

The Second Decade of H₂¹⁸O: Line Positions and Energy Levels

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Spectra of ¹⁸O-enriched water vapor have been recorded between 11 300 and 13 600 cm⁻¹ by means of Fourier-transform spectroscopy. The analysis has led to the determination for the first time of accurate values of the rotational energy levels of the interacting vibrational states (131), (211), (013), (230), (112), and (310) which belong to the second decade of H₂¹⁸O. © 1995 Academic Press, Inc.

I. INTRODUCTION

The purpose of the work is, besides atmospheric applications, the understanding of highly excited vibrational states of a light asymmetric top molecule. The H₂¹⁸O absorption has been recently investigated between 5900 and 8800 cm⁻¹ (1), covering the 2ν + δ spectral region and between 9500 and 11 500 cm⁻¹ (2), covering the 3ν spectral region, where ν is a quantum of the stretching vibration and δ is a quantum of the bending vibration. We present here a study of the 3ν + δ region between 11 300 and 13 600 cm⁻¹ which corresponds, to our knowledge, to the highest studied excited vibrational states of H₂¹⁸O.

The analysis of the spectrum has allowed us to determine accurate rotational energy levels for the six highly excited states (see Table I) (131), (211), (013), (230), (112), and (310) which belong to the second decade of interacting states of H₂¹⁸O.

II. EXPERIMENTAL DETAILS

The experimental details and data reduction have previously been discussed (2, 3), so only the details relevant to the present study are given. The spectrum was recorded at the National Solar Observatory (Kitt Peak, AZ) using the McMath Fourier transform spectrometer. The unapodized resolution was 0.012 cm⁻¹. The water vapor was contained in a 6-m-long White-type cell allowing an absorption path length of 434 m. The sample used contained ¹⁸O water at 73% concentration and also HDO and ¹⁷O isotopic variants as impurities but with contents less than 1.5%. The rest of the gas was H₂¹⁶O. A natural water vapor spectrum was also recorded in order to assign easily the lines of the H₂¹⁶O isotopic species. The uncertainty in the line positions is estimated to be typically 10⁻³ cm⁻¹, varying from 0.1 × 10⁻³ cm⁻¹ for strong and well-isolated lines to 5 × 10⁻³ cm⁻¹ for the weakest ones. In the 11 300 to 12 700 cm⁻¹ spectral range, 1445 lines were found with peak absorptions ranging from 0.007 to 0.975. Among them a comparison with natural water spectrum shows that about 450 lines belong to H₂¹⁶O.

TABLE I
Observed Absorption Bands of $H_2^{18}O$ in the $0.8 \mu m$ Region

VIB	N	INT	Spectral range cm^{-1}	Imin	Imax
131	110	0.00377	11600.0	12325.9	0.69
211	277	0.11510	11778.8	12633.4	0.69
013	131	0.00752	12293.4	12695.5	0.80
230	19	0.00022	11618.2	11865.6	0.69
310	100	0.00757	11796.9	12395.5	0.80
112	128	0.00414	12119.2	12633.9	0.80

Note. VIB, vibrational assignment of the upper state; N, number of assigned lines; INT, sum of the intensities of the individual assigned lines in $\text{cm}^{-2} \cdot \text{atm}^{-1}$; and I min and I max, minimum and maximum observed line intensities in $10^{-5} \text{ cm}^{-2} \cdot \text{atm}^{-1}$.

III. ANALYSIS AND RESULTS

Twelve resonating vibrational states are involved in the studied spectral region: 10 states form the so-called second decade of the water molecule which includes the interacting states {(070), (051), (150), (230), (131), (032), (310), (211), (112), (013)}, and 2 vibrational states (080) and (160) which belong to the first pentadecade. During the study, the levels of 6 vibrational states have been observed; the $7\nu_2$, $5\nu_2 + \nu_3$, $\nu_1 + 5\nu_2$, $3\nu_2 + 2\nu_3$, $8\nu_2$, and $\nu_1 + 6\nu_2$ bands were so weak that they could not be observed.

A special approach was used for the identification of the other weak bands because it is difficult to find two or more lines sharing the same upper level. There is then no confirmation of assignments by the observation of combination differences. The line assignment process was performed in parallel with the fitting of the rotational constants to obtain better predicted line positions and relative strengths. Such a procedure indeed often permits the identification of weak lines which cannot be assigned by the usual combination difference methods.

The positions and assignments of the observed lines are listed in Table II and from these lines, the energy levels reported in Table III together with their uncertainties were derived. It is worth noting that for the very weak $2\nu_1 + 3\nu_2$ band only 10 levels were determined (3 are determined from only one line each).

The $H_2^{18}O$ spectrum in this region is complicated by numerous resonances. In total, 23 resonance terms are needed to explain the spectrum. The following comments can be made:

A. Strong perturbations of line positions and intensities were observed for the $2\nu_1 + \nu_2 + \nu_3$ band which is the strongest band in this region:

1. There is a strong Coriolis resonance coupling the levels of the (211) and (310) states which appears for small rotational quantum numbers ($J = 2$) and the mixing coefficients reach 20–35%. Typical examples are the interaction of the (211) [826] level at $13\ 066.4103 \text{ cm}^{-1}$ with the (310) [818] level at $13\ 071.9954 \text{ cm}^{-1}$ (the mixing coefficients are 69 and 23%, respectively) and the interaction of (211) [716] at $12\ 794.1485 \text{ cm}^{-1}$ with (310) [726] at $12\ 788.3330 \text{ cm}^{-1}$ (the mixing coefficients are 82 and 11%).

2. There is a strong Fermi resonance coupling the levels of the (131) state with those of (211) beginning at small rotational quantum numbers. For example, the

TABLE II

List of the Experimental Absorption Lines of H₂¹⁸O between 11 300 and 13 600 cm⁻¹

Sigma, cm ⁻¹	Depth, %	VIB	J'	K' _a	K' _c	J''K'a''Kc''	Sigma, cm ⁻¹	Depth, %	VIB	J'	K' _a	K' _c	J''K'a''Kc''		
11305.0772	0.0080						11797.9151	0.0110	131	1	0	1	0	0	0
11315.9097	0.0220						11799.8058	0.0250	131	2	1	1	2	1	2
11318.3153	0.0100						11802.3127	0.0360	131	3	2	2	3	2	1
11319.4771	0.0100						11808.6443	0.0240	131	2	2	1	2	2	0
11328.8793	0.0070						11809.0009	0.0100	230	4	0	4	3	1	3
11337.8504	0.0060						11810.8977	0.0220	211	11	0	11	12	0	12
11338.1359	0.0070						11810.8977	0.0220	211	11	1	11	12	1	12
11347.0760	0.0150						11810.9460	0.0100							
11373.8592	0.0100						11811.0757	0.0740	131	2	2	0	2	2	1
11383.5537	0.0060						11813.6995	0.0130	131	3	2	1	3	2	2
11404.8532	0.0070						11819.3890	0.0530	131	2	0	2	1	0	1
11573.0549	0.0070						11820.7483	0.0060	211	10	2	8	11	2	9
11584.4905	0.0080						11820.9913	0.0170	131	4	2	2	4	2	3
11600.0769	0.0140	131	7	1	7	8 1 8	11821.9796	0.0090	230	4	1	4	3	0	3
11604.4331	0.0100						11823.5152	0.0140	131	2	1	2	1	1	1
11608.1455	0.0060						11827.5339	0.0070							
11618.2302	0.0070	230	3	1	2	4 2 3	11828.6583	0.0060	131	6	3	4	6	3	3
11623.0648	0.0110	131	6	2	4	7 2 5	11828.6583	0.0060	230	2	2	1	2	1	2
11623.4289	0.0200	131	6	0	6	7 0 7	11836.7724	0.0400	131	2	1	1	1	1	0
11625.0259	0.0090						11838.4075	0.0240	131	3	0	3	2	0	2
11625.0547	0.0080						11839.5570	0.0180	131	5	3	3	5	3	2
11625.2751	0.0090	131	6	1	6	7 1 7	11840.8967	0.0610	131	3	1	3	2	1	2
11625.3499	0.0070	230	2	2	1	3 3 0	11841.8343	0.0420	211	10	0	10	11	0	11
11625.3499	0.0070	230	4	0	4	5 1 5	11842.0037	0.0100	211	9	4	6	10	4	7
11626.2035	0.0140	131	6	1	5	7 1 6	11842.7351	0.0080	211	5	1	4	6	3	3
11634.2714	0.0130	230	4	1	4	5 0 5	11844.7597	0.0100	230	4	2	3	4	1	4
11643.5842	0.0150	131	5	1	4	6 1 5	11845.9788	0.0150	131	4	3	2	4	3	1
11643.5842	0.0150	230	3	0	3	4 1 4	11847.7673	0.0210	211	9	3	7	10	3	8
11646.2456	0.0110	131	5	0	5	6 0 6	11848.0745	0.0080							
11649.5563	0.0270	131	5	1	5	6 1 6	11848.2814	0.0440	131	4	3	1	4	3	2
11656.6193	0.0080	131	6	3	3	7 3 4	11849.3699	0.0640	131	3	3	1	3	3	0
11660.0746	0.0240	131	4	1	3	5 1 4	11849.7155	0.0320	131	3	3	0	3	3	1
11660.9118	0.0080	230	2	0	2	3 1 3	11850.7911	0.0100	131	6	3	3	6	3	4
11661.1937	0.0090						11855.0457	0.0610	131	4	0	4	3	0	3
11667.3359	0.0380	131	4	0	4	5 0 5	11855.4580	0.0320	211	8	3	5	9	3	6
11667.9130	0.0210	131	5	2	4	6 2 5	11856.7365	0.0230	131	4	1	4	3	1	3
11670.2319	0.0120	230	4	2	3	5 1 4	11859.7104	0.0100							
11673.0857	0.0150	131	4	1	4	5 1 5	11859.8454	0.0380	211	9	2	8	10	2	9
11674.1875	0.0070						11860.2554	0.0150	211	9	1	8	10	1	9
11674.4511	0.0210	131	4	2	2	5 2 3	11861.8585	0.0250	131	3	1	2	2	1	1
11678.5521	0.0110	230	1	0	1	2 1 2	11862.0432	0.0210	211	8	4	4	9	4	5
11681.8472	0.0150	131	3	1	2	4 1 3	11862.6916	0.0140							
11684.7381	0.0120	230	2	1	2	3 0 3	11865.6288	0.0100	230	2	2	1	1	1	0
11687.0973	0.0190	131	3	0	3	4 0 4	11868.2114	0.0460	211	8	2	6	9	2	7
11690.8395	0.0110	131	4	2	3	5 2 4	11869.8573	0.0230	131	5	0	5	4	0	4
11694.5252	0.0090	230	3	0	3	3 1 2	11871.0739	0.0560	131	5	1	5	4	1	4
11696.0577	0.0480	131	3	1	3	4 1 4	11871.3534	0.0340	211	9	0	9	10	0	10
11696.9879	0.0090						11872.0943	0.0940	211	9	1	9	10	1	10
11679.8735	0.0090						11872.8190	0.0110	211	3	1	3	4	3	2
11699.9032	0.0180	131	5	3	3	6 3 4	11874.1773	0.0110	211	8	5	3	9	5	4
11703.9917	0.0140	131	3	2	1	4 2 2	11876.5176	0.0200	211	8	3	6	9	3	7
11704.3003	0.0070						11877.1335	0.0120							
11705.9112	0.0430	131	2	1	1	3 1 2	11877.3296	0.0230	211	4	1	3	5	3	2
11706.8079	0.0510	131	2	0	2	3 0 3	11879.6346	0.0410	131	3	2	2	2	2	1
11714.4896	0.0350	131	3	2	2	4 2 3	11882.4204	0.0190	211	4	0	4	5	2	3
11715.5156	0.0100	230	1	0	1	1 1 0	11885.1605	0.0450	131	6	0	6	5	0	5
11718.6960	0.0180	131	2	1	2	3 1 3	11885.4695	0.0070	310	8	3	6	9	2	7
11721.8438	0.0190	131	4	3	1	5 3 2	11883.6731	0.0150	131	3	2	1	2	2	0
11726.0844	0.0080	131	4	3	2	5 3 3	11884.0443	0.0170	131	6	1	6	5	1	5
11727.9864	0.0180	131	1	0	1	2 0 2	11885.5534	0.0620	131	4	1	3	3	1	2
11731.4684	0.0140	131	1	1	0	2 1 1	11885.7659	0.0100							
11733.7526	0.0270	131	2	2	0	3 2 1	11887.0661	0.0880	211	8	1	7	9	1	8
11734.3584	0.0180						11887.3601	0.0340	211	8	2	7	9	2	8
11738.6726	0.0110	131	2	2	1	3 2 2	11887.5539	0.0080							
11741.0742	0.0370	131	1	1	1	2 1 2	11887.7099	0.0320	211	7	3	4	8	3	5
11747.0027	0.0110	131	3	1	3	3 1 2	11889.7462	0.0110	131	6	4	3	6	4	2
11749.1292	0.0110	131	5	4	2	6 4 3	11891.7999	0.0200							
11750.9536	0.0290	131	0	0	0	1 0 1	11892.6706	0.0200	131	6	4	2	6	4	3
11751.1110	0.0080	131	3	3	0	4 3 1	11894.1355	0.0420	211	7	2	5	8	2	6
11752.3836	0.0200	131	3	3	1	4 3 2	11895.0376	0.0140	131	7	0	7	6	0	6
11763.5348	0.0110	230	1	1	0	1 0 1	11895.3682	0.0370	131	5	4	2	5	4	1
11765.4722	0.0070	131	2	1	2	2 1 1	11895.7291	0.0330	131	7	1	7	6	1	6
11766.3722	0.0080						11895.8382	0.0140	131	5	4	1	5	4	2
11772.9133	0.0100						11896.4258	0.0070							
11773.2080	0.0080	131	5	2	4	5 2 3	11897.3596	0.0180	211	7	4	3	8	4	4
11776.4198	0.0120	131	4	4	0	5 4 1	11898.5176	0.0260	131	4	4	1	4	4	0
11778.0393	0.0420	131	1	1	1	1 1 0	11898.5692	0.0730	131	4	4	0	4	4	1
11778.8133	0.0060	211	12	0	12	13 0 13	11900.2695	0.0780	211	8	1	8	9	1	9
11778.8133	0.0060	211	12	1	12	13 1 13	11901.3276	0.1850	211	8	0	8	9	0	9
11780.5090	0.0150	131	6	5	1	7 5 2	11903.0180	0.0520	211	7	4	4	8	4	5
11780.5090	0.0150	230	3	1	2	3 0 3	11904.8769	0.1060	211	7	3	5	8	3	6
11789.5101	0.0140	131	1	1	0	1 1 1	11906.4198	0.0120							
11796.9948	0.0070	310	6	2	5	7 3 4	11906.8250	0.0100	211	7	5	2	8	5	3
11797.3197	0.0090	23													

TABLE II—Continued

<i>Sigma, cm⁻¹</i>	<i>Depth, km</i>	<i>VIB</i>	<i>J'</i>	<i>Ka'</i>	<i>Kc'</i>	<i>J''Ka''Kc''</i>	<i>Sigma, cm⁻¹</i>	<i>Depth, km</i>	<i>VIB</i>	<i>J'</i>	<i>Ka'</i>	<i>Kc'</i>	<i>J''Ka''Kc''</i>
11907.4852	0.0250	211	7	5	3	8 5 4	11986.6404	0.4040	211	4	3	1	5 3 2
11908.7302	0.0100						11987.2914	0.0140	310	6	3	4	6 4 3
11908.8133	0.0530	131	4	2	2	3 2 1	11988.0256	0.0610	211	6	0	6	6 2 5
11909.4783	0.0180	131	7	3	5	8 1 8	11990.2385	0.1640	211	4	3	2	5 3 3
11909.7126	0.0100						11990.4411	0.0260	131	6	3	3	5 3 2
11913.8218	0.1750	211	7	2	6	8 2 7	11991.1514	0.0110	310	6	2	5	6 3 4
11914.6539	0.0480	211	7	1	6	8 1 7	11992.2265	0.0090	310	4	0	4	5 1 5
11917.2342	0.0100	211	7	6	2	8 6 3	11992.5938	0.1640	211	4	4	0	5 4 1
11917.6775	0.0080						11992.8068	0.0650	211	4	4	1	5 4 2
11919.2612	0.0110						11993.3372	0.2940	211	4	2	3	5 2 4
11919.7465	0.0470	131	5	2	4	4 2 3	11995.8419	0.0910	310	4	1	4	5 0 5
11920.8491	0.1750	211	6	3	3	7 3 4	11996.1852	0.0080					
11921.0892	0.2440	211	6	2	4	7 2 5	11996.5025	0.0370	211	6	1	5	6 3 4
11923.7156	0.0070						11997.7226	0.0240	211	6	1	6	6 1 5
11927.2392	0.0120	211	2	1	1	3 3 0	11998.7718	0.0070					
11928.8567	0.0160						11999.6696	0.0120	310	5	3	2	5 4 1
11928.4097	0.1340	211	7	0	7	8 0 8	12000.1092	0.0160	310	4	3	2	4 4 1
11928.7716	0.3420	211	7	1	7	8 1 8	12000.4430	0.0320	310	4	2	3	5 1 4
11929.5358	0.0330	131	6	1	5	5 1 4	12000.6592	0.0090					
11929.7455	0.0140	131	7	4	4	8 2 7	12000.8109	0.0100					
11930.9920	0.0970	211	6	4	2	7 4 3	12001.5085	0.0080					
11932.8207	0.0150	211	3	0	3	4 2 2	12002.5274	0.0080					
11933.4557	0.0680	211	6	3	4	7 3 5	12002.9146	0.0100					
11933.5271	0.0340	211	6	4	3	7 4 4	12003.5324	0.8350	211	4	0	4	5 0 5
11933.5271	0.0340	131	5	2	3	4 2 2	12003.7345	0.0200					
11933.6821	0.0160						12003.7644	0.0240	211	4	1	3	4 3 2
11934.8501	0.1940	310	6	2	5	7 1 6	12004.6449	0.4620	211	4	1	4	5 1 5
11935.3371	0.0350	131	6	4	3	7 2 6	12006.6378	0.0190					
11935.6747	0.0120	211	8	0	8	8 2 7	12008.2656	0.0070	211	9	3	7	9 3 6
11938.0567	0.0390	131	6	2	5	5 2 4	12008.6972	0.0080	310	1	1	1	2 2 0
11938.0567	0.0390	211	6	5	1	7 5 2	12009.2626	0.0130	310	5	2	4	5 3 3
11938.2497	0.0180	211	6	5	2	7 5 3	12009.5330	0.0070					
11938.4926	0.0090						12009.6528	0.3660	211	3	2	1	4 2 2
11940.1911	0.1900	211	6	1	5	7 1 6	12010.1436	0.4440	211	3	1	2	4 1 3
11940.5541	0.0090						12010.4539	0.0350	211	5	0	5	5 2 4
11942.9907	0.1020	211	6	2	5	7 2 6	12012.2325	0.0070	131	7	3	4	6 3 3
11944.2111	0.0120	310	6	0	6	7 1 7	12013.2128	0.0120	310	3	0	3	4 1 4
11944.5808	0.0110	131	4	3	2	3 3 1	12015.2843	0.0400	211	7	2	6	7 2 5
11944.8799	0.0330	310	6	1	6	7 0 7	12015.3725	0.0140	310	1	1	0	2 2 1
11945.2671	0.0300	131	4	3	1	3 3 0	12015.4094	0.0070					
11947.0477	0.0140	211	6	6	1	7 6 2	12016.9953	0.1570	211	3	3	0	4 3 1
11947.0477	0.0140	211	6	6	0	7 6 1	12017.5182	0.0200	131	5	4	2	4 4 1
11949.5033	0.1680	211	5	2	3	6 2 4	12017.7090	0.0080	131	5	4	1	4 4 0
11949.7118	0.0130	131	5	4	2	6 2 5	12018.1742	0.4010	211	3	3	1	4 3 2
11951.6262	0.0150	131	6	5	1	6 5 2	12018.9409	0.0110					
11951.6262	0.0150	131	6	5	2	6 5 1	12019.0320	0.7310	211	3	2	2	4 2 3
11954.0948	0.0550	131	5	5	1	5 5 0	12019.1134	0.0100	032	3	3	0	4 2 3
11954.0948	0.0550	131	5	5	0	5 5 1	12019.5104	0.0380	310	4	2	3	4 3 2
11954.2508	0.1110	211	5	3	2	6 3 3	12020.8821	0.0730	310	3	1	3	4 0 4
11954.6988	0.5400	211	6	0	6	7 0 7	12025.2447	0.0070	310	7	2	5	7 3 4
11954.9147	0.2290	211	6	1	6	7 1 7	12026.0471	0.5170	211	3	0	3	4 0 4
11956.4966	0.0220						12026.6391	0.0120	310	3	2	2	3 3 1
11958.0350	0.0130	310	2	2	1	3 3 0	12027.2256	0.1190	211	5	1	5	5 1 4
11958.3581	0.0240	131	6	2	4	5 2 3	12028.1987	0.0150					
11960.1657	0.2060	211	5	1	4	6 1 5	12028.2816	0.9100	211	3	1	3	4 1 4
11961.9297	0.3110	211	5	3	3	6 3 4	12028.9587	0.1330	211	4	0	4	4 2 3
11963.5338	0.1540	211	5	4	2	6 4 3	12032.5964	0.0230	310	3	2	1	3 3 0
11966.8031	0.0140						12034.2271	0.0090	310	4	2	2	4 3 1
11967.0741	0.0090						12034.7726	0.0090					
11967.6750	0.4980	211	5	2	4	6 2 5	12035.1640	0.0080					
11967.9506	0.0140	131	5	3	2	4 3 1	12035.4256	0.0180	310	5	2	3	5 3 2
11968.0761	0.0290	211	7	1	7	7 1 6	12036.6591	0.8820	211	2	1	1	3 1 2
11968.1620	0.0480	211	5	5	1	6 5 2	12037.5153	0.4350					
11968.1620	0.0480	211	5	5	0	6 5 1	12037.5939	0.0130	310	4	3	2	5 2 3
11968.6777	0.0330	310	5	2	4	6 1 5	12038.9120	0.0200	131	6	4	2	5 4 1
11968.7411	0.0130						12039.9675	0.6680	211	2	2	0	3 2 1
11969.0961	0.0240	310	5	0	5	6 1 6	12040.3763	0.0070	211	8	3	6	8 3 5
11970.6716	0.0180	310	5	1	5	6 0 6	12040.6939	0.0100	131	6	4	3	6 2 4
11971.5702	0.0170	310	2	1	2	3 2 1	12041.7730	0.0090					
11973.8753	0.0080	211	2	0	2	3 2 1	12042.5257	0.0500	211	3	0	3	3 2 2
11974.5498	0.0090	310	5	4	1	5 5 0	12044.6076	0.3090	211	2	2	1	3 2 2
11975.8991	0.0130						12046.0359	0.7110	310	2	1	2	3 0 3
11976.9415	0.0070	310	7	3	5	7 4 4	12047.1757	0.0160	310	5	1	4	5 2 3
11979.1773	0.6080	211	4	2	2	5 2 3	12048.3391	0.7780	211	2	0	2	3 0 3
11979.7748	0.3410	211	5	0	5	6 0 6	12050.7539	0.0120	310	1	0	1	2 1 2
11980.2401	0.7230	211	5	1	5	6 1 6	12051.1996	0.0770	211	2	0	2	2 2 1
11981.1306	0.0090						12051.3523	0.5560	211	2	1	2	3 1 3
11981.3920	0.0100	211	7	1	6	7 3 5	12053.5208	0.0120					
11981.6755	0.0080						12055.0059	0.0120	131	5	4	2	5 2 3
11981.6972	0.0090						12055.0572	0.0780	211	4	1	4	4 1 3
11983.0374	0.0080	211	8	2	7	8 2 6	12057.4097	0.0090					
11984.6982	0.7120	211	4	1	3	5 1 4	12058.1206	0.0270					
11986.3649	0.0110						12059.0438	0.0110	310	4	1	3	4 2 2

TABLE II—Continued

Sigma, cm ⁻¹	Depth, χ	VIB	J'	Ka'	Kc'	J''Ka''Kc''	Sigma, cm ⁻¹	Depth, χ	VIB	J'	Ka'	Kc'	J''Ka''Kc''	
12060.6233	0.0140	131	7	4	4	6	4	3	12127.4608	0.4000				
12061.2507	0.0080	211	9	4	6	9	4	5	12129.3401	0.0080				
12062.4100	0.5260								12129.9227	0.0100	310	2	1	1
12063.7170	0.4310	211	1	1	0	2	1	1	12130.5533	0.6310	211	2	1	1
12064.1551	0.0190	310	3	0	3	3	1	2	12131.2115	0.0090				
12064.2318	0.0100								12131.4972	0.0140				
12064.4534	0.0350	310	3	1	2	3	2	1	12132.0041	0.0090				
12065.0684	0.0110	310	2	1	1	2	2	0	12133.5367	0.0340	211	8	3	5
12067.0345	0.0530	211	7	3	5	7	3	4	12136.1571	0.0160	211	6	1	5
12069.5154	0.5600	211	1	0	1	2	0	2	12136.5726	0.0910	211	5	2	3
12071.0346	0.4910								12137.1034	0.0100	310	2	0	2
12072.9676	0.2060	211	5	2	4	5	2	3	12137.9596	0.0080				
12073.5504	0.0180	310	1	1	1	2	0	2	12138.9279	0.0240	310	3	1	2
12073.9572	0.8420	211	1	1	1	2	1	2	12139.4430	0.4090	211	1	0	1
12074.0702	0.0080								12141.7730	0.0160	310	3	1	2
12074.7445	0.0090								12142.0251	0.0120	310	3	2	1
12078.4876	0.0100								12142.3504	0.0140	112	4	3	2
12079.2274	0.3700	211	3	1	3	3	1	2	12143.3790	0.1660	211	3	1	2
12080.1311	0.0080								12143.4749	0.0540	310	1	1	1
12080.1475	0.0080	211	8	4	5	8	4	4	12144.9879	0.0070				
12082.2235	0.4910								12145.4445	0.5000				
12084.9895	0.0080	211	9	5	5	9	5	4	12146.9619	0.0090				
12086.8409	0.0080								12149.9170	0.5220				
12087.6076	0.0530	211	6	3	4	6	3	3	12150.7173	0.0100	310	6	2	4
12087.7143	0.0300	310	1	0	1	1	1	0	12151.0910	0.1110	211	6	2	4
12090.1106	0.0090								12151.8238	0.6170				
12093.0418	0.8320	211	0	0	0	1	0	1	12155.4546	0.0170				
12093.9541	0.0730	211	7	4	4	7	4	3	12155.7340	0.0090	112	8	1	8
12094.8612	0.0100	211	8	5	4	8	5	3	12156.1730	0.5110	211	2	1	2
12096.4192	0.0290	211	8	5	3	8	5	4	12156.6419	0.0090				
12098.0248	0.0090	131	6	5	1	5	5	0	12158.0498	0.0320	310	3	0	3
12098.1338	0.2770	211	2	1	2	2	1	1	12158.1007	0.0130	112	4	2	3
12100.2879	0.0090	211	4	2	2	5	0	5	12158.6176	0.5980	310	2	1	2
12100.6063	0.0260	211	8	4	4	8	4	5	12159.2303	0.2600	211	4	1	3
12101.5833	0.3580	211	5	3	3	5	3	2	12160.9207	0.8870	211	2	0	2
12101.9062	0.0270	211	7	4	3	7	4	4	12161.0028	0.0110				
12102.6500	0.0650	211	7	5	3	7	5	2	12161.2743	0.0080				
12102.8757	0.0080	211	3	2	1	4	0	4	12161.8598	0.0170	310	5	2	3
12103.0425	0.0200	211	7	5	2	7	5	3	12161.9586	0.0130	112	5	2	3
12103.2339	0.0700	211	6	4	3	6	4	2	12165.3977	0.0070				
12104.3777	0.0080								12167.0540	0.0140	112	7	1	6
12105.6588	0.1900	211	6	4	2	6	4	3	12167.5187	0.8790	211	2	1	1
12106.1495	0.0080								12167.7589	0.0210	211	7	2	5
12106.2441	0.0130								12168.7497	0.0110	310	4	1	3
12106.8528	0.7440	211	3	2	2	3	2	1	12169.3719	0.0080				
12108.3200	0.4430	310	6	6	6	7	1	7	12170.3830	0.0280				
12109.1140	0.0600	211	6	5	2	6	5	1	12170.9465	0.0090	112	3	3	1
12109.1847	0.1630	211	6	5	1	6	5	2	12171.0325	0.0210	112	3	3	0
12109.7741	0.4060	211	5	4	2	5	4	1	12172.1884	0.0290	310	3	1	3
12110.1322	0.2990	211	4	3	2	4	3	1	12173.0405	0.0150				
12110.3002	0.1590	211	5	4	1	5	4	2	12173.1215	0.9600	211	3	1	3
12110.9224	0.8870	211	1	1	1	1	1	0	12173.2317	0.0110				
12111.1335	0.0710								12174.5243	0.0080	310	7	3	4
12112.2645	0.1440	211	5	3	2	5	3	3	12175.8724	0.0090	310	4	0	4
12112.5004	0.0520	211	3	0	3	2	2	0	12176.1292	0.0550	211	5	1	4
12112.5004	0.0520								12176.9974	0.0160				
12113.0777	0.6630	211	4	3	1	4	3	2	12177.3536	0.6820	211	3	0	3
12114.4261	0.0180	211	2	2	0	3	0	3	12179.4368	0.0310	211	2	2	1
12114.5746	0.7060	211	2	2	1	2	2	0	12179.8826	0.0190				
12114.5746	0.7060	211	5	5	0	5	5	1	12180.1593	0.0100	112	4	2	2
12114.6810	0.3290	211	4	4	1	4	4	0	12181.3154	0.1600	211	3	2	2
12114.7435	0.6970	211	4	4	0	4	4	1	12183.5473	0.0130	310	4	1	4
12115.0159	0.1610	211	6	3	3	6	3	4	12183.7409	0.0120				
12115.1587	0.9080	211	3	3	1	3	3	0	12183.9477	0.0370	112	7	0	7
12115.6032	0.5370	211	3	3	0	3	3	1	12184.1765	0.7600	211	3	2	2
12115.8233	0.0070								12184.2586	0.0120	032	3	3	0
12116.4903	0.0110	310	4	2	3	3	3	0	12184.4142	0.0160	310	6	1	5
12116.7809	0.0210	211	4	0	4	3	2	1	12184.4142	0.0160	112	7	1	7
12117.2909	0.9570	211	2	2	0	2	2	1	12184.4964	0.0210	211	8	2	6
12117.4060	0.0100								12186.2702	0.0610	211	4	2	3
12118.0268	0.1310	211	6	6	1	6	6	0	12188.2926	0.6510	211	4	1	4
12118.0268	0.1310	211	6	6	0	6	6	1	12188.9990	0.0070				
12118.3135	0.0110								12189.3290	0.3770	211	3	2	1
12119.2003	0.0120	112	4	4	1	5	5	0	12189.4010	0.0170				
12119.3563	0.3690	211	3	2	1	3	2	2	12190.1582	0.5960	211	3	1	2
12121.7570	0.5160	211	1	1	0	1	1	1	12190.6103	0.0090	310	5	0	5
12122.2750	0.0220	211	7	3	4	7	3	5	12191.2427	0.9750	211	4	0	4
12122.2750	0.0220	211	8	1	7	7	3	4	12193.1005	0.0110	112	3	2	2
12123.1606	0.0070								12193.6157	0.0090	112	3	1	3
12125.0952	0.0250	310	1	1	0	1	0	1	12193.7184	0.0370	310	5	1	4
12125.7156	0.4630	211	4	2	2	4	2	3	12194.0790	0.1340	211	5	2	4
12127.1479	0.0140								12195.1910	0.5810				
12127.2262	0.0120								12196.5405	0.0350	211	6	1	5
									12197.0834	0.0070				

TABLE II—Continued

Sigma, cm ⁻¹	Depth, km	VIB	J'	Ka'	Kc'	J''Ka''Kc''	Sigma, cm ⁻¹	Depth, km	VIB	J'	Ka'	Kc'	J''Ka''Kc''
12198.3188	0.0660	310	2	2	1	1 1 0	12244.7189	0.5460					
12198.4443	0.0090						12245.6209	0.1840	211	6	3	4	5 3 3
12199.5828	0.0090						12246.9619	0.0670	211	10	1	10	9 1 9
12200.9983	0.0350	112	3	2	1	4 3 2	12247.0307	0.1890	211	10	0	10	9 0 9
12201.5409	0.0200	131	5	4	2	4 2 3	12247.1534	0.0470	310	7	2	6	6 1 5
12201.6774	0.0120						12248.0200	0.4350					
12201.7579	0.9420	211	5	1	5	4 1 4	12249.3900	0.4840					
12202.0286	0.4840						12250.3484	0.0100					
12202.7491	0.4500	211	4	2	3	3 2 2	12250.8770	0.0880	211	6	4	3	5 4 2
12203.1455	0.0210	112	6	2	5	7 1 6	12251.8991	0.2400	211	6	4	2	5 4 1
12203.3869	0.6040	211	5	0	5	4 0 4	12252.3031	0.1130	211	11	0	11	10 0 10
12203.6143	0.0090						12252.3031	0.1130	211	11	1	11	10 1 10
12204.3461	0.0100	310	7	2	6	7 1 7	12252.9682	0.1920	211	7	1	6	6 1 5
12204.6132	0.0090	310	6	1	6	5 0 5	12253.7380	0.0090					
12204.7434	0.0260	211	6	2	5	6 0 6	12254.1863	0.0490	211	6	4	3	6 2 4
12204.8894	0.0400	211	7	3	5	7 1 6	12254.6702	0.4570	211	6	3	3	5 3 2
12204.8894	0.0400	310	2	2	0	1 1 1	12255.5755	0.0770	211	6	5	1	5 5 0
12205.0391	0.0190	211	6	3	4	6 1 5	12256.0596	0.0550	310	3	0	0	2 2 1
12205.1319	0.0310	131	7	3	5	6 1 6	12256.3155	0.0460	211	12	0	12	11 0 11
12207.6329	0.0220						12256.3155	0.0469	211	12	1	12	11 1 11
12207.7518	0.6260						12256.3831	0.6230	211	6	2	4	5 2 3
12208.1905	0.0370	112	5	1	4	6 2 5	12256.6709	0.1260	211	8	2	7	7 2 6
12208.7398	0.2110	211	4	3	2	3 3 1	12258.2980	0.0350	112	4	0	4	5 1 5
12208.9515	0.0590	211	5	3	3	5 1 4	12259.0742	0.0190					
12210.0624	0.5210	211	4	3	1	3 3 0	12260.1349	0.3240	211	8	1	7	7 1 6
12210.1758	0.9250	211	4	1	3	3 1 2	12260.8126	0.0190	112	2	1	1	3 2 2
12210.8977	0.0580	112	6	1	6	7 0 7	12261.2013	0.3530	131	7	4	4	6 2 5
12211.9595	0.0450	211	7	2	6	7 0 7	12261.2013	0.3530	211	7	3	5	6 3 4
12213.2748	0.0070						12261.7649	0.0970	112	4	1	4	5 0 5
12213.3021	0.0100	211	9	3	7	9 1 8	12264.5600	0.0100	112	5	3	2	5 4 1
12213.4535	0.0120						12265.4705	0.0330	112	4	2	3	5 1 4
12213.5365	0.8360	211	4	2	2	3 2 1	12266.1991	0.1800	211	9	2	8	8 2 7
12213.6854	0.4970	211	6	1	6	5 1 5	12268.4924	0.0650	211	9	1	8	8 1 7
12213.6854	0.4970	310	7	0	7	6 1 6	12268.6214	0.1710	211	7	4	4	6 4 3
12213.9504	0.0410	310	3	2	2	2 1 1	12271.3252	0.0550					
12214.4298	0.8770	211	6	0	6	5 0 5	12271.6123	0.0610	211	7	4	3	6 4 2
12215.0924	0.0080	310	6	1	5	5 2 4	12271.8384	0.0260					
12215.2704	0.0140						12271.9498	0.0710	310	4	3	2	3 2 1
12216.0323	0.0140	211	4	3	2	4 1 3	12272.6879	0.0070					
12216.1070	0.0100						12273.1193	0.1540	211	7	2	5	6 2 4
12217.8926	0.0100						12273.3644	0.0100	310	4	2	2	3 1 3
12218.1184	0.0150						12273.6923	0.0260					
12218.7558	0.0120						12273.7754	0.0670	211	7	5	3	6 5 2
12219.4211	0.0210	310	7	2	5	6 3 4	12273.9215	0.0260	211	7	5	2	6 5 1
12219.5058	0.7930	211	5	2	4	4 2 3	12274.0169	0.0180	112	1	1	1	2 2 0
12220.8298	0.0200	211	8	1	7	8 1 8	12274.9397	0.0680	211	8	3	6	7 3 5
12224.2818	0.0140						12275.4115	0.0160					
12224.4241	0.7390	211	7	1	7	6 1 6	12275.6337	0.0070					
12224.5858	0.0230	211	3	3	1	3 1 2	12276.4286	0.1190	211	7	3	4	6 3 3
12225.5104	0.0170	112	4	1	3	5 2 4	12278.8779	0.0320					
12225.9209	0.1900	310	4	2	3	3 1 2	12279.1223	0.1030	112	3	0	3	4 1 4
12226.1016	0.6590						12279.4123	0.0180	310	4	3	1	3 2 2
12226.4197	0.0190						12280.9083	0.0540	112	1	1	0	2 2 1
12226.5428	0.4160	211	5	1	4	4 1 3	12281.7338	0.0120	112	5	0	5	5 1 4
12227.0123	0.0640	211	2	2	0	1 0 1	12282.3552	0.0210					
12227.7639	0.0760	131	6	4	3	5 2 4	12284.3074	0.0140					
12228.0208	0.5530	211	5	3	3	4 3 2	12284.5368	0.0130	112	4	2	3	4 3 2
12229.7483	0.0130						12284.6865	0.0340	211	8	4	5	7 4 6
12230.8613	0.0090						12284.8412	0.0250	310	5	3	3	4 2 2
12231.4989	0.0100						12285.7286	0.0150					
12231.8583	0.0130	211	9	2	8	9 0 9	12285.9582	0.2130	211	8	2	6	7 2 5
12231.9231	0.2360	211	5	4	2	4 4 1	12286.3518	0.0940	211	9	3	7	8 3 6
12232.1613	0.2910	211	5	3	2	4 3 1	12287.1908	0.0150	112	4	1	4	4 2 3
12232.1613	0.2910	211	5	4	1	4 4 0	12287.9993	0.1080	211	4	2	2	3 0 3
12232.5788	0.2290	211	8	1	8	7 1 7	12288.2922	0.0080					
12233.3175	0.0110	112	5	2	4	6 1 5	12289.7522	0.0090					
12233.8074	0.5440	211	8	0	8	7 0 7	12291.5455	0.0970	211	8	4	4	7 4 3
12234.0676	0.0130						12293.1636	0.0640	310	6	3	4	5 2 3
12234.7500	0.0730	112	5	0	5	6 1 6	12293.4079	0.0070	013	8	1	7	9 1 8
12235.0565	0.1300	310	5	2	4	4 1 3	12294.1731	0.0070					
12235.4198	0.2640	211	6	2	5	5 2 4	12295.0577	0.0210					
12235.9193	0.0440	310	3	2	1	2 1 2	12295.7066	0.1660	211	8	3	5	7 3 4
12236.2815	0.3920	211	5	2	3	4 2 2	12297.6027	0.0180	310	7	3	5	6 2 4
12236.5607	0.5890						12297.9656	0.0150					
12238.0468	0.0230	112	2	1	2	3 2 1	12298.1427	0.0360	112	2	0	2	3 1 3
12238.1841	0.3900	310	6	2	5	5 1 4	12298.9937	0.0110	112	3	2	2	4 1 3
12239.1961	0.0110	211	7	4	4	7 2 5	12299.8203	0.0480	211	9	4	6	8 4 5
12239.8084	0.0070						12301.2038	0.0520	310	8	3	6	7 2 5
12240.2277	0.1330	211	9	0	9	8 0 8	12301.6095	0.0140	112	5	2	3	5 3 2
12240.8975	0.3440	211	9	1	9	8 1 8	12301.9793	0.0110	112	4	3	2	5 2 3
12241.8454	0.0130						12302.2978	0.0220					
12242.5933	0.0440	112	3	1	2	4 2 3	12302.9077	0.0120	211	3	3	0	2 1 1
12243.5254	0.5900	211	6	1	5	5 1 4	12303.3252	0.0090	112	3	1	3	3 2 2
12244.2261	0.0080	112	6	1	6	6 2 5							

TABLE II—Continued

Sigma, cm ⁻¹	Depth, X	VIB	J'	Ka'	Kc'	J''Ka''Kc''	Sigma, cm ⁻¹	Depth, X	VIB	J'	Ka'	Kc'	J''Ka''Kc''
12304.8737	0.0170						12372.4230	0.0150					
12305.8476	0.0410	310	5	3	2	4 2 3	12375.1063	0.0090	310	7	3	4	6 2 5
12306.2459	0.0090	211	6	4	2	6 2 5	12375.3761	0.0100					
12306.9904	0.0430	211	10	2	8	9 2 7	12376.7866	0.0260	310	6	5	2	5 4 1
12307.2389	0.0220	211	9	5	5	8 5 4	12377.0123	0.0100	013	2	0	2	3 2 1
12308.1659	0.0150	013	8	0	8	9 0 9	12377.2609	0.0110	310	6	5	1	5 4 2
12308.2744	0.0440	310	4	4	1	3 3 0	12377.4958	0.0300	211	6	2	4	5 0 5
12308.5297	0.0170	310	4	4	0	3 3 1	12380.4539	0.0150	013	4	4	0	5 4 1
12308.7112	0.0100	112	4	0	4	4 1 3	12380.6571	0.0080	013	4	4	1	5 4 2
12309.7349	0.0090						12382.8521	0.0660	013	4	2	2	5 2 3
12311.0957	0.0250						12383.4836	0.0260	211	5	3	3	4 1 4
12311.4228	0.0190						12383.9165	0.0350	013	4	3	1	5 3 2
12311.8975	0.0080						12384.6787	0.0290	013	5	0	5	6 0 6
12312.0228	0.0110						12385.3157	0.0730	013	5	1	5	6 1 6
12312.5085	0.0850	112	2	1	2	3 0 3	12386.5869	0.0160	211	4	4	0	3 2 1
12313.4792	0.0310	112	5	1	4	5 2 3	12387.1559	0.0130	013	4	3	2	5 3 3
12314.0219	0.0090						12387.6591	0.0110					
12315.0578	0.0080						12390.4936	0.0870	013	4	1	3	5 1 4
12315.5696	0.0210	112	2	1	2	2 2 1	12390.6292	0.0900	112	1	1	0	1 0 1
12316.5322	0.0800	112	1	0	1	2 1 2	12392.5901	0.0080	211	4	4	1	3 2 2
12317.3212	0.0130	310	5	2	3	4 1 4	12393.8568	0.0120	211	7	3	4	6 1 5
12318.4764	0.0200	211	3	3	1	2 1 2	12395.4150	0.0340	013	4	2	3	5 2 4
12318.4764	0.0200						12395.5337	0.0140	310	7	5	2	6 4 3
12319.0508	0.0090	013	7	1	6	8 1 7	12395.6443	0.0410	112	2	1	1	2 0 2
12319.4858	0.0600	211	4	3	1	3 1 2	12399.8585	0.0080	013	6	1	5	6 3 4
12319.5603	0.0120						12402.9564	0.0120	112	2	0	2	1 1 1
12320.7367	0.0200						12404.8771	0.0820	112	3	1	2	3 0 3
12321.4010	0.0100						12405.9519	0.0280	112	4	2	2	4 1 3
12321.6615	0.0150						12406.2214	0.0110					
12322.5443	0.0130	013	7	2	6	8 2 7	12407.4067	0.0850	112	3	2	1	3 1 2
12322.6870	0.0090						12407.7417	0.0080	112	3	1	2	2 2 1
12324.8095	0.0140	013	6	3	3	7 3 4	12407.9425	0.1110	013	4	0	4	5 0 5
12325.0250	0.0090						12408.7975	0.0210	112	1	1	1	0 0 0
12325.2292	0.0170	112	4	1	3	4 2 2	12408.9750	0.0600	112	5	2	3	5 1 4
12325.8999	0.0090						12409.5732	0.0080	013	4	1	3	4 3 2
12325.9767	0.0090	131	6	5	1	5 3 2	12410.6709	0.0150	112	7	3	4	7 2 5
12326.9161	0.0100						12411.1951	0.0310	013	3	2	1	4 2 2
12327.2661	0.0150	310	5	4	2	4 3 1	12411.4072	0.0090					
12328.8991	0.0230	013	6	2	4	7 2 5	12411.5328	0.0230	211	6	4	2	5 2 3
12328.9425	0.0390	310	5	4	1	4 3 2	12411.9573	0.0310	013	3	3	0	4 3 1
12329.0109	0.0080	013	6	4	2	7 4 3	12411.9573	0.0310	112	2	2	0	2 1 1
12329.5048	0.0250	211	5	2	3	4 0 4	12412.3122	0.0130					
12329.7138	0.0210						12413.0650	0.0350	013	3	3	1	4 3 2
12330.0682	0.0510	112	3	0	3	3 1 2	12414.7419	0.0410	013	3	1	2	4 1 3
12330.4144	0.0490	112	3	1	2	3 2 1	12415.2080	0.0160					
12330.7909	0.0130	112	2	1	1	2 2 0	12415.9450	0.0220	211	5	4	2	4 2 3
12332.4621	0.0170	112	2	2	1	3 1 2	12416.0545	0.0110	112	6	3	3	6 2 4
12332.5775	0.0150						12417.9656	0.0130	112	6	2	4	6 1 5
12333.2755	0.0080						12418.4569	0.0220	112	4	1	3	4 0 4
12334.6784	0.0330	013	7	1	7	8 1 8	12419.8269	0.0830	013	3	2	2	4 2 3
12334.8648	0.0070						12421.0037	0.0100	211	6	3	4	5 1 5
12334.9632	0.0080						12422.5641	0.0080	211	7	4	3	6 2 4
12335.9580	0.0230	112	0	0	0	1 1 1	12423.9618	0.0480	112	3	0	3	2 1 2
12338.0579	0.0260	211	5	3	2	4 1 3	12424.1822	0.0380	112	5	3	2	5 2 3
12338.8125	0.0100						12425.0902	0.0670	112	2	1	2	1 0 1
12338.8768	0.0180	112	1	1	1	2 0 2	12426.3532	0.0480	112	2	2	1	2 1 2
12340.1916	0.0130						12429.9640	0.0500	013	3	0	3	4 0 4
12343.1607	0.0090	310	6	4	3	5 3 2	12430.5560	0.0160					
12343.3750	0.0300	310	6	4	3	5 3 2	12431.9019	0.1370	013	3	1	3	4 1 4
12343.5457	0.0290	013	6	1	5	7 1 6	12432.2318	0.0220	112	3	2	2	3 1 3
12344.9226	0.0280	112	2	0	2	2 1 1	12433.3689	0.0180	013	4	0	4	4 2 3
12346.1631	0.0100						12433.5617	0.0160	211	8	3	5	7 1 6
12346.2864	0.0100	013	6	2	5	7 2 6	12434.0489	0.0160	112	4	3	1	4 2 2
12348.2446	0.0100						12434.5924	0.0380	112	5	1	4	5 0 5
12349.2670	0.0130	211	4	3	2	3 1 3	12434.9299	0.0070	112	4	1	3	3 2 2
12349.6525	0.0110						12436.7884	0.0150	211	8	4	4	7 2 5
12350.7778	0.0130						12438.1534	0.0240	112	3	1	3	2 0 2
12353.4968	0.0700	112	1	0	1	1 1 0	12439.0141	0.0100					
12354.4975	0.0110	310	7	4	4	6 3 3	12439.8160	0.0770	013	2	2	0	3 2 1
12354.5669	0.0110	013	5	3	2	6 3 3	12440.0035	0.0480	112	4	2	3	4 1 4
12355.3827	0.0160	013	5	2	3	6 2 4	12440.1105	0.1340	013	2	1	1	3 1 2
12357.8530	0.0100	013	5	4	2	6 4 3	12441.2615	0.0090	211	6	4	3	5 2 4
12358.0926	0.0130	310	5	5	1	4 4 0	12441.9497	0.0170	112	4	0	4	3 1 3
12358.1481	0.0340	310	5	5	0	4 4 1	12442.8769	0.0410	112	3	3	0	3 2 1
12360.0140	0.0190	013	6	1	6	7 1 7	12444.0918	0.0090					
12360.2333	0.0500	013	6	0	6	7 0 7	12444.2731	0.0270	013	2	2	1	3 2 2
12361.1830	0.0250	013	5	3	3	6 3 4	12446.4441	0.0080	013	3	0	3	3 2 2
12361.4979	0.0100						12448.5212	0.0380	112	4	3	2	4 2 3
12361.5980	0.0090						12448.8531	0.0100	112	3	3	1	3 2 2
12362.0376	0.0600	211	6	3	3	5 1 4	12449.2840	0.0120	112	5	2	4	5 1 5
12366.1051	0.0070	310	7	5	2	7 2 5	12449.4758	0.0530	112	4	1	4	3 0 3
12367.0875	0.0220	013	5	1	4	6 1 5	12449.9547	0.0110	112	5	3	3	5 2 4
12367.0875	0.0220	310	6	0	6	5 1 5	12451.4787	0.1630	013	2	0	2	3 0 3
12370.9268	0.0460	013	5	2	4	6 2 5	12452.0808	0.0150	112	6	3	4	6 2 5

TABLE II—Continued

TABLE III

Experimental Levels of the Vibrational States (211), (013), (310), (131), (112), and (230) of H₂¹⁸O

J	K _a	K _c	State (211) Energy, cm ⁻¹	Delta, 10-3cm ⁻¹	State (013) Energy, cm ⁻¹	Delta, 10-3cm ⁻¹	J	K _a	K _c	State (211) Energy, cm ⁻¹	Delta, 10-3cm ⁻¹	State (013) Energy, cm ⁻¹	Delta, 10-3cm ⁻¹
0	0	0	12116.7966	0.10	12520.1241	3.65	7	0	7	12669.3218	0.33	13075.6072	1.53
1	0	1	12139.4429	0.14	12543.2289	0.04	7	1	7	12669.7701	0.21	13075.6756	1.15
1	1	1	12152.9457	0.05	12555.3721	0.77	7	2	6	12794.1485	0.04	13198.5460	0.61
1	1	0	12158.5055	0.09	12561.0839	0.04	7	2	5	12874.3569	0.37	13283.4554	4.81
2	0	2	12184.6752	0.60	12587.8151	0.09	7	3	4	12935.0374	0.69	13342.8054	5.03
2	1	2	12192.9213	0.92	12595.8898	1.32	7	4	4	13019.6542	0.14	13421.6620	2.71
2	1	1	12209.5418	0.15	12612.9931	0.09	7	4	3	13023.8006	1.26	13425.3595	5.24
2	2	1	12249.3636	0.48	12649.0279	0.78	7	5	3	13153.8534	1.12		
2	2	0	12250.7667	0.33	12650.6154	0.53	7	5	2	13154.0338	1.80		
3	0	3	12247.2807	0.66	12651.1975	0.31	7	6	2	13316.6694	5.91		
3	1	3	12252.1100	0.23	12655.7305	0.47	7	6	1	13316.6707	0.96		
3	1	2	12284.9466	0.06	12689.5448	0.03	8	0	8	12817.5851	0.04	13224.4047	1.26
3	2	2	12317.6519	0.27	12718.4472	0.44	8	1	8	12816.5639	1.10	13224.3903	2.80
3	2	1	12324.1119	0.18	12725.6534	0.47	8	1	7	12961.8286	0.45	13368.1706	0.41
3	3	1	12397.4658	0.22	12792.3564	0.07	8	2	7	12963.2687	0.22	13371.6812	1.76
3	3	0	12397.6972	0.80	12792.6502	1.14	8	2	6	13066.4103	0.30	13476.0022	2.80
4	0	4	12327.5789	0.52	12731.9888	0.22	8	3	6	13087.7020	0.88		
4	1	4	12329.8602	0.06	12734.1577	12.72	8	4	5	13135.2554	0.64		
4	1	3	12383.0583	0.32	12788.8539	0.18	8	4	5	13206.5846	2.27		
4	2	3	12407.5045	0.36	12809.5791	2.61	8	4	4	13217.2429	1.59		
4	2	2	12424.3352	0.44	12828.0088	1.24	8	5	4	13342.0682	9.44		
4	3	2	12490.8345	0.18	12887.7521	1.23	9	0	9	12981.1400	0.20	13390.2831	1.90
4	3	1	12492.3689	0.50	12889.6474	0.22	9	1	9	12981.8960	0.10	13390.2813	1.71
4	4	1	12597.3526	1.47	12985.1989	2.38	9	1	8	13147.9879	0.88		
4	4	0	12597.3866	0.65	12985.2457	1.07	9	2	8	13148.1133	1.87	13554.7403	4.43
5	0	5	12424.6210	0.39	12829.5248	0.13	9	3	7	13288.0560	1.34		
5	1	5	12425.5860	0.04	12830.6616	0.02	9	4	6	13416.4545	2.11		
5	1	4	12501.3452	0.65	12908.2664	1.33	9	5	5	13553.6082	2.11		
5	2	4	12518.1255	0.07	12921.3781	1.41							
5	2	3	12550.7405	0.20	12956.6202	0.10	10	0	10	13163.2882	0.02		
5	3	3	12607.3118	0.18	13006.5660	0.88	10	1	10	13163.2552	0.72		
5	3	2	12612.8605	0.28	13013.1720	3.12							
5	4	2	12714.5669	0.12	13108.8858	0.11	11	0	11	13362.0946	4.74		
5	4	1	12714.8444	0.29	13109.1012	1.93	11	1	11	13362.1035	1.37		
5	5	1	12848.2385	0.94	13225.9536	1.67	11	1	10	13568.0949	4.59		
5	5	0	12848.2768	0.94	13225.9499	1.67							
6	0	6	12538.4763	0.14	12944.0106	0.28	12	0	12	13577.7737	4.29		
6	1	6	12538.9008	0.06	12944.0005	0.34	12	1	12	13577.7775	1.71		
6	1	5	12641.8855	0.57	13045.2405	0.30							
6	2	5	12649.5879	0.39	13052.8842	0.26							
6	2	4	12701.5415	0.26	13109.3504	1.22							
6	3	4	12746.2170	0.19	13148.0734	2.41							
6	3	3	12760.3982	0.14	13164.3576	0.84							
6	4	3	12855.4218	0.82	13253.6699	6.06							
6	4	2	12856.6916	0.45	13254.7130	2.19							
6	5	2	12989.2288	0.81									
6	5	1	12989.2598	1.05	13368.2952	4.15							
6	6	1	13151.2198	1.89	13513.9380	5.16							
6	6	0	13151.2224	1.10	13513.9376	5.16							

Note. JK_aK_c is the rotational assignment of the level, and Delta corresponds to one standard deviation.

levels (131) [643] and (211) [625] separated by 3 cm⁻¹ have mixing coefficients of 20 and 78%.

3. There is a strong linestrength redistribution among the resonating lines. More precisely, the lines belonging to the weakest band borrow part of their intensities from a stronger band through the mixing of the wavefunctions. For example, lines involving the levels (310) [836] and (112) [818] could not be observed in the spectrum in the absence of a resonance with the [826] level of the (211) state.

4. The level (211) [818], because of a complicated resonance coupling with the levels of the (131), (230), (310) states is shifted down by about 1 cm⁻¹ from its unperturbed position and its position is inverted as compared to that of the level (211) [808].

TABLE III—Continued

J	K _a	K _c	State Energy, cm ⁻¹	(310) Delta, 10 ⁻³ cm ⁻¹	State Energy, cm ⁻¹	(311) Delta, 10 ⁻³ cm ⁻¹	J	K _a	K _c	State Energy, cm ⁻¹	(112) Sigma, 10 ⁻³ cm ⁻¹	State Energy, cm ⁻¹	(230) Sigma, 10 ⁻³ cm ⁻¹
0	0	0			11774.7084	1.63	0	0	0	12372.7066	2.81		
1	0	1	12129.7400	2.35	11797.9144	0.69	1	0	1	12395.5204	0.25	11757.5398	0.80
1	1	1	12143.4763	1.41	11820.0627	0.00	1	1	1	12408.8005	2.73		
1	1	0	12148.8492	0.88	11826.2578	0.94	1	1	0	12414.3841	0.02	11787.2896	6.98
2	0	2	12173.8520	4.34	11843.1441	0.29	2	0	2	12439.7107	0.29	11802.4795	4.01
2	1	2	12182.3724	0.01	11860.2638	0.04	2	1	2	12448.8453	0.26	11821.0746	0.04
2	1	1	12199.8508	0.74	11878.7946	0.83	2	1	1	12465.5713	2.40		
2	2	1	12240.3422	0.08	11943.4278	0.38	2	2	1	12505.3434	1.28	11907.6520	4.27
2	2	0	12241.6380	1.44	11944.5515	0.03	2	2	0	12506.7518	2.56		
3	0	3	12237.0390	1.41	11908.3330	1.84	3	0	3	12502.9505	0.23	11867.4101	2.26
3	1	3	12242.1158	0.11	11919.8854	0.29	3	1	3	12508.0807	0.02		
3	1	2	12275.2525	1.09	11956.6485	1.63	3	1	2	12541.2133	0.28	11619.8477	2.16
3	2	2	12308.7366	2.66	12013.1104	0.94	3	2	2	12573.7993	0.21		
3	2	1	12314.9064	1.90	12018.4539	2.44	3	2	1	12580.2895	0.16		
3	3	1			12131.6761	1.12	3	3	1	12653.6183	1.11		
3	3	0	12389.5379	2.47	12131.8117	1.44	3	3	0	12653.6753	1.08		
4	0	4	12317.4410	0.86	11991.3823	0.12	4	0	4	12583.5150	1.76	11950.5669	1.69
4	1	4	12319.8861	2.32	11998.3026	1.59	4	1	4	12585.8114	0.77	11958.3170	0.92
4	1	3	12373.5039	1.30	12058.4355	0.47	4	1	3	12639.6856	4.71		
4	2	3	12398.8029	0.81	12105.0072	3.46	4	2	3	12663.8303	1.51	12068.5901	2.26
4	2	2	12414.9307	1.42	12119.6107	1.23	4	2	2	12680.7550	0.10		
4	3	2	12482.7512	1.87	12226.6806	0.40	4	3	2	12747.1397	1.15		
4	3	1	12484.1679	5.37	12227.5731	1.01	4	3	1	12748.5065	1.20		
4	4	1	12590.5817	1.09	12381.1905	2.31	4	4	1	12852.8834	1.21		
4	4	0	12590.6245	2.73	12381.2128	0.18	4	4	0	12852.8839	4.49		
5	0	5	12414.4402	1.77	12091.0914	0.22	5	0	5	12680.0953	0.75		
5	1	5	12415.5176	3.01	12094.9021	0.07	5	1	5	12681.4710	4.66		
5	1	4	12492.3359	2.15	12184.7644	2.80	5	1	4	12758.6388	1.40		
5	2	4	12509.8586	0.64	12218.3638	0.32	5	2	4	12774.4996	1.57		
5	2	3	12541.1514	1.83	12247.9859	1.55	5	2	3	12807.3380	2.17		
5	3	3	12599.3000	2.25	12345.2853	0.08	5	3	3	12864.1122	3.57		
5	3	2	12604.4648	2.39	12348.6528	2.35	5	3	2	12869.3402	0.05		
5	4	2	12707.9683	4.30	12500.1620	1.07	5	4	2	12970.1897	3.23		
5	4	1	12708.2333	0.54	12500.5821	0.23	5	4	1	12970.2582	0.43		
5	5	1	12840.7655	4.31	12687.7778	0.78	5	5	1	13098.8298	4.20		
5	5	0	12840.7919	1.47	12687.7741	0.78	5	5	0	13098.6604	1.73		
6	0	6	12528.1973	3.16	12207.2068	0.27	6	0	6	12794.0588	6.80		
6	1	6	12528.6586	1.12	12209.2605	0.81	6	1	6	12794.6756	0.70		
6	1	5	12629.2601	0.05	12327.8971	0.78	6	2	5	12904.8373	0.65		
6	2	5	12636.5443	0.34	12352.2244	1.20	6	2	4	12959.1463	0.50		
6	2	4	12691.8975	4.44	12403.5167	0.62	6	3	4	13002.5326	1.27		
6	3	4	12738.3230	1.32	12487.2678	14.0	6	4	3	13111.2713	4.24		
6	3	3			12496.1703	2.15							
6	4	3	12848.8889	6.01	12641.9325	1.13	7	0	7	12924.9461	1.19		
6	4	2	12850.2483	8.29	12643.7047	0.98	7	1	7	12925.3294	3.10		
6	5	2	12981.5795	1.85	12831.7410	2.02	7	1	6	13048.9658	1.37		
6	5	1	12981.8051	5.21	12831.7077	4.11	7	3	4	13191.1235	4.25		
7	0	7	12659.0313	0.11	12339.8836	7.02	8	0	8	13073.4208	4.97		
7	1	7			12341.0751	0.15	8	1	8	13071.9939	2.41		
7	2	6	12788.3330	0.68			8	3	6	13347.8218	7.15		
7	2	5	12884.7985	4.79									
7	3	5	12898.8388	1.38									
7	3	4	12925.5570	0.19	12670.8420	8.58	9	1	9	13234.7796	1.73		
7	4	4	13013.1070	2.63	12811.6557	3.07							
7	5	2	13146.5621	4.46									
8	3	6	13081.6564	0.87									

B. In addition to the usual Coriolis, Darling-Dennison, and Fermi resonances, the interactions between (211) and (032), (310) and (131), (310) and (013), and (310) and (032) had to be taken into account.

C. Very complicated mixings of states were found; indeed, there were cases where three or more states were mixed simultaneously:

—the levels (211)[826] at 13 066.4103 cm⁻¹, (310)[836] at 13 081.6564 cm⁻¹ and (112)[818] at 13 071.9939 cm⁻¹

—the levels (211)[625] at 12 649.5879 cm⁻¹, (310)[615] at 12 629.2601 cm⁻¹ and (131)[643] at 12 641.9325 cm⁻¹.

D. It was necessary to introduce in the energy level calculations the highly excited "dark" states (032), (150), and (051). Indeed, these dark states perturb through resonances the positions of the observed energy levels. They were then introduced in the calculations and some of their Hamiltonian constants were varied during the fit. The so-called HEL (highly excited local) resonances (4) were taken into account for the analysis of the perturbations affecting some rotational levels of the (230) and (131) vibrational states; this resonance is due to a coupling between these states and the (080) vibrational state, formally belonging to the 4ν higher polyade. The same situation takes place for the rotational levels of the (310) and (112) states which interact with (160).

IV. CONCLUSION

Using water vapor Fourier-transform spectra recorded between 11 300 and 13 600 cm⁻¹, we have obtained a set of accurate rotational energy levels for six interacting vibrational states belonging to the second decade of H₂¹⁸O. These results improve the knowledge of the H₂¹⁸O absorption spectrum in the near-infrared region.

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