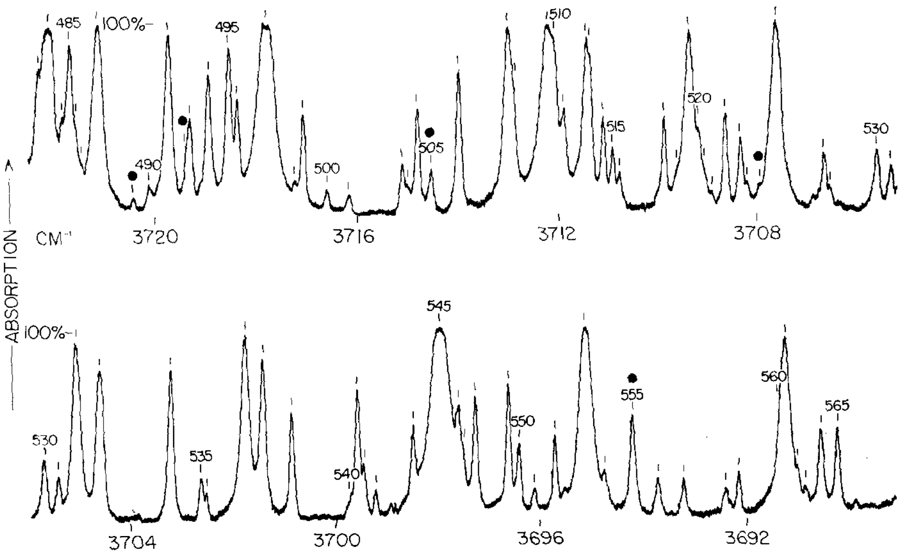
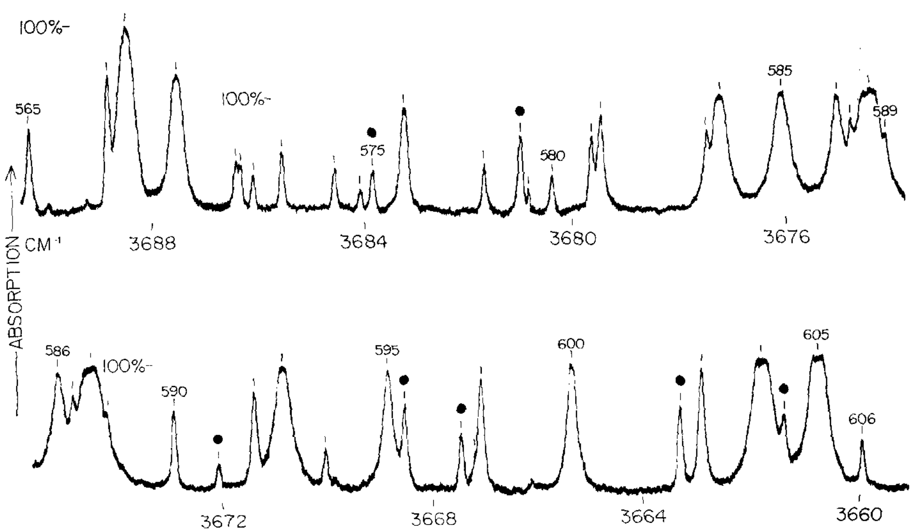


FIG. 5. (Part 9)



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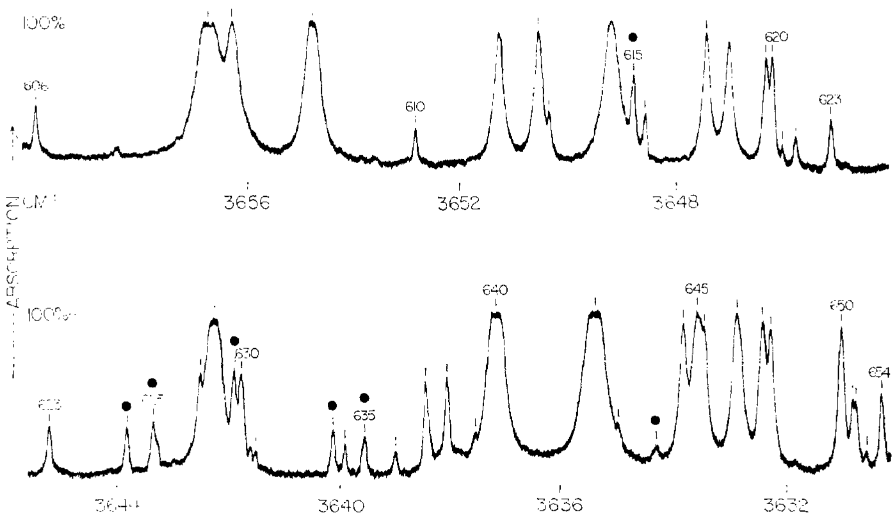

FIG. 5. (Part 11)

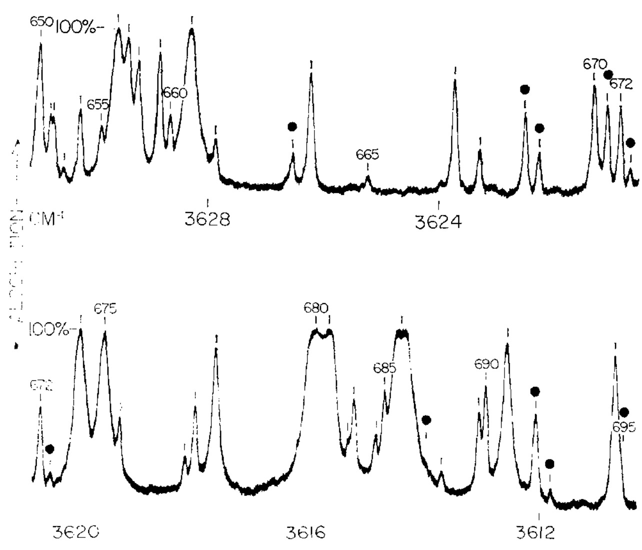

FIG. 5. (Part 12)

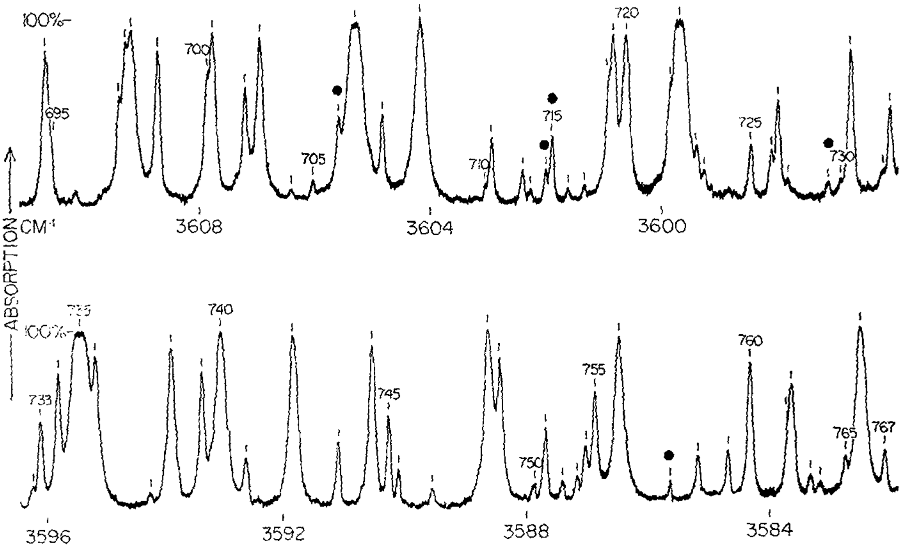

FIG. 5. (Part 13)

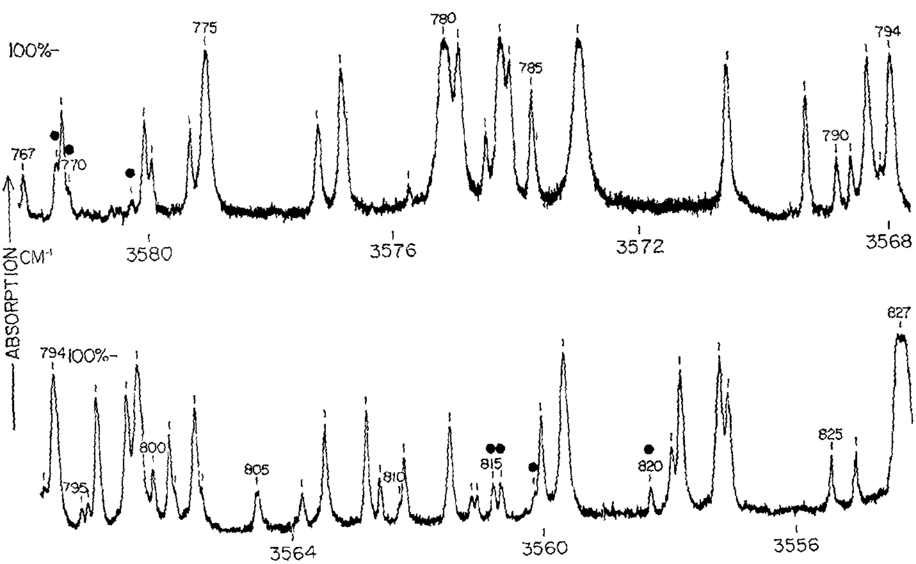

FIG. 5. (Part 14)

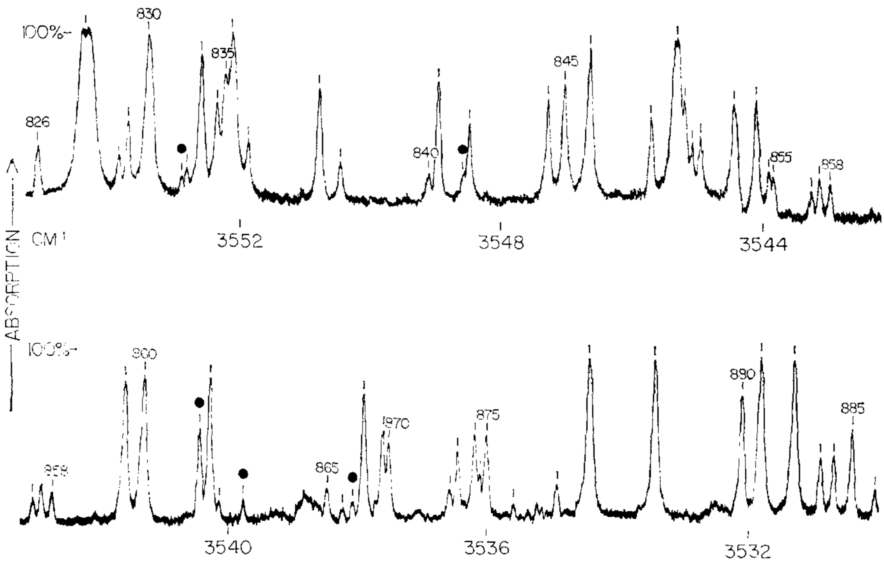

Fig. 5. (Part 15)

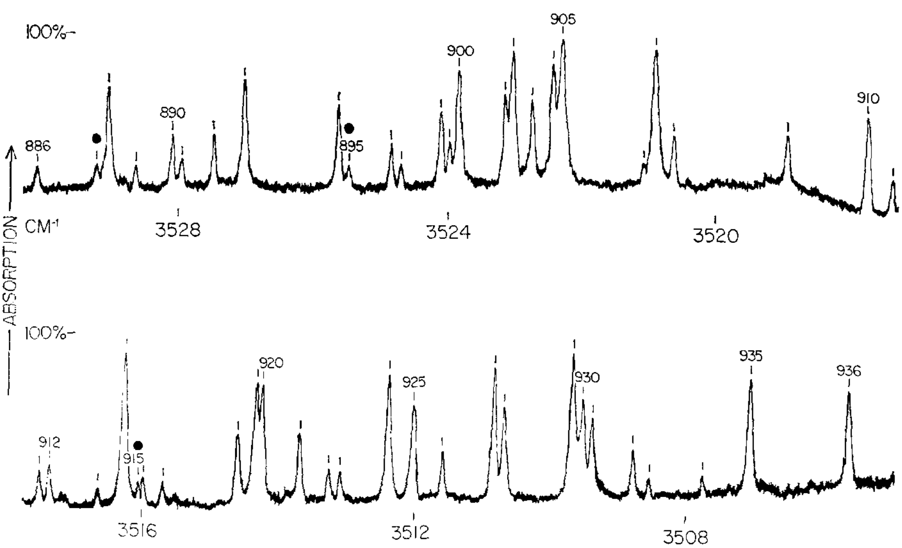

Fig. 5. (Part 16)

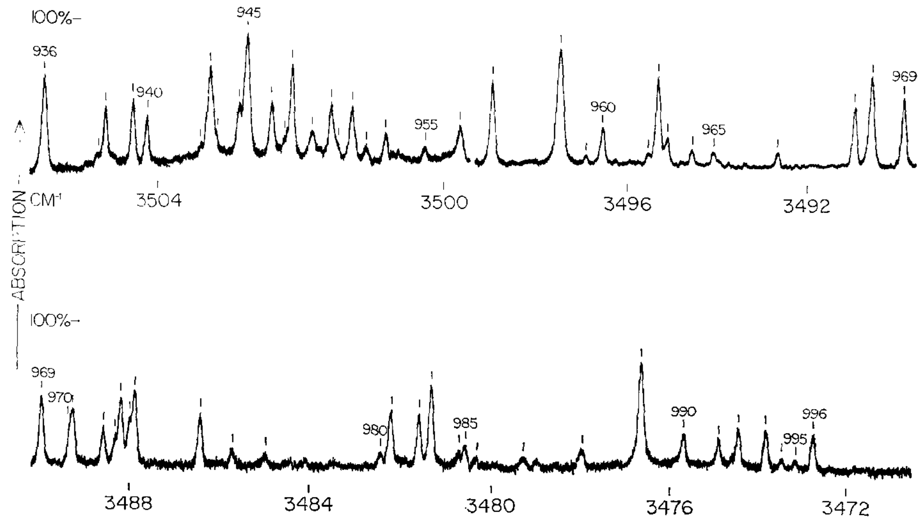

FIG. 5. (Part 17)

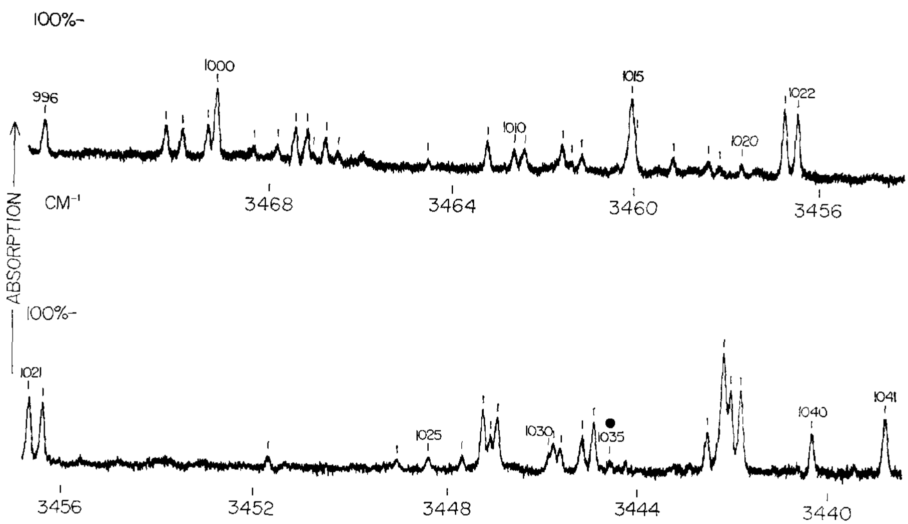

FIG. 5. (Part 18)

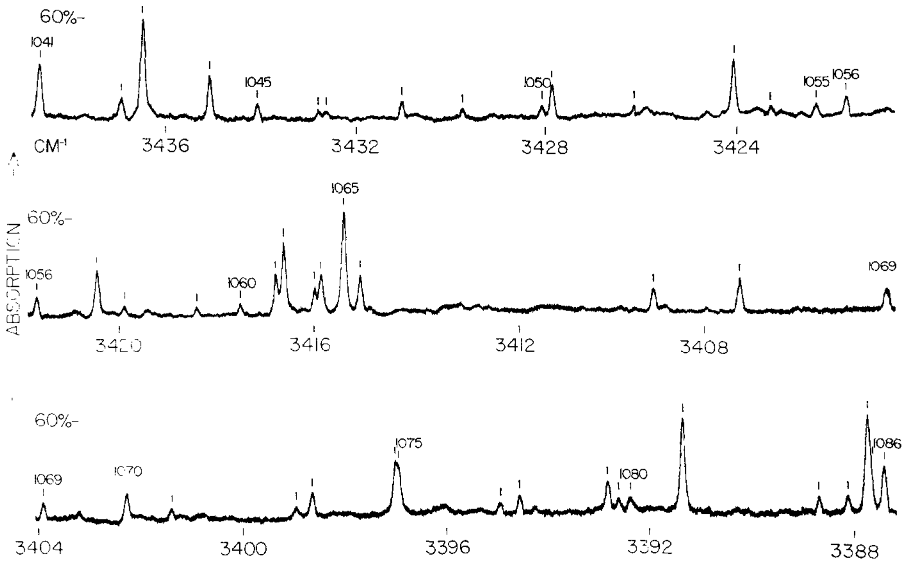

Fig. 5. (Part 19)

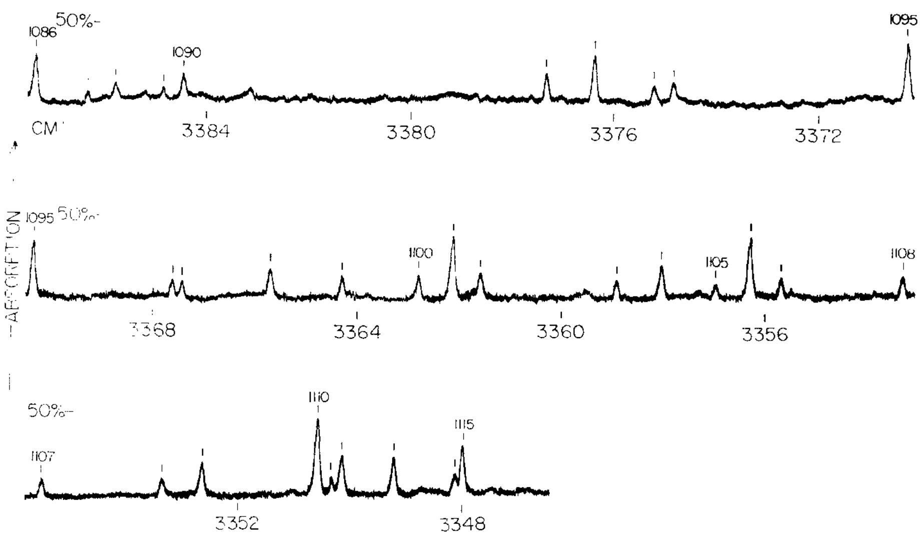

Fig. 5. (Part 20)

Band Origins:

From Eqs. (13a), (14a), (15a), and (16a) one can calculate the band origins of the ν_1 and ν_3 bands of $H_2{}^{18}O$; the values obtained are $\nu_1 = 3649.68_0$ cm^{-1} and $\nu_3 = 3741.58_1$ cm^{-1}. They agree within ±0.01 cm^{-1} with the values derived from observed transitions involving $J' = K'_{-1} = K''_{+1} = 0$ and the energy levels of the ground state given in Table I. Using Eq. (17) values of $\nu_3 = 3748.36$ cm^{-1} and $\nu_1 = 3653.15$ cm^{-1} were derived for the $H_2{}^{17}O$ molecule.

ACKNOWLEDGMENTS

We wish to express our thanks to Dr. W. S. Benedict for many valuable discussions.

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REFERENCES

1. G. HERZBERG, "Infrared and Raman Spectra of Polyatomic Molecules." Van Nostrand, Princeton, New Jersey, 1962; H. C. ALLEN AND P. C. CROSS, "Molecular Vib-Rotors." Wiley, New York, 1963.
2. P. E. FRALEY AND K. NARAHARI RAO, *Appl. Opt.* **2**, 1127 (1963).
3. K. NARAHARI RAO, C. J. HUMPHREYS AND D. H. RANK, "Wavelength Standards in the Infrared." Academic Press, New York, 1966.
4. P. E. FRALEY AND K. NARAHARI RAO, *J. Opt. Soc. Am.* **55**, 1091 (1965).
5. H. R. GORDON AND T. K. MCCUBBIN, JR., *J. Mol. Spectry.* **19**, 137 (1966).
6. P. E. FRALEY AND K. NARAHARI RAO, *J. Mol. Spectry.* **19**, 131 (1966).
7. P. E. FRALEY, Ph.D. dissertation, The Ohio State University, 1966.
8. R. A. HILL, *J. Mol. Spectry.* **24**, 100 (1967).

TABLE II

ANALYSIS OF THE ν_1 AND ν_3 BANDS OF $H_2{}^{18}O$

(In the last column 181 refers to ν_1 and 183 refers to ν_3)

Line No.	Wave number (vac.cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
0001	4028.573	24	7	3	4	6	1	5	183
0002	4027.330	32	5	4	2	4	2	3	183
0003	4027.038	42	6	4	2	5	2	3	183
0006	4018.466	6	5	4	1	4	1	4	181
0008	4011.811	17							
0008	4011.811	17	5	4	1	4	0	4	183
0009	4010.750	50	6	2	4	5	0	5	183
0010	4009.717	4							
0012	4007.809	5							
0013	4004.009	45	5	3	3	4	1	4	183
0014	4001.004	8							
0015	4000.853	7	11	4	7	10	4	6	183
0016	4000.730	12	4	4	1	3	2	2	183
0017	3996.562	4							
0019	3994.725	28	4	4	0	3	2	1	183
0020	3993.300	64	6	3	3	5	1	4	183
0024	3989.798	12	11	3	8	10	3	7	183
0028	3982.655	7							
0029	3982.525	51	6	4	3	5	1	4	181
0031	3981.521	17							
0032	3981.284	31	10	4	6	9	4	5	183
0034	3979.880	9							
0035	3977.177	11	12	2	10	11	2	9	183
0037	3976.014	8							
0039	3975.516	55	10	3	7	9	3	6	183
0041	3974.415	16	9	5	4	8	4	5	181
0042	3974.277	16	13	2	12	12	2	11	183
0047	3968.420	7	8	6	3	7	5	2	181
0048	3968.191	17	5	4	2	4	1	3	181
0049	3968.026	18	11	4	8	10	4	7	183
0050	3966.857	23	4	3	2	3	1	3	183
0051	3966.435	8	11	5	7	10	5	6	183
0052	3965.260	14	11	2	9	10	2	8	183
0054	3964.228	15	9	5	5	8	4	4	181
0056	3963.265	20	10	5	6	9	4	5	181
0061	3961.147	36	13	1	13	12	1	12	183
0062	3960.844	28	12	1	11	11	1	10	183
0063	3960.651	12	12	2	11	11	2	10	183
0064	3960.234	40	11	3	9	10	3	8	183
0066	3959.084	50	5	2	3	4	0	4	183
0068	3958.018	51	5	3	2	4	1	3	183
0069	3957.696	4							
0070	3957.407	55	9	3	6	8	3	5	183
0073	3953.536	65	10	2	8	9	2	7	183
0076	3952.056	28	10	5	5	9	5	4	183
0077	3950.865	7							
0079	3950.131	23	10	4	7	9	4	6	183
0081	3948.507	11	4	4	1	3	1	2	181
0085	3947.039	28	11	1	10	10	1	9	183
0086	3946.968	65	12	0	12	11	0	11	183

TABLE II (Continued)

Line No.	Wave number (vac.cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
0087	3946.796	37	8	5	4	7	5	3	181
0088	3946.612	54	11	2	10	10	2	9	183
0089	3946.194	12	6	5	1	6	3	4	183
0090	3945.035	34	10	3	8	9	3	7	183
0092	3943.649	13							
0093	3943.031	35	9	4	5	8	4	4	183
0097	3941.412	62	9	2	7	8	2	6	183
0098	3941.025	3	5	5	1	5	3	2	183
0102	3939.122	15							
0104	3937.105	76	4	3	1	3	1	2	183
0105	3935.634	90	8	3	5	7	3	4	183
0109	3933.881	47	3	3	1	2	1	2	183
0110	3933.015	77	10	1	9	9	1	8	183
0112	3932.426	81	11	1	11	10	1	10	183
0113	3932.145	70	10	2	9	9	2	8	183
0114	3930.776	65	9	4	6	8	4	5	183
0117	3928.522	78	9	3	7	8	3	6	183
0118	3928.323	30	7	5	2	6	4	3	181
0120	3927.456	94	8	2	6	7	2	5	183
0121	3927.106	14	7	5	3	6	4	2	181
0123	3924.932	50	9	5	5	8	5	4	183
0126	3924.273	39	7	3	4	6	2	5	181
0129	3921.757	5	6	4	2	6	2	5	183
0132	3918.943	78	9	1	8	8	1	7	183
0133	3918.344	30	3	3	0	2	1	1	183
0133	3918.344	30	5	3	3	4	0	4	181
0134	3917.694	88	8	4	4	7	4	3	183
0135	3917.552	95	10	0	10	9	0	9	183
0137	3917.217	88	9	2	8	8	2	7	183
0140	3915.010	5	9	6	3	8	6	2	183
0141	3914.832	20	9	6	4	8	6	3	183
0142	3914.205	92	4	2	2	3	0	3	183
0144	3913.491	51	7	4	3	6	3	4	181
0146	3911.147	15	7	3	4	6	3	3	183
0147	3910.335	90	7	2	5	6	2	4	183
0147	3910.335	90	8	3	6	7	3	5	183
0147	3910.335	90	8	4	5	7	4	4	183
0149	3906.891	4	4	4	0	4	2	3	183
0152	3905.881	10	6	5	1	5	4	2	181
0152	3905.881	10	6	5	1	5	4	2	181
0153	3905.668	20	6	5	2	5	4	1	181
0155	3904.925	89	8	1	7	7	1	6	183
0157	3903.854	51	8	5	3	7	5	2	183
0158	3903.141	11	8	4	5	7	3	4	181
0159	3902.948	30	8	5	4	7	5	3	183
0160	3902.337	95	9	1	9	8	1	8	183
0163	3901.534	75	8	2	7	7	2	6	183
0167	3898.241	24	10	2	9	10	0	10	183
0168	3897.988	30	10	1	9	10	1	10	183
0169	3897.566	9	10	1	9	10	1	10	183

TABLE II (Continued)

Line No.	Wave number (vac. cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
0177	3892.854	47	8	6	2	7	6	1	183
0176	3893.587	12							
0178	3892.035	74	7	4	3	6	4	2	183
0180	3891.558	32	7	4	4	6	3	3	181
0182	3890.876	96	7	1	6	6	1	5	183
0182	3890.876	96	7	3	5	6	3	4	183
0183	3889.648	95	6	2	4	5	2	3	183
0184	3888.635	77	7	4	4	6	4	3	183
0185	3887.314	44	6	4	2	5	3	3	181
0186	3886.942	90	8	0	8	7	0	7	183
0187	3886.767	84	8	1	8	7	1	7	183
0189	3885.949	90	6	3	3	5	3	2	183
0191	3884.879	92	7	2	6	6	2	5	183
0193	3883.882	7	4	3	2	3	0	3	181
0194	3883.295	58	5	5	0	4	4	1	181
0195	3882.843	48	6	3	3	5	2	4	181
0195	3882.843	48	9	2	8	9	0	9	183
0196	3882.144	8	9	1	8	9	1	9	183
0197	3882.021	11	8	7	1	7	7	0	183
0200	3880.768	44	7	5	2	6	5	1	183
0201	3880.505	64	7	5	3	6	5	2	183
0207	3877.405	55	3	2	1	2	0	2	183
0208	3876.280	95	6	1	5	5	1	4	183
0209	3875.152	78	6	4	3	5	3	2	181
0211	3874.141	55							
0217	3871.192	90	7	0	7	6	0	6	183
0218	3870.825	94	7	1	7	6	1	6	183
0219	3870.606	47	7	6	2	6	6	1	183
0220	3870.133	94	6	3	4	5	3	3	183
0221	3869.535	7	6	4	3	6	2	4	183
0223	3867.406	80	6	4	2	5	4	1	183
0224	3867.213	19	8	2	7	8	0	8	183
0225	3866.678	85	6	2	5	5	2	4	183
0226	3866.217	67	6	4	3	5	4	2	183
0228	3865.852	88	5	2	3	4	2	2	183
0229	3865.622	44	8	1	7	8	1	8	183
0232	3863.477	5	10	2	8	10	2	9	183
0233	3863.332	43	5	2	3	4	1	4	181
0234	3863.005	60	5	4	1	4	3	2	181
0236	3862.277	67	5	4	2	4	3	1	181
0239	3859.619	88	5	1	4	4	1	3	183
0240	3859.226	16	7	4	4	7	2	5	183
0241	3857.827	74	6	5	1	5	5	0	183
0241	3857.827	74	6	5	2	5	5	1	183
0241	3857.827	74	6	5	2	5	5	1	183
0244	3855.296	110	6	0	6	5	0	5	183
0246	3854.434	130	6	1	6	5	1	5	183
0250	3851.627	105	5	2	4	4	2	3	183
0250	3851.627	105	7	2	6	7	0	7	183
0253	3849.222	10	9	4	6	9	2	7	183

TABLE II (Continued)

Line No.	Wave number (vac.cm^{-1})	% Abs.	J'	K'_{-1}	K'_{1}	J"	K''_{-1}	K''_{1}	Band
0255	3848.548	96	5	3	3	4	3	2	183
0256	3848.114	38	7	1	6	7	1	7	183
0257	3847.747	66	2	2	0	1	0	1	183
0261	3845.697	9	9	2	7	9	2	8	183
0264	3843.830	110	5	3	2	4	2	3	181
0265	3843.566	82	5	4	1	4	4	0	183
0266	3843.315	86	5	4	2	4	4	1	183
0269	3839.785	150	4	1	3	3	1	2	183
0269	3839.785	150	4	2	2	3	2	1	183
0270	3839.294	100	5	0	5	4	0	4	183
0271	3839.067	55	4	4	1	3	3	0	181
0273	3837.433	130	5	1	5	4	1	4	183
0274	3836.838	35	6	3	4	5	2	3	181
0276	3835.996	45	6	2	5	6	0	6	183
0278	3834.518	48	7	3	5	7	1	6	183
0280	3833.624	25	4	3	2	4	1	3	183
0284	3829.484	94	4	2	3	3	2	2	183
0285	3829.302	71	6	1	5	6	1	6	183
0288	3827.656	97	4	3	1	3	3	0	183
0291	3826.344	83	4	3	2	3	3	1	183
0292	3826.202	80	5	2	4	5	0	5	183
0293	3825.998	41	8	2	6	8	2	7	183
0295	3825.096	21	5	3	3	4	2	2	181
0298	3823.132	100	4	0	4	3	0	3	183
0300	3820.756	95	4	1	4	3	1	3	183
0305	3817.230	96	3	1	2	2	1	1	183
0306	3816.428	70	4	3	1	3	2	2	181
0308	3815.900	89	4	2	2	3	1	3	181
0311	3813.225	10	8	2	7	7	1	6	181
0312	3812.974	70	4	2	3	4	0	4	183
0313	3812.546	93	3	2	1	2	2	0	183
0315	3809.424	63	4	3	2	3	2	1	181
0316	3809.199	63	5	1	4	5	1	5	183
0318	3807.444	110	3	2	2	2	2	1	183
0320	3806.110	120	3	0	3	2	0	2	183
0321	3804.981	35	7	2	5	7	2	6	183
0322	3804.586	85	3	2	2	3	0	3	183
0323	3804.072	3							
0325	3801.513	150	3	1	3	2	1	2	183
0328	3800.146	49	2	2	1	2	0	2	183
0336	3793.532	5	9	3	6	9	3	7	183
0337	3792.616	140	2	1	1	1	1	0	183
0338	3791.315	78	3	3	0	2	2	1	181
0339	3791.198	21	6	2	5	5	1	4	181
0341	3789.890	46	3	3	1	2	2	0	181
0343	3789.253	12	7	7	0	7	6	1	181
0344	3788.902	92	4	1	3	4	1	4	183
0346	3788.461	7	3	3	0	3	0	3	181
0347	3788.057	13	9	1	8	9	0	9	181
0348	3786.934	140	2	0	2	1	0	1	183

TABLE II (Continued)

Line No.	Wave Number (vac.cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
0353	3784.351	81	6	2	4	6	2	5	183
0354	3781.990	97	2	1	2	1	1	1	183
0355	3781.634	15							
0356	3780.942	21	5	2	4	4	1	3	181
0361	3777.694	10	7	1	7	6	0	6	181
0362	3777.052	74	3	2	1	2	1	2	181
0362	3777.052	74	7	0	7	6	1	6	181
0363	3775.811	11	7	6	1	7	5	2	181
0364	3773.950	5	8	2	7	8	1	8	181
0365	3773.483	45	8	3	5	8	3	6	183
0366	3773.279	8	8	6	3	8	5	4	181
0369	3770.460	87	3	1	2	3	1	3	183
0371	3769.335	57	4	2	3	3	1	2	181
0372	3768.921	35	6	1	5	5	3	2	183
0374	3767.702	6							
0375	3767.048	11	6	1	5	5	2	4	181
0377	3766.141	77	5	2	3	5	2	4	183
0379	3765.082	94	1	0	1	0	0	0	183
0382	3762.489	53	6	1	6	5	0	5	181
0384	3762.016	4	10	4	6	10	4	7	183
0385	3761.332	21	5	5	1	5	4	2	181
0386	3761.088	42	5	5	0	5	4	1	181
0387	3760.884	20	6	0	6	5	1	5	181
0389	3759.418	45	6	5	2	6	4	3	181
0390	3759.045	52	7	2	6	7	1	7	181
0392	3758.271	17	6	5	1	6	4	2	181
0394	3757.373	12	7	5	3	7	4	4	181
0395	3756.996	47	7	3	4	7	3	5	183
0397	3755.670	110	2	1	1	2	1	2	183
0399	3755.167	43	3	2	2	2	1	1	181
0400	3754.723	16	7	1	6	7	0	7	181
0402	3753.666	33	7	5	2	7	4	3	181
0406	3751.904	100	4	2	2	4	2	3	183
0409	3750.360	10	8	3	6	8	2	7	181
0414	3748.668	5	4	0	4	3	2	1	183
0418	3746.285	95	6	3	3	6	3	4	183
0419	3746.066	22	5	0	5	4	2	2	183
0420	3745.547	103	1	1	0	1	1	1	183
0425	3743.815	55	5	0	5	4	1	4	181
0426	3742.560	95	3	2	1	3	2	2	183
0427	3742.397	80	5	4	2	5	3	3	181
0428	3742.086	90	4	4	1	4	3	2	181
0430	3741.301	77	3	0	3	2	2	0	183
0432	3740.615	64	4	4	0	4	3	1	181
0434	3740.019	13	6	2	4	5	3	3	181
0434	3740.019	13	7	3	5	7	2	6	181
0437	3738.000	160	2	2	0	2	2	1	183
0443	3736.553	76	5	4	1	5	3	2	181
0444	3736.385	18	6	1	5	6	0	6	181
0445	3735.847	15	R30 ($\nu_1 + \nu_3$) of CO_2						

TABLE II (Continued)

Line No.	Wave number (vac. cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
0446	3735.351	160	2	2	1	2	2	0	183
0447	3734.944	140	1	1	1	1	1	0	183
0449	3734.491	42							
0452	3733.474	5	8	2	6	8	1	7	181
0453	3732.867	73	4	1	4	3	0	3	181
0456	3731.903	25							
0457	3731.515	30	6	3	4	6	2	5	181
0458	3731.038	105	3	3	0	3	3	1	183
0459	3730.608	160	3	3	1	3	3	0	183
0459	3730.608	160	4	3	1	4	3	2	183
0460	3730.129	125	3	2	2	3	2	1	183
0461	3729.721	24	R20	($\nu_1 + \nu_3$)		of	CO_2		
0463	3729.309	44	6	4	2	6	3	3	181
0464	3728.425	18	R18	($\nu_1 + \nu_3$)		of	CO_2		
0465	3728.176	7	10	1	9	9	3	6	183
0466	3727.723		4	3	2	4	3	1	183
0468	3726.763	56	8	4	4	8	4	5	183
0471	3726.110	8	3	2	1	4	0	4	183
0473	3725.388	10	5	3	3	5	2	4	181
0474	3725.267	40	4	0	4	3	1	3	181
0479	3723.970	95	2	1	2	2	1	1	183
0481	3722.860	125	4	4	0	4	4	1	183
0482	3722.338	72	7	4	3	7	4	4	183
0483	3722.144	115	5	3	3	5	3	2	183
0485	3721.724	88	5	4	1	5	4	2	183
0486	3721.545	33	4	3	2	4	2	3	181
0487	3721.528	12							
0488	3721.169	100	5	4	2	5	4	1	183
0488	3721.169	100	6	4	2	6	4	3	183
0491	3719.756	94	4	2	3	4	2	2	183
0493	3719.329	46	7	4	3	7	3	4	181
0495	3718.572	88	3	1	3	2	0	2	181
0495	3718.572	88	6	4	3	6	4	2	183
0496	3718.384	60	4	2	3	4	1	4	181
0497	3717.815	125	0	0	0	1	0	1	183
0498	3717.251	14							
0499	3717.076	53	5	1	4	5	0	5	181
0502	3715.109	24	7	2	5	7	1	6	181
0503	3714.982	11	4	1	3	3	2	2	181
0506	3713.986	75	3	3	0	3	2	1	181
0506	3713.986	75	7	4	4	7	4	3	183
0507	3713.006	92	5	5	0	5	5	1	183
0510	3712.078	75	6	3	4	6	3	3	183
0512	3711.479	89	6	5	1	6	5	2	183
0513	3711.378	75	6	5	2	6	5	1	183
0517	3709.894	47	7	5	2	7	5	3	183
0518	3709.656	19							
0519	3709.400	96	7	5	3	7	5	2	183
0521	3709.093	16							
0523	3708.672	50	8	5	3	8	5	4	183

TABLE II (Continued)

Line No.	Wave number (vac.cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
0524	3708.395	37	3	2	2	3	1	3	181
0525	3708.263	10	9	5	4	9	5	5	183
0527	3707.693	99	3	1	3	3	1	2	183
0528	3706.741	27	4	3	1	4	2	2	181
0528	3706.741	27	8	5	4	8	5	3	183
0530	3705.716	26	8	4	5	8	4	4	183
0532	3705.077	96	5	2	4	5	2	3	183
0533	3704.639	82	3	0	3	2	1	2	181
0534	3703.271	81	2	1	2	1	0	1	181
0535	3702.684	21	9	5	5	9	5	4	183
0538	3701.457	87	6	6	0	6	6	1	183
0539	3700.905	58	2	2	1	2	1	2	181
0540	3699.782	6	P18 $(\nu_1 + \nu_3)$ of CO_2						
0541	3699.626	72	7	6	2	7	6	1	183
0542	3699.493	25	6	2	4	6	1	5	181
0544	3698.543	45	4	1	3	4	0	4	181
0545	3698.004	125	1	1	1	2	1	2	183
0546	3697.655	54	5	2	3	4	4	0	183
0547	3697.549	25	8	6	2	8	6	3	183
0548	3697.316	60	5	3	2	5	2	3	181
0549	3696.668	68	7	3	5	7	3	4	183
0551	3696.172	8	P22 $(\nu_1 + \nu_3)$ of CO_2						
0552	3695.772	39	6	3	3	6	2	4	181
0553	3695.169	115	1	0	1	2	0	2	183
0555	3694.266	53	7	3	4	7	2	5	181
0559	3692.230	19	9	4	6	9	4	5	183
0566	3688.812	77	5	2	3	5	1	4	181
0568	3687.534	110	1	1	0	2	1	1	183
0568	3687.534	110	4	1	4	4	1	3	183
0569	3686.429	33	2	2	0	2	1	1	181
0570	3686.334	34	8	7	1	8	7	2	183
0571	3686.090	25	3	1	2	2	2	1	181
0572	3685.534	48	1	1	1	0	0	0	181
0574	3684.046	14	9	7	3	9	7	2	183
0576	3683.203	85	3	1	2	3	0	3	181
0576	3683.203	85	3	2	1	3	1	2	181
0577	3681.676	35	2	0	2	1	1	1	181
0579	3680.826	14							
0581	3679.608	60	6	2	5	6	2	4	183
0584	3677.176	105	2	0	2	2	2	1	183
0584	3677.176	105	2	1	2	3	1	3	183
0588	3674.352	150	2	0	2	3	0	3	183
0589	3674.019	53	8	8	0	8	8	1	183
0590	3672.792	60	2	1	1	2	0	2	181
0591	3671.953	22	10	4	7	10	4	6	183
0592	3671.283	76	3	0	3	3	2	2	183
0598	3667.161	16							
0599	3667.023	78	1	1	0	1	0	1	181
0600	3665.326	88	2	2	1	3	2	2	183
0602	3662.917	83	5	1	5	5	1	4	183

TABLE II (Continued)

Line No.	Wave number (vac. cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
0603	3661.766	140	2	1	1	3	1	2	183
0605	3660.741	150	2	2	0	3	2	1	183
0607	3656.733	140	3	1	3	4	1	4	183
0609	3654.814	110	3	0	3	4	0	4	183
0609	3654.814	110	7	2	6	7	2	5	183
0613	3650.443	29	9	3	7	9	3	6	183
0620	3646.359	70	5	0	5	5	2	4	183
0621	3646.173	8	6	6	1	5	5	0	182
0628	3642.299	105	3	2	2	4	2	3	183
0630	3641.810	62	5	2	3	6	1	6	181
0632	3641.575	9							
0636	3639.015	12							
0637	3638.472	55	6	1	6	6	1	5	183
0639	3637.580	17							
0640	3637.188	130	3	1	2	4	1	3	183
0640	3637.188	130	4	1	4	5	1	5	183
0641	3635.418	140	4	0	4	5	0	5	183
0645	3633.587	95	3	3	1	4	3	2	183
0646	3633.442	76	4	1	3	4	3	2	183
0647	3632.873	99	3	2	1	4	2	2	183
0648	3632.420	94	3	3	0	4	3	1	183
0649	3632.271	80	3	2	1	4	1	4	181
0649	3632.271	80	4	2	2	5	1	5	181
0650	3631.028	88	1	0	1	1	1	0	181
0653	3630.576	8	R24 $(2\nu_2 + \nu_3)$ of CO_2						
0654	3630.311	47	1	0	1	2	2	0	183
0655	3629.918	35	3	1	2	3	3	1	183
0658	3629.269	80	6	1	5	6	3	4	183
0659	3628.872	81	6	0	6	6	2	5	183
0662	3627.920	24	8	2	7	8	2	6	183
0665	3625.182	4	R16 $(2\nu_2 + \nu_3)$ of CO_2						
0666	3623.631	67	2	0	2	2	1	1	181
0672	3620.717	52	4	4	0	5	3	3	181
0674	3620.031	99	4	2	3	5	2	4	183
0676	3619.342	43	7	1	6	7	3	5	183
0680	3615.945	120	5	1	5	6	1	6	183
0681	3615.661	110	5	0	5	6	0	6	183
0681	3615.661	110	4	4	1	5	3	2	181
0684	3614.852	33	5	5	0	6	4	3	181
0686	3614.404	160	4	1	3	5	1	4	183
0686	3614.404	160	7	1	7	7	1	6	183
0688	3613.707	8	5	5	1	6	4	2	181
0690	3612.940	70	0	0	0	1	1	1	181
0694	3610.703	77	3	0	3	3	1	2	181
0696	3609.441	40	7	0	7	7	2	6	183
0699	3608.771	83	3	1	2	3	2	1	181
0700	3607.940	53	2	1	1	2	2	0	181
0701	3607.830	85	4	3	2	5	3	3	183
0704	3606.457	4	2	2	1	3	1	2	181
0705	3606.088	9							

TABLE II (Continued)

Line No.	Wave number (vac.cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
0707	3605.381	100	4	2	2	5	2	3	183
0708	3604.905	44	8	1	7	8	3	6	183
0709	3604.249	98	4	3	1	5	3	2	183
0710	3603.131	6	P12 $(2\nu_2 + \nu_3)$ of CO_2						
0716	3601.700	6							
0717	3601.418	7	P14 $(2\nu_2 + \nu_3)$ of CO_2						
0719	3600.946	90	4	4	1	5	4	2	183
0720	3600.732	90	4	4	0	5	4	1	183
0722	3599.798	96	5	2	4	6	2	5	183
0726	3598.261	24	3	1	3	3	3	0	183
0728	3597.968	8	P18 $(2\nu_2 + \nu_3)$ of CO_2						
0730	3597.068	8							
0731	3596.905	82	5	4	1	6	3	4	181
0732	3596.416	10							
0734	3595.949	76	5	1	4	5	2	3	181
0735	3595.599	100	6	1	6	7	1	7	183
0735	3595.599	100	6	0	6	7	0	7	183
0737	3594.409	5	P22 $(2\nu_2 + \nu_3)$ of CO_2						
0738	3594.066	85	1	0	1	2	1	2	181
0739	3593.547	70	2	1	2	2	2	1	181
0740	3593.235	93	5	1	4	6	1	5	183
0741	3592.814	25	7	3	4	8	2	7	181
0742	3592.024	88	4	0	4	4	1	3	181
0742	3592.024	88	5	3	2	6	2	5	181
0743	3591.269	35	8	1	8	8	1	7	183
0743	3591.269	35	8	2	6	8	4	5	183
0744	3590.691	84	2	1	2	3	0	3	181
0745	3590.413	47	6	3	3	7	2	6	181
0746	3590.247	20	6	3	3	7	2	6	181
0747	3589.687	6	7	2	5	7	4	4	183
0753	3587.250	10	9	1	8	9	3	7	183
0759	3584.762	23	6	5	2	7	4	3	181
0760	3584.383	70	5	4	2	6	3	3	181
0762	3583.679	57	3	1	3	3	2	2	181
0764	3583.228	6	P34 $(2\nu_2 + \nu_3)$ of CO_2						
0766	3582.460	95	5	3	3	6	3	4	183
0767	3582.071	23	6	2	4	6	3	3	181
0769	3581.443	55	5	2	3	5	3	2	181
0773	3579.969	30	6	1	5	6	2	4	181
0775	3579.081	90	5	2	3	6	2	4	183
0776	3577.235	47	7	2	5	7	3	4	181
0777	3576.854	76	2	0	2	3	1	3	181
0778	3576.772	37	4	2	2	4	3	1	181
0779	3575.771	8	5	2	3	5	4	2	183
0780	3575.158	94	7	0	7	8	0	8	183
0780	3575.158	94	7	1	7	8	1	8	183
0781	3574.930	85	5	4	2	6	4	3	183
0783	3574.239	92	5	3	2	6	3	3	183
0783	3574.239	92	6	2	5	7	2	6	183
0784	3574.100	79	5	4	1	6	4	2	183

TABLE II (Continued)

Line No.	Wave number (vac.cm^{-1})	% Abs.	J'	K'_{-1}	K'_{1}	J"	K''_{-1}	K''_{1}	Band
0785	3573.807	60	3	2	1	3	3	0	181
0787	3572.953	93	6	1	5	7	1	6	183
0788	3570.574	74	4	1	4	4	2	3	181
0789	3569.292	59	5	0	5	5	1	4	181
0791	3568.570	26	9	1	9	9	1	8	183
0794	3567.921	78	3	2	2	3	1	3	181
0795	3567.500	8	10	1	9	10	3	8	183
0796	3567.398	10	9	0	9	9	2	8	183
0797	3567.238	67	3	1	3	4	0	4	181
0799	3566.568	88	5	5	0	6	5	1	183
0799	3566.568	88	5	5	1	6	5	2	183
0804	3565.572	15	8	2	6	8	3	5	181
0808	3562.928	58	4	2	3	4	3	2	181
0809	3562.715	16	7	5	2	8	4	5	181
0812	3561.586	48	3	0	3	4	2	2	183
0819	3559.753	85	3	0	3	4	1	4	181
0821	3558.062	33	7	1	6	7	2	5	181
0822	3557.918	77	6	3	4	7	3	5	183
0823	3557.293	85	1	1	0	2	2	1	181
0824	3557.155	62	7	4	3	8	3	6	181
0825	3555.546	23	5	1	5	5	3	2	183
0826	3555.148	28	5	2	4	5	3	3	181
0827	3554.398	94	6	2	4	7	2	5	183
0827	3554.398	94	8	0	8	9	0	9	183
0830	3553.412	90	7	2	6	8	2	7	183
0832	3552.818	13	7	5	3	8	4	4	181
0833	3552.595	80	7	1	6	8	1	7	183
0834	3552.341	52	2	1	1	3	3	0	183
0836	3552.099	88	6	3	3	7	3	4	183
0838	3550.749	61	1	1	1	2	2	0	181
0840	3549.023	13	7	3	4	7	4	3	181
0841	3548.876	65	6	4	3	7	4	4	183
0846	3546.500	84	6	4	2	7	4	3	183
0847	3545.552	45	10	0	10	10	2	9	183
0848	3545.174	89	4	1	4	5	0	5	181
0850	3544.922	32	6	0	6	6	1	5	181
0851	3544.795	35	6	3	3	6	4	2	181
0852	3544.190	55	6	2	5	6	3	4	181
0853	3543.870	58	4	2	3	5	1	4	181
0859	3541.625	69	4	0	4	5	1	5	181
0860	3541.329	72	6	4	3	7	3	4	181
0861	3540.484	48	6	5	2	7	5	3	183
0862	3540.323	70	6	5	1	7	5	2	183
0865	3538.524	12	4	3	1	4	4	0	181
0866	3538.281	4	5	3	3	6	2	4	181
0868	3537.958	63	2	1	1	3	2	2	181
0869	3537.664	40	5	3	2	5	4	1	181
0870	3537.579	33	4	3	2	4	4	1	181
0871	3536.648	12	2	1	2	3	3	1	183
0875	3536.088	42	6	1	6	6	2	5	181

TABLE II (Continued)

Line No.	Wave number (vac.cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
0877	3535.010	14	5	3	3	5	4	2	181
0878	3534.514	80	7	3	5	8	3	6	183
0879	3533.526	80	9	1	9	10	1	10	183
0880	3532.215	62	8	2	7	9	2	8	183
0881	3531.848	80	8	1	7	9	1	8	183
0882	3531.352	80	3	1	2	4	3	1	183
0882	3531.352	80	7	2	5	8	2	6	183
0883	3530.954	26	6	3	4	6	4	3	181
0885	3530.470	42	6	6	0	7	6	1	183
0886	3530.116	5	7	2	6	7	3	5	181
0889	3528.660	7	6	2	5	6	4	2	183
0897	3524.689	9	7	3	5	7	4	4	181
0900	3523.842	62	5	1	5	6	0	6	181
0902	3523.034	74	7	4	4	8	4	5	183
0904	3522.432	67	7	3	4	8	3	5	183
0905	3522.302	83	5	0	5	6	1	6	181
0906	3521.101	10							
0907	3520.943	79	3	1	2	4	2	3	181
0908	3520.663	25	7	0	7	7	1	6	181
0910	3517.813	49	7	4	3	8	4	4	183
0912	3517.309	17	8	5	4	9	4	5	181
0913	3516.601	6	9	5	4	10	4	7	181
0914	3516.215	77	2	1	2	3	2	1	181
0916	3515.947	11	7	1	7	7	2	6	181
0917	3515.661	6	8	3	6	8	4	5	181
0918	3514.578	32	5	2	4	6	1	5	181
0919	3514.286	60	4	0	4	5	2	3	183
0920	3514.213	59	7	5	3	8	5	4	183
0921	3513.681	34	7	5	2	8	5	3	183
0922	3513.251	13	8	2	7	8	3	6	181
0924	3512.389	67	10	0	10	11	0	11	183
0925	3512.028	49	8	3	6	9	3	7	183
0927	3510.848	69	9	2	8	10	2	9	183
0928	3510.698	47	9	1	8	10	1	9	183
0929	3509.707	79	8	2	6	9	2	7	183
0933	3508.602	7	5	4	1	5	5	0	181
0934	3507.678	4	7	4	3	7	5	2	181
0934	3507.678	4	6	4	2	6	5	1	181
0935	3507.009	64	4	1	3	5	3	2	183
0936	3505.605	54	4	1	3	5	2	4	181
0937	3504.852	5							
0939	3504.357	40	7	6	2	8	6	3	183
0941	3503.398	8							
0943	3503.198	16							
0944	3502.870	32	7	4	4	8	3	5	181
0945	3502.758	81	6	1	6	7	0	7	181
0948	3502.115	59	6	0	6	7	1	7	181
0950	3501.563	35	6	3	4	7	2	5	181
0952	3501.271	32	3	1	3	4	3	2	183
0954	3500.798	17	6	4	3	6	5	2	181

TABLE II (Continued)

Line No.	Wave number (vac.cm^{-1})	% Abs.	J'	K'_{-1}	K'_{1}	J"	K''_{-1}	K''_{1}	Band
0955	3500.245	6							
0957	3499.112	56	2	2	0	3	3	1	181
0957	3499.112	56	5	3	2	5	5	1	183
0958	3497.581	81	2	2	1	3	3	0	181
0958	3497.581	81	8	4	5	9	4	6	183
0959	3496.991	3	8	4	5	9	4	6	183
0959	3496.991	3	8	0	8	8	1	7	181
0960	3496.617	25	8	4	5	8	5	4	181
0961	3495.595	8	6	4	2	5	3	3	182
0962	3495.377	60	8	3	5	9	3	6	183
0964	3494.612	9	8	1	8	8	2	7	181
0965	3494.133	7	5	3	3	5	5	0	183
0966	3492.710	7	7	7	1	8	7	2	183
0967	3491.013	42	11	1	11	12	1	12	183
0968	3490.654	62	5	1	4	6	2	5	181
0969	3489.933	47	9	3	7	10	3	8	183
0970	3489.315	17	10	2	9	11	2	10	183
0971	3489.238	32	10	1	9	11	1	10	183
0972	3488.578	22	9	2	7	10	2	8	183
0974	3488.192	43	8	4	4	9	4	5	183
0976	3487.902	50	6	2	5	7	1	6	181
0976	3487.902	50	8	5	4	9	5	5	183
0977	3486.442	32	8	5	3	9	5	4	183
0982	3481.608	35	7	1	7	8	0	8	181
0983	3481.343	57	7	0	7	8	1	8	181
0988	3478.027	11	8	6	2	9	6	3	183
0989	3476.740	71	3	2	1	4	3	2	181
0990	3475.803	16	5	1	4	6	3	3	183
0992	3474.613	27	6	1	5	7	2	6	181
0993	3474.005	25	3	1	3	4	2	2	181
0994	3473.658	4	9	0	9	9	1	8	181
0995	3473.346	4	10	2	9	10	3	8	181
0996	3472.961	22	9	4	6	10	4	7	183
0997	3470.353	23	9	3	6	10	3	7	183
0999	3469.436	23	12	1	12	13	1	13	183
1000	3469.254	48	3	2	2	4	3	1	181
1001	3468.440	7	5	4	2	4	3	1	182
1002	3467.928	8	10	3	8	11	3	9	183
1003	3467.544	22	11	2	10	12	2	11	183
1004	3467.288	20	10	2	8	11	2	9	183
1007	3466.612	5	8	7	1	9	7	2	183
1008	3464.660	4	3	2	1	4	4	0	183
1009	3463.383	14	7	2	6	8	1	7	181
1010	3462.806	11	8	4	5	9	3	6	181
1012	3461.755	13	4	1	4	5	3	3	183
1012	3461.755	13	9	5	5	10	5	6	183
1015	3460.276	44	8	1	8	9	0	9	181
1016	3460.187	17	8	0	8	9	1	9	181
1017	3459.271	9	5	0	5	6	2	4	183
1018	3458.527	6	9	5	4	10	5	5	183

TABLE II (Continued)

Line No.	Wave number (vac. cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
1019	3458.261	5	3	2	2	4	4	1	183
1020	3457.809	5	9	4	5	10	2	8	183
1021	3456.879	37	4	2	2	5	3	3	181
1022	3456.599	35	7	1	6	8	2	7	181
1023	3451.800	7	9	6	4	10	6	3	183
1024	3449.069	4	10	4	7	11	4	8	183
1026	3447.684	5	13	1	13	14	1	14	183
1029	3446.935	30	10	3	7	11	3	8	183
1030	3445.817	10	11	3	9	12	3	10	183
1031	3445.737	16	4	2	2	5	4	1	183
1032	3445.599	14	12	1	11	13	1	12	183
1034	3444.887	28	4	4	1	3	3	0	182
1037	3442.141	70	3	3	0	4	4	1	181
1038	3441.996	48	3	3	1	4	4	0	181
1039	3441.781	48	5	2	3	6	3	4	181
1040	3440.188	23	8	2	7	9	1	8	181
1041	3438.654	31	9	0	9	10	1	10	181
1042	3436.933	11	8	1	7	9	2	8	181
1043	3436.488	60	4	2	3	5	3	2	181
1044	3435.089	25	6	1	5	7	3	4	183
1045	3434.061	7	8	3	6	9	2	7	181
1047	3432.658	3							
1049	3429.798	4							
1050	3428.124	5	5	2	3	6	4	2	183
1051	3427.911	17	6	2	4	7	3	5	181
1052	3426.205	4							
1053	3424.048	34	4	1	4	5	2	3	181
1060	3417.562	5	9	2	8	10	1	9	181
1061	3416.824	22	10	1	10	11	0	11	181
1062	3416.657	41	4	3	1	5	4	2	181
1063	3416.019	15	9	1	8	10	2	9	181
1064	3415.894	22	5	1	5	6	3	4	183
1065	3415.430	61	4	3	2	5	4	1	181
1066	3415.095	21	7	2	5	8	3	6	181
1067	3409.095	11	6	2	4	7	4	3	183
1068	3407.326	20	5	3	2	4	2	3	182
1069	3404.293	6	3	0	3	4	3	2	181
1070	3402.612	12	6	3	4	5	2	3	182
1071	3401.699	3	8	2	6	9	3	7	181
1072	3399.190	3	5	2	4	6	4	3	183
1073	3398.866	12	6	0	6	7	2	5	183
1075	3397.116	17	5	2	4	6	3	3	181
1076	3395.099	4	10	2	9	11	1	10	181
1077	3394.619	9	11	0	11	12	1	12	181
1081	3391.429	50	5	3	2	6	4	3	181
1082	3388.627	5	5	2	3	4	1	4	182
1083	3388.071	5	5	3	3	4	2	2	182
1084	3387.680	50	4	4	1	5	5	0	181
1085	3387.599	17	4	4	0	5	5	1	181
1086	3387.362	25	5	3	3	6	4	2	181

TABLE II (Continued)

Line No.	Wave number (vac.cm^{-1})	% Abs.	J'	K'_{-1}	K'_{1}	J"	K''_{-1}	K''_{1}	Band
1087	3386.326	3	9	2	7	10	3	8	181
1089	3384.771	4	7	1	6	8	3	5	183
1091	3377.212	13	4	3	1	3	2	2	182
1092	3376.271	25	4	3	1	5	5	0	183
1093	3375.098	8	6	3	3	7	4	4	181
1094	3374.715	10	4	3	2	5	5	1	183
1095	3370.257	30	4	3	2	3	2	1	182
1097	3367.430	7	5	1	5	6	2	4	181
1100	3362.856	11	5	4	2	6	5	1	181
1101	3362.196	35	5	4	1	6	5	2	181
1103	3358.925	5	6	2	5	7	4	4	183
1104	3358.068	15	7	3	4	8	4	5	181
1106	3356.265	33	6	3	4	7	4	3	181
1108	3353.421	7							
1109	3352.677	17	5	3	2	6	5	1	183
1109	3352.677	17	8	2	6	9	4	5	183
1110	3350.489	45	3	3	0	2	2	1	182
1111	3350.224	5	6	4	3	6	3	4	182
1112	3350.029	21	6	2	5	7	3	4	181
1113	3349.045	20	3	3	1	2	2	0	182
1114	3347.890	7	4	4	1	4	3	2	182
1115	3347.746	26	5	3	3	6	5	2	183

TABLE III

IMPURITY LINES DUE TO THE ν_1 AND ν_3 BANDS OF $H_2{}^{17}O$

(In the last column 171 refers to ν_1 and 173 refers to ν_3)

Line No.	Wave number (vac. cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
0096	3942.407	8	9	2	7	8	2	6	173
0100	3940.169	4	10	1	9	9	1	8	173
0101	3939.500	5	11	1	11	10	1	10	173
0107	3934.609	11	8	2	6	7	2	5	173
0124	3924.627	11	10	0	10	9	0	9	173
0145	3912.042	10	8	1	7	7	1	6	173
0148	3909.371	12	9	1	9	8	1	8	173
0170	3897.216	10	7	3	5	6	3	4	173
0171	3896.478	27	6	2	4	5	2	3	173
0174	3893.941	24	8	0	8	7	0	7	173
0175	3893.772	10	8	1	8	7	1	7	173
0179	3891.730	25	7	2	6	6	2	5	173
0205	3878.191	14	7	0	7	6	0	6	173
0206	3877.802	33	7	1	7	6	1	6	173
0214	3873.217	11	6	2	5	5	2	4	173
0215	3872.593	15	5	2	3	4	2	2	173
0238	3861.377	19	6	1	6	5	1	5	173
0245	3854.827	47	5	3	3	4	3	2	173
0258	3846.707	56	4	1	3	4	2	2	173
0259	3846.413	49	4	2	2	3	2	1	173
0260	3846.241	31	5	0	5	4	0	4	173
0263	3844.327	56	5	1	5	4	1	4	173
0275	3836.154	23	4	2	3	3	2	2	173
0279	3834.016	25	4	3	1	3	3	0	173
0281	3832.764	4	5	2	4	5	0	5	173
0281	3832.764	4	4	3	2	3	3	1	173
0283	3830.054	58	4	0	4	3	0	3	173
0289	3827.377	37	4	1	4	3	1	3	173
0297	3824.021	34	3	1	2	2	1	1	173
0302	3819.222	16	3	2	1	2	2	0	173
0310	3814.166	38	3	2	2	2	2	1	173
0312	3812.974	70	3	0	3	2	0	2	173
0314	3811.787	10	3	2	2	3	0	3	173
0317	3808.401	58	3	1	3	2	1	2	173
0330	3799.389	50	2	1	1	1	1	0	173
0334	3795.516	14	4	1	3	4	1	4	173
0335	3793.743	55	2	0	2	1	0	1	173
0340	3790.663	4	6	2	4	6	2	5	173
0345	3788.756	33	2	1	2	1	1	1	173
0367	3771.845	24	1	0	1	0	0	0	173
0383	3762.345	35	2	1	1	2	1	2	173
0391	3758.413	22	4	2	2	4	2	3	173
0415	3747.606	5	5	4	2	5	3	3	171
0417	3746.915	7	4	4	1	4	3	2	171
0428	3742.086	90	2	2	1	2	2	0	173
0429	3741.717	56	1	1	1	1	1	0	173
0438	3737.652	55	3	3	0	3	3	1	173
0439	3737.180	55	3	3	1	3	3	0	173
0440	3736.979	38	4	3	1	4	3	2	173
0441	3736.884	68	3	2	2	3	2	1	173

TABLE III (Continued)

Line No.	Wave number (vac.cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
0451	3734.173	43	4	3	2	4	3	1	173
0462	3729.405	42	4	4	0	4	4	1	173
0467	3727.513	15	5	4	2	5	4	1	173
0477	3724.544	47	0	0	0	1	0	1	173
0489	3720.454	7	7	4	4	7	4	3	173
0492	3719.414	27	5	5	1	5	5	0	173
0505	3714.524	20	3	1	3	3	1	2	173
0526	3708.002	11	3	0	3	2	1	2	171
0555	3694.266	53	1	1	0	2	1	1	173
0575	3683.816	30	2	1	2	3	1	3	173
0578	3680.978	60	2	0	2	3	0	3	173
0591	3671.953	22	2	2	1	3	2	2	173
0596	3668.478	59	2	1	1	3	1	2	173
0597	3667.406	40	2	2	0	3	2	1	173
0601	3663.319	55	3	1	3	4	1	4	173
0604	3661.385	50	3	0	3	4	0	4	173
0615	3648.890	55	3	2	2	4	2	3	173
0624	3643.876	26	3	1	2	4	1	3	173
0625	3643.388	33	4	1	4	5	1	5	173
0629	3641.942	65	4	0	4	5	0	5	173
0633	3640.148	26	3	3	1	4	3	2	173
0635	3639.581	24	3	2	1	4	2	2	173
0643	3634.315	8	1	0	1	1	1	0	171
0663	3626.520	20	4	2	3	5	2	4	173
0668	3622.387	47	5	1	5	6	1	6	173
0669	3622.147	21	5	0	5	6	0	6	173
0671	3620.949	50	4	1	3	5	1	4	173
0673	3620.538	5	4	4	1	5	3	2	171
0687	3614.150	41	4	3	2	5	3	3	173
0692	3612.061	51	4	2	2	5	2	3	173
0693	3611.801	5	3	1	2	3	2	1	171
0695	3610.599	31	4	3	1	5	3	2	173
0706	3605.653	43	5	2	4	6	2	5	173
0714	3602.091	14	6	1	6	7	1	7	173
0715	3601.984	36	6	0	6	7	0	7	173
0729	3597.296	5	1	0	1	2	1	2	171
0757	3585.713	10	5	2	3	6	2	4	173
0768	3581.548	30	7	1	7	8	1	8	173
0770	3581.337	14	5	4	2	6	4	3	173
0771	3580.311	7	6	2	5	7	2	6	173
0815	3560.902	16	6	2	4	7	2	5	173
0816	3560.775	17	8	0	8	9	0	9	173
0817	3560.250	10	1	1	0	2	2	1	171
0820	3558.384	10	6	3	3	7	3	4	173
0831	3552.902	8	6	4	2	7	4	3	173
0842	3548.480	12	4	1	4	5	0	5	171
0861	3540.484	48	7	3	5	8	3	6	173
0864	3539.788	7	9	1	9	10	1	10	173
0867	3538.130	7	8	1	7	9	1	8	173
0887	3529.229	6	7	4	4	8	4	5	173

TABLE III (Continued)

Line No.	Wave number (vac.cm^{-1})	% Abs.	J'	K'_{-1}	K'_1	J"	K''_{-1}	K''_1	Band
0895	3525.469	8	5	0	5	6	1	6	171
0915	3516.008	8	8	2	6	9	2	7	173
1035	3444.538	4	3	3	0	4	4	1	171