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The Emission Spectrum of Hot Water in the Region between 370 and 930 cm^{-1}

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An emission spectrum of the water molecule at a temperature of 1550°C has been recorded in the range from 373 to 933 cm^{-1}. More than 4000 pure rotational lines were observed with the strongest belonging to the ground state (000) and the first excited bending vibrational level (010). Transitions involving rotational quantum numbers J and K_a significantly higher than previously recorded have been assigned.

I. INTRODUCTION

The pure rotational spectrum of water at room temperature has been studied in the millimeter wave, submillimeter wave, and far infrared regions (*1–9*). Even more studies have been devoted to the rovibrational bands of water (*10–21*) including overtones with wavenumbers as high as 25 000 cm^{-1}. Among the IR and near IR studies are the classic works by Flaud, Camy-Peyret, and co-workers (*10, 11*) on the oxyacetylene flame spectra of water at temperatures as high as 2900 K. Information on the energy levels for high values of the rotational quantum numbers J and K_a are derived mostly from the transitions in these flame spectra. The ground state energy levels up to $J = 35$ and $K_a = 20$ were derived in Ref. (*10*) and the levels of the first excited bending state (010) up to $J = 32$ and $K_a = 14$ were reported in Ref. (*11*). These energy levels were used for a comprehensive atlas of the water lines (*22*) and for the assignment of a hot water spectrum (*9*).

The energy levels derived from the flame spectra have been used in numerous theoretical papers, in which effective Hamiltonians were developed for the theoretical treatment of the highly excited rotational states of water molecule (*3, 4, 23–27*). Within the framework of the variational approach, the fitting of the potential energy surface of water was accomplished using these energy levels as the input data (*28–34*).

Experimental information on highly excited rotational levels of water in the ground and lower vibrational states is very important and is widely used in many applications. For example, the infrared spectrum of a sunspot (*36, 37*) contains thousands of molecular absorption features. Many of these lines belong to the water molecule but most of the lines do not have rovibrational assignments. This spectrum awaits detailed assignment and the obvious step toward this goal is the study of the high temperature water spectrum in the laboratory.

The present study of the hot water spectrum was motivated both by the desire to extend the rotational energy levels higher than those reported in the literature and by the necessity of understanding the sunspot spectrum in more detail.

II. EXPERIMENTAL DETAILS

A high resolution emission spectrum of hot H_2O was recorded with the Bruker IFS 120 HR Fourier transform spectrometer located at the University of Waterloo. The spectrum was recorded using a KBr beamsplitter with a liquid helium cooled Si:B detector in the region 350–1000 cm^{-1} with a resolution of 0.01 cm^{-1}. The lower limit of the spectrum was set by the transmission of the KBr beamsplitter and the detector response, while the upper limit was determined by a cold filter.

Water vapor flowed continuously from a room temperature glass container into the hot cell. The cell was a 1.2 m long by 5 cm diameter mullite ($3Al_2O_3 \cdot 2SiO_2$) tube with KRS-5 windows attached at each end. The mullite tube was placed inside a commercial CM Rapid Temperature Furnace and the pressure maintained at approximately 15 Torr with a vacuum pump. The tube was slowly heated to a temperature of 1550°C. It was necessary to have a constant flow of water vapor since the water vapor reacted rapidly with the hot walls of the tube. Higher temperatures were not obtained because the mullite tube cracked at 1550°C.

III. ANALYSIS

The spectrum was reduced by fitting the water lines with Voigt profiles to determine line position, width, and relative intensity using PC-DECOMP, an interactive spectral analysis program developed by J. W. Brault. The laboratory data were calibrated using J. W. C. Johns' H_2O measurements (*8*) and a calibration factor of 1.00 004 870 768 was applied to correct the observed line positions.

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TABLE 1

Assigned Line Frequencies of the Hot Water Spectrum with Intensities Higher than 0.1 r.u.

Wavenumber	Intensity	J'	K'_a	K'_c	J	K_a	K_c	(0v0)
407.30521	0.0772	19	4	16	18	3	15	(000)
418.96138	0.1094	19	4	15	18	5	14	(000)
423.23867	0.0754	20	3	17	19	4	16	(000)
423.75482	0.1107	20	4	17	19	3	16	(000)
424.87537	0.1083	23	0	23	22	1	22	(000)
425.16224	0.1165	22	1	21	21	2	20	(010)
425.43655	0.1074	22	2	21	21	1	20	(000)
432.46246	0.1046							OH
433.39106	0.1044							OH
435.35756	0.1177	11	5	6	10	4	7	(010)
436.95054	0.1184	20	4	16	19	5	15	(000)
438.07435	0.1290	24	0	24	23	1	23	(010)
438.12334	0.1026	21	6	15	20	7	14	(000)
439.88645	0.1673	21	3	18	20	4	17	(000)
440.17247	0.1031	21	4	18	20	3	17	(000)
441.21862	0.1404	22	2	20	21	3	19	(000)
441.22887	0.1535	22	3	20	21	2	19	(000)
441.70186	0.1050	22	3	20	21	2	19	(010)
441.87974	0.2018	24	0	24	23	1	23	(000)
442.21655	0.2051	20	5	16	19	4	15	(000)
442.25198	0.1257	23	1	22	22	2	21	(010)
442.42334	0.1552	23	2	22	22	1	21	(000)
446.12087	0.1307	9	8	1	8	7	2	(010)
447.41481	0.1008	13	6	8	12	5	7	(000)
449.27890	0.2260	23	7	16	22	8	15	(000)
449.69817	0.1511	10	7	4	9	6	3	(010)
449.79489	0.1385	10	7	3	9	6	4	(010)
454.08393	0.2339	21	4	17	20	5	16	(000)
456.34126	0.1663	22	3	19	21	4	18	(000)
456.50106	0.2446	22	4	19	21	3	18	(000)
457.14058	0.1132	21	5	17	20	4	16	(000)
457.83898	0.2792	23	3	21	22	2	20	(000)
458.03151	0.1137	23	2	21	22	3	20	(010)
458.04729	0.1342	23	3	21	22	2	20	(010)
458.75505	0.2546	25	0	25	24	1	24	(000)
459.25771	0.1533	24	1	23	23	2	22	(010)
459.79574	0.1919	15	6	10	14	5	9	(000)
460.83250	0.1744	21	5	16	20	6	15	(000)
461.64610	0.1903	16	6	11	15	5	10	(000)
462.64262	0.2112	17	6	12	16	5	11	(000)
463.14425	0.1527	11	4	7	10	3	8	(010)
463.30281	0.1860	9	9	0	8	8	1	(010)
463.38157	0.2292	12	6	7	11	5	6	(010)
464.35772	0.1881	18	6	13	17	5	12	(000)
464.75076	0.1533							OH
465.87552	0.1514							OH

Wavenumber	Intensity	J'	K'_a	K'_c	J	K_a	K_c	(0v0)
499.08242	0.2584	23	5	18	22	6	17	(000)
499.78570	0.1787							OH
502.19364	0.3375	13	6	7	12	5	8	(010)
502.61196	0.1098	24	4	20	23	5	19	(000)
502.93212	0.2643	10	10	0	9	9	1	(010)
503.21357	0.2593	24	5	20	23	4	19	(000)
503.97049	0.1396	9	3	7	8	0	8	(010)
504.38274	0.1514	13	5	8	12	4	9	(000)
504.61545	0.2658	25	3	22	24	4	21	(000)
504.64520	0.1340	25	4	22	24	3	21	(000)
506.68047	0.2714	26	3	24	25	2	23	(000)
506.74287	0.1175	23	6	18	22	5	17	(000)
507.92176	0.2117	14	7	8	13	6	7	(000)
508.56081	0.2445	28	1	28	27	0	27	(000)
509.04550	0.2584	27	1	26	26	2	25	(000)
510.58378	0.1248	12	4	8	11	3	9	(000)
513.39309	0.2377	11	9	2	10	8	3	(010)
514.76864	0.2043	13	5	8	12	4	9	(010)
514.91255	0.1692	14	6	8	13	5	9	(000)
517.18934	0.1398	25	4	21	24	5	20	(000)
517.78161	0.2005	13	7	7	12	6	6	(010)
518.41450	0.1591	14	7	7	13	6	8	(000)
518.78710	0.1481	24	6	19	23	5	18	(000)
519.14188	0.2550	12	8	5	11	7	4	(010)
519.20352	0.1916	12	8	4	11	7	5	(010)
520.13515	0.1825	12	4	8	11	3	9	(010)
520.35162	0.1501	26	4	23	25	3	22	(000)
520.58546	0.2056	13	7	6	12	6	7	(010)
522.58329	0.1798	27	2	25	26	3	24	(000)
522.74032	0.2001	15	7	9	14	6	8	(000)
524.87378	0.2413	29	0	29	28	1	28	(000)
525.34551	0.2087	28	2	27	27	1	26	(000)
528.29060	0.3110	11	10	1	10	9	2	(010)
529.67325	0.1457							OH
530.54049	0.1211							OH
531.06871	0.1713							OH
532.13805	0.1699							OH
532.55170	0.2063	14	6	8	13	5	9	(010)
533.19198	0.3359	16	7	10	15	6	9	(000)
534.24968	0.2605	13	9	5	12	8	4	(000)
534.26268	0.2398							art
534.27895	0.2706	13	9	4	12	8	5	(000)
535.85486	0.2487	27	3	24	26	4	23	(000)
536.46687	0.1768	10	4	7	9	1	8	(010)
536.61132	0.2142	11	3	8	10	2	9	(010)
536.94751	0.2873	14	8	7	13	7	6	(000)
537.84470	0.3694	12	9	3	11	8	4	(010)

Wavenumber	Intensity	J'	K'_a	K'_c	J	K_a	K_c	(0v0)
568.30274	0.4270	15	7	8	14	6	9	(010)
568.94562	0.1504	30	3	28	29	2	27	(000)
571.28617	0.1647	13	4	9	12	3	10	(000)
572.88411	0.1932	32	0	32	31	1	31	(000)
572.94282	0.3620	16	7	9	15	6	10	(000)
573.32095	0.1837	31	2	30	30	1	29	(000)
574.53908	0.3161	14	10	5	13	9	4	(000)
574.55568	0.2366	14	10	4	13	9	5	(000)
575.15347	0.4192	12	12	0	11	11	1	(010)
575.56939	0.3121							art
575.58194	0.3326	13	12	1	12	11	2	(000)
576.69533	0.2298	17	7	11	16	6	10	(010)
577.23550	0.3603	16	8	9	15	7	8	(000)
577.73289	0.4783	13	10	4	12	9	3	(010)
580.21560	0.4751	15	9	7	14	8	6	(000)
580.22725	0.1264							art
580.43439	0.3818	15	9	6	14	8	7	(000)
580.73232	0.1318	12	3	9	11	2	10	(000)
580.84027*	0.2818	20	7	14	19	6	13	(010)
581.00694*	0.2796	20	7	14	19	6	13	(010)
581.14986	0.2195	30	4	27	29	3	26	(000)
581.25267	0.2889	18	7	12	17	6	11	(010)
581.61518	0.3224	13	4	9	12	3	10	(010)
583.38113	0.3781	16	8	8	15	7	9	(000)
584.20394	0.3717	13	13	0	12	12	1	(000)
584.25344	0.1079	11	4	8	10	1	9	(010)
584.70802	0.1298	12	5	8	11	2	9	(000)
585.25851	0.4978	14	9	6	13	8	5	(010)
585.29478	0.3545	14	9	5	13	8	6	(010)
586.62282	0.3378	15	8	8	14	7	7	(010)
588.13178	0.4402	15	8	7	14	7	8	(010)
588.77838	0.4158	14	11	4	13	10	3	(000)
588.99047	0.1433	32	2	31	31	1	30	(000)
590.63946	0.5212	13	11	3	12	10	2	(010)
592.05514	0.1154	10	6	5	9	3	6	(000)
592.11412	0.1537	11	5	7	10	2	8	(010)
592.75489	0.2084							OH
593.70280	0.1272							OH
593.80898	0.1318							OH
593.88832	0.4256	17	8	10	16	7	9	(000)
594.18763	0.2485	16	7	9	15	6	10	(010)
594.94996	0.1055							OH
597.87173	0.3210							art
597.88868	0.4747	15	10	6	14	9	5	(000)
597.90376	0.3303	15	10	5	14	9	6	(000)
600.45911	0.4495	14	12	3	13	11	2	(000)
600.66240	0.4628	16	6	10	15	5	11	(000)

466.85554	0.1282							OH
468.05342	0.1534	19	6	14	18	5	13	(000)
470.50693	0.1043	12	7	5	11	6	6	(000)
470.64555	0.1433	22	4	18	21	5	17	(000)
470.88177	0.2750	10	8	3	9	7	2	(010)
471.85437	0.1833	12	5	7	11	4	8	(010)
472.41776	0.1682	22	5	18	21	4	17	(000)
472.61404	0.1896	23	3	20	22	4	19	(000)
472.70423	0.1130	23	4	20	22	3	19	(000)
473.34816	0.2522	11	7	5	10	6	4	(010)
473.69864	0.2109	11	7	4	10	6	5	(010)
474.18431	0.1221	24	3	22	23	2	21	(010)
474.29606	0.3065	24	3	22	23	2	21	(000)
474.37711	0.2693	20	6	15	19	5	14	(000)
475.08999	0.1708	12	6	6	11	5	7	(010)
475.49734	0.3083	26	1	26	25	0	25	(000)
476.00912	0.2466	25	2	24	24	1	23	(000)
478.14645	0.2286	13	6	8	12	5	7	(010)
480.31431	0.1251	22	5	17	21	6	16	(000)
480.73132	0.1173	9	2	7	8	1	8	(010)
483.28368	0.1360	21	6	16	20	5	15	(000)
486.80013	0.2641	23	4	19	22	5	18	(000)
487.83063	0.1599	23	5	18	22	4	19	(000)
488.39672	0.2380	14	6	9	13	5	8	(010)
488.52555	0.2399	10	9	1	9	8	2	(010)
488.70675	0.1482	24	3	21	23	4	20	(000)
488.75795	0.2732	24	4	21	23	3	20	(000)
489.57321	0.1535	13	7	7	12	6	6	(000)
490.57922	0.2469	25	3	23	24	2	22	(000)
492.10020	0.2448	27	1	27	26	0	26	(000)
492.59836	0.3244	26	2	25	25	1	24	(000)
493.68548	0.2629	22	6	17	21	5	16	(000)
494.13252	0.1394	13	7	6	12	6	7	(000)
494.15008	0.1201	15	6	10	14	5	9	(010)
494.17121	0.1405	23	6	17	22	7	16	(000)
494.28165	0.2564	22	6	17	21	5	16	(000)
495.16398	0.2138	18	6	13	17	5	12	(010)
495.25026	0.2738	11	8	4	10	7	3	(010)
495.26578	0.2513	11	8	3	10	7	4	(010)
496.17999	0.3424	12	7	6	11	6	5	(010)
496.31042	0.3216	16	6	11	15	5	10	(010)
496.39507	0.1536	17	6	12	16	5	11	(010)
497.13882	0.1536							OH
497.24411	0.2952	12	7	5	11	6	6	(010)
497.95896	0.1262							OH
498.16329	0.2155	23	5	18	22	6	17	(000)
498.75866	0.1731							OH
537.99484	0.3072	14	8	6	13	7	7	(000)
538.27415	0.2523	28	3	26	27	2	25	(000)
538.83496	0.1417	21	7	15	20	6	14	(000)
539.14306	0.4393	17	7	11	16	6	10	(000)
539.56964	0.2376	12	11	1	11	10	2	(000)
539.58613	0.2094							art
539.63238	0.3246	20	7	14	19	6	13	(000)
539.82100	0.2456	22	7	16	21	6	15	(000)
540.13149	0.1172							art
540.14835	0.3809	11	11	0	10	10	1	(010)
540.95752	0.2224	19	7	13	18	6	12	(000)
541.03491	0.2254	30	1	30	29	0	29	(000)
541.30157	0.3794	18	7	12	17	6	11	(000)
541.49465	0.2444	29	1	28	28	2	27	(000)
542.45282	0.2867	13	8	6	12	7	5	(010)
542.47003	0.2511							art
542.65487	0.3800	13	8	5	12	7	6	(010)
544.06961	0.2914	14	7	7	13	6	8	(010)
544.26008	0.3258	15	7	8	14	6	9	(000)
549.15711	0.3280	24	7	18	23	6	17	(000)
550.19349	0.3077	12	12	0	11	11	1	(000)
551.17472	0.1993	28	4	25	27	3	24	(000)
553.23923	0.3763	12	10	2	11	9	3	(000)
553.73506	0.2275	29	2	27	28	3	26	(000)
554.48878	0.2255	15	7	9	14	6	8	(010)
554.63534	0.2606	15	6	9	14	5	10	(000)
557.03969	0.2167	31	0	31	30	1	30	(000)
557.19993	0.2878	14	5	9	13	4	10	(000)
557.48804	0.2318	30	2	29	29	1	28	(000)
557.54557	0.3244	14	9	6	13	8	5	(000)
557.61690	0.3415	14	9	5	13	8	6	(000)
557.98437	0.3036	15	8	8	14	7	7	(000)
560.44380	0.1387	10	3	8	9	0	9	(010)
560.66066	0.3146	15	8	7	14	7	8	(000)
561.81939	0.3416	13	9	5	12	8	4	(010)
561.82984	0.3878	13	9	4	12	8	5	(010)
562.46483	0.1300							OH
562.76517	0.1223							OH
563.87255	0.1345							OH
564.31234	0.1821	14	5	9	13	4	10	(010)
564.86756	0.1755	10	5	6	9	2	7	(010)
565.02529	0.3796	14	8	7	13	7	6	(010)
565.61262	0.3399	14	8	6	13	7	7	(010)
565.62834	0.3848	12	11	1	11	10	2	(010)
566.27120	0.1464	29	3	26	28	4	25	(000)
567.61545	0.3267	15	6	9	14	5	10	(010)
567.75501	0.3361	16	7	10	15	6	9	(010)
600.73934	0.5430	13	12	2	12	11	1	(010)
601.72375	0.6402	14	10	5	13	9	4	(010)
602.12444	0.4878	16	9	8	15	8	7	(000)
602.72913	0.4290	16	9	7	15	8	8	(000)
604.44870	0.1486	11	6	6	10	3	7	(010)
605.86831	0.4598	17	7	10	16	6	11	(000)
606.71780	0.5039	17	8	9	16	7	10	(000)
606.86993	0.4710	16	8	9	15	7	8	(010)
607.01311	0.4826	18	8	11	17	7	10	(000)
608.08854	0.3454	15	9	7	14	8	6	(010)
608.13399	0.5096	13	13	1	12	12	0	(010)
608.20167	0.4872	15	9	6	14	8	7	(010)
608.48603	0.1846	16	6	10	15	5	11	(010)
609.68135	0.4107	14	13	1	13	12	2	(000)
609.71656	0.1523	11	2	9	10	1	10	(010)
610.38170	0.2933	16	8	8	15	7	9	(010)
612.24055	0.1885	24	8	17	23	7	16	(000)
612.63289	0.4486	15	11	4	14	10	5	(000)
614.57714	0.3551	15	5	10	14	4	11	(000)
615.13815	0.5979	14	11	3	13	10	4	(010)
615.87635	0.3337	19	8	12	18	7	11	(000)
616.45096	0.4927	14	14	0	13	13	1	(000)
618.17573	0.1552	11	3	9	10	0	10	(010)
618.85541	0.3326	22	8	15	21	7	14	(000)
619.65315	0.4188	15	5	10	14	4	11	(010)
619.66553	0.1175							art
620.32273	0.4357	20	8	13	19	7	12	(000)
620.57768	0.2130	12	6	7	11	3	8	(000)
620.65238	0.4576	16	10	7	15	9	6	(000)
620.69547	0.4417	16	10	6	15	9	7	(000)
621.03814	0.1934	21	8	14	20	7	13	(000)
622.88476	0.3786	17	7	10	16	6	11	(010)
623.05277	0.4289	17	9	9	16	8	8	(000)
624.16601	0.1355							OH
624.56303	0.4970	17	9	8	16	8	9	(000)
624.81813	0.4694	15	12	3	14	11	4	(000)
625.17351	0.5586	15	10	5	14	9	6	(010)
625.20825	0.2137	17	8	10	16	7	9	(010)
625.33542	0.1182							OH
625.66428	0.2852	12	5	8	11	2	9	(010)
625.78240	0.5645	14	12	2	13	11	3	(010)
626.32268	0.2354	13	5	9	12	2	10	(000)
630.21788	0.4920	16	9	8	15	8	7	(010)
630.53386	0.3255	16	9	7	15	8	8	(010)
631.51448	0.4401	18	8	10	17	7	11	(000)
632.68428	0.4843	17	8	9	16	7	10	(010)
632.77024	0.3230	14	4	10	13	3	11	(000)

TABLE 1—*Continued*

Wavenumber	Intensity	J'	K'_a	K'_c	J	K_a	K_c	(0v0)
633.09023	0.1261	12	2	10	11	1	11	(000)
633.81065	0.5675	14	13	1	13	12	2	(010)
634.59131	0.5063	15	13	2	14	12	3	(000)
635.11455	0.2971	12	4	9	11	1	10	(010)
635.39734	0.1004	12	3	10	11	0	11	(000)
635.94640	0.5407	16	11	5	15	10	6	(000)
639.09858	0.5944	15	11	4	14	10	5	(010)
639.25833	0.5547	14	14	0	13	13	1	(010)
639.97283	0.2179	13	3	10	12	2	11	(000)
640.88868	0.3989	18	8	11	17	7	10	(010)
642.01050	0.5580	15	14	1	14	13	2	(000)
642.23218	0.2664	13	6	8	12	3	9	(000)
642.65853	0.6405	18	9	10	17	8	9	(000)
642.78348	0.5673	17	10	8	16	9	7	(000)
642.91061	0.5273	17	10	7	16	9	8	(000)
644.18769	0.3768	18	7	11	17	6	12	(000)
645.51864	0.1442	14	4	10	13	3	11	(010)
646.09504	0.4727	18	9	9	17	8	10	(000)
647.04629	0.5352	15	15	0	14	14	1	(000)
648.02989	0.4940	16	10	7	15	9	6	(010)
648.05219	0.2888	16	10	6	15	9	7	(010)
648.62802	0.5403	16	12	4	15	11	5	(000)
650.26380	0.5349	15	12	3	14	11	4	(010)
651.50878	0.2383	17	9	9	16	8	8	(010)
651.58078	0.2059	13	4	10	12	1	11	(000)
652.30117	0.4796	17	9	8	16	8	9	(010)
652.36965	0.4983	17	6	11	16	5	12	(000)
653.79697	0.1258							OH
655.47558	0.3429	17	6	11	16	5	12	(010)
658.69005	0.6255	17	11	6	16	10	7	(000)
658.87174	0.6582	19	8	11	18	7	12	(000)
658.87174	0.6582	15	13	2	14	12	3	(010)
658.91865	0.5117	16	13	3	15	12	4	(000)
660.42037	0.3966	19	9	11	18	8	10	(000)
661.48313	0.3112	20	8	13	19	7	12	(010)
662.48822	0.5839	16	11	5	15	10	6	(010)
664.19669	0.5926	18	10	9	17	9	8	(000)
664.53574	0.4585	18	10	8	17	9	9	(000)
664.77462	0.1175							art
664.78334	0.1161	13	5	9	12	2	10	(010)
665.00942	0.5423	15	14	1	14	13	2	(010)
666.43201	0.3017	13	3	10	12	2	11	(010)
666.92459	0.5867	16	14	2	15	13	3	(000)
667.65486	0.5083	19	9	10	18	8	11	(000)
668.67687	0.5493	15	15	0	14	14	1	(010)
670.11273	0.4234	14	6	9	13	3	10	(000)
670.25455	0.2865	17	10	8	16	9	7	(010)

Wavenumber	Intensity	J'	K'_a	K'_c	J	K_a	K_c	(0v0)
702.30630	0.3356	19	11	9	18	10	8	(000)
702.37810	0.4514	19	11	8	18	10	9	(000)
703.69963	0.4930	17	17	0	16	16	1	(000)
703.71594	0.1567	14	4	11	13	1	12	(000)
703.76382	0.2503	15	6	10	14	3	11	(000)
704.29680	0.4268	20	10	11	19	9	10	(000)
705.36109	0.1135	11	5	6	10	2	9	(000)
705.77654	0.4767							art
705.77643	0.4861	18	13	5	17	12	6	(000)
706.16387	0.2940	20	10	10	19	9	11	(000)
707.08304	0.4109	17	13	4	16	12	5	(010)
707.44311	0.3722	18	11	8	17	10	7	(010)
707.45721	0.1447	18	11	7	17	10	8	(010)
707.67042*	0.2445	20	9	12	19	8	11	(010)
708.26088	0.2546	14	5	10	13	2	11	(010)
708.33956	0.2448	18	6	12	17	5	13	(000)
709.75494	0.2825	15	4	11	14	3	12	(010)
712.57127	0.2118	19	10	10	18	9	9	(010)
712.97183	0.3603	19	10	9	18	9	10	(010)
713.05216	0.4932	21	9	12	20	8	13	(000)
713.79192	0.2222	12	7	6	11	4	7	(000)
714.40047	0.4915	17	14	3	16	13	4	(010)
714.81549	0.6264	18	14	4	17	13	5	(000)
716.55537	0.6760	19	12	7	18	11	8	(000)
718.65746	0.3193	15	5	11	14	2	12	(000)
719.49361	0.4805	17	15	2	16	14	3	(010)
720.10263	0.4903	18	12	7	17	11	6	(010)
721.23345	0.2598	14	6	9	13	3	10	(010)
721.42276	0.1431	13	7	7	12	4	8	(000)
721.75104	0.6394	18	15	3	17	14	4	(000)
722.37214	0.4364	17	17	0	16	16	1	(010)
722.48368	0.2880	21	10	12	20	9	11	(000)
722.91670	0.4218	17	16	1	16	15	2	(010)
723.10053	0.6088	20	11	10	19	10	9	(000)
723.28313	0.3919	20	11	9	19	10	10	(000)
726.00050	0.4869	21	8	13	20	7	14	(000)
726.39964	0.5578	21	10	11	20	9	12	(000)
726.62928	0.6715	18	16	2	17	15	3	(000)
728.28407	0.6706	19	13	6	18	12	7	(000)
728.56502	0.1129	14	3	11	13	2	12	(010)
728.95342	0.1838	19	11	9	18	10	8	(010)
728.99050	0.3976	19	11	8	18	10	9	(010)
729.41598	0.6410	18	17	1	17	16	2	(000)
729.94740	0.6295	18	18	0	17	17	1	(000)
730.22320	0.4921	18	13	6	17	12	5	(010)
730.54469	0.3868	14	7	8	13	4	9	(000)
732.44626	0.3347	20	10	11	19	9	10	(010)

Wavenumber	Intensity	J'	K'_a	K'_c	J	K_a	K_c	(0v0)
763.26527	0.1852	22	11	11	21	10	12	(000)
763.49275	0.2520	20	12	9	19	11	8	(010)
763.78639	0.2249	24	10	15	23	9	14	(000)
766.73727	0.3414	19	6	13	18	5	14	(000)
767.14864	0.2933	23	10	13	22	9	14	(000)
767.20415	0.2580	19	15	5	18	14	4	(010)
767.26388	0.3629	16	5	12	15	2	13	(000)
767.30775	0.2556	23	9	14	22	8	15	(000)
768.02110	0.4484	20	15	5	19	14	6	(000)
770.08621	0.1778	19	19	1	18	18	0	(010)
771.40923	0.6035	21	13	8	20	12	9	(000)
771.75382	0.1903	19	16	4	18	15	3	(010)
772.57363	0.1004	16	4	12	15	3	13	(010)
773.63854	0.2553	19	18	2	18	17	1	(010)
773.83385	0.2216	19	17	3	18	16	2	(010)
774.00120	0.5466	20	16	4	19	15	5	(000)
774.53229	0.3054	20	13	8	19	12	7	(010)
778.11966	0.5172	20	17	3	19	16	4	(000)
778.70499	0.3984	20	20	1	19	19	0	(000)
778.77158	0.4053	22	12	11	21	11	10	(000)
778.88644	0.2152	22	12	10	21	11	11	(000)
780.37298	0.4918	20	18	2	19	17	3	(000)
780.66034	0.4359	20	19	2	19	18	1	(000)
781.79343	0.5054	21	14	7	20	13	8	(000)
782.44360	0.3227	23	11	12	22	10	13	(000)
783.29377	0.1945	21	12	9	20	11	10	(010)
783.48504	0.1349	20	14	7	19	13	6	(010)
783.76246	0.2464	17	6	12	16	3	13	(000)
783.79347	0.2157	16	6	11	15	3	12	(010)
785.57960	0.2196	17	7	11	16	4	12	(000)
788.38963	0.2196	15	3	12	14	2	13	(010)
789.94558	0.2435	20	15	6	19	14	5	(010)
790.12837	0.4959	21	15	6	20	14	7	(000)
791.49878	0.1025	0	0	0	0	0	0	art
791.50969	0.3349	21	7	14	20	6	15	(000)
791.97967	0.1252	22	13	9	21	12	10	(000)
792.01535	0.4598	22	13	10	21	12	9	(000)
793.70547	0.1439	14	3	12	13	0	13	(010)
793.90849	0.1848	13	6	7	12	3	10	(000)
794.12159	0.2282	18	5	13	17	4	14	(000)
794.67518	0.2074	20	16	5	19	15	4	(010)
795.69543	0.1536	21	13	8	20	12	9	(010)
796.57162	0.4249	21	16	5	20	15	6	(000)
797.18824	0.2277	24	11	14	23	10	13	(000)
797.55087	0.1782	20	17	4	19	16	3	(010)
797.60820	0.1224	20	19	2	19	18	1	(010)
798.12288	0.1195	23	12	12	22	11	11	(000)

670.31846	0.5213	17	10	7	16	9	8	(010)
671.36049	0.3754	14	5	10	13	2	11	(000)
671.75283	0.4293	18	9	10	17	8	9	(010)
671.86728	0.5751	17	12	5	16	11	6	(000)
672.67373	0.6014	16	15	1	15	14	2	(000)
673.57662	0.2120	18	9	9	17	8	10	(010)
674.15507	0.5165	16	12	4	15	11	5	(010)
674.53197	0.2964	16	5	11	15	4	12	(000)
675.62922	0.4858	20	9	12	19	8	11	(000)
676.09636	0.5364	16	16	0	15	15	1	(000)
676.55000	0.1517	12	3	10	11	0	11	(010)
679.24772	0.1172	16	5	11	15	4	12	(010)
679.77495	0.3179	19	8	11	18	7	12	(010)
680.81836	0.5320	18	11	8	17	10	7	(000)
680.84398	0.4064	18	11	7	17	10	8	(000)
682.24652	0.1567	12	6	7	11	3	8	(010)
682.65079	0.4845	17	13	4	16	12	5	(000)
683.29582	0.4766	16	13	3	15	12	4	(010)
684.77335	0.3801	19	10	10	18	9	9	(000)
685.28085	0.4680	17	11	6	16	10	7	(010)
685.59269	0.5134	19	10	9	18	9	10	(000)
687.47605	0.2254	21	9	13	20	8	12	(000)
687.98667	0.1086	13	4	10	12	1	11	(010)
688.33863	0.4757	19	7	12	18	6	13	(000)
689.03754	0.1578	13	2	11	12	1	12	(000)
689.72957	0.3166	20	9	11	19	8	12	(000)
690.02014	0.2722	20	8	12	19	7	13	(000)
690.05509	0.4528	16	14	3	15	13	2	(010)
690.22063	0.1359	13	3	11	12	0	12	(000)
691.19311	0.5173	17	14	3	16	13	4	(000)
691.37971	0.1349	19	9	11	18	8	10	(010)
691.79103	0.4157	18	10	9	17	9	8	(010)
691.95960	0.1955	18	10	8	17	9	9	(010)
693.11754	0.3870	15	4	11	14	3	12	(000)
693.52831	0.2483	19	7	12	18	6	13	(010)
694.48554	0.4650	16	15	2	15	14	1	(010)
694.51611	0.5792	18	12	6	17	11	7	(000)
695.28114	0.3893	22	9	14	21	8	13	(000)
696.52345	0.4286	16	16	1	15	15	0	(010)
697.05479	0.2115	14	3	11	13	2	12	(000)
697.44090	0.4530	17	12	5	16	11	6	(010)
697.56964	0.5178	17	15	3	16	14	2	(000)
697.91839	0.1411	11	6	5	10	3	8	(000)
698.46870	0.1818	23	9	15	22	8	14	(000)
698.77006*	0.1111	24	9	16	23	8	15	(000)
699.65764*	0.1152	24	9	16	23	8	15	(000)
701.77622	0.4661	17	16	1	16	15	2	(000)
732.51092	0.1988	13	2	11	12	1	12	(010)
733.38132	0.1280	20	10	10	19	9	11	(010)
734.98112	0.5245	17	5	12	16	4	13	(000)
737.79052	0.6404	19	14	5	18	13	6	(000)
737.85031	0.2445	20	7	13	19	6	14	(000)
737.95872	0.6405	20	12	9	19	11	8	(000)
737.97236	0.3222	20	12	8	19	11	9	(000)
738.04973	0.4628	18	14	5	17	13	4	(010)
738.45629	0.2110	22	9	13	21	8	14	(000)
738.87926	0.4915	22	10	13	21	9	12	(000)
740.56995	0.1629	11	7	4	10	4	7	(010)
741.20236	0.2949	17	5	12	16	4	13	(010)
742.00289	0.2901	14	4	11	13	1	12	(010)
742.06775	0.4951	16	6	11	15	3	12	(000)
742.12768	0.4469	19	12	8	18	11	7	(010)
742.43352	0.1039	12	6	6	11	3	9	(000)
743.12339	0.3231	21	11	11	20	10	10	(000)
743.34735	0.2416	15	7	9	14	4	10	(000)
743.57704	0.5860	21	11	10	20	10	11	(000)
743.72649	0.4309	18	15	4	17	14	3	(010)
744.21132	0.1628	14	2	12	13	1	13	(000)
744.81380	0.2705	14	3	12	13	0	13	(000)
745.23143	0.6514	19	15	4	18	14	5	(000)
746.58395	0.2422	22	10	12	21	9	13	(000)
747.31583	0.3938	18	16	3	17	15	2	(010)
747.96251	0.3273	18	18	1	17	17	0	(010)
748.78707	0.3674	18	17	2	17	16	1	(010)
749.74234	0.1273	15	6	10	14	3	11	(010)
749.77536	0.3139	20	11	10	19	10	9	(010)
749.86908	0.1269	20	11	9	19	10	10	(010)
750.16491	0.6721	20	13	7	19	12	8	(000)
750.69458	0.6660	19	16	3	18	15	4	(000)
751.18495	0.3086	16	4	12	15	3	13	(000)
752.26512	0.4034	15	3	12	14	2	13	(000)
752.71128	0.4227	19	13	7	18	12	6	(010)
752.88465	0.2351	23	10	14	22	9	13	(000)
754.20060	0.6575	19	17	2	18	16	3	(000)
754.86499	0.1329	15	5	11	14	2	12	(010)
754.92380	0.5795	19	19	0	18	18	1	(000)
755.68307	0.6026	19	18	1	18	17	2	(000)
755.98181	0.2605	15	4	12	14	1	13	(000)
758.71268	0.3065	21	12	10	20	11	9	(000)
758.73833	0.5374	21	12	9	20	11	10	(000)
760.11674	0.6202	20	14	6	19	13	7	(000)
761.00294	0.3462	19	14	6	18	13	5	(010)
761.47289	0.4148	16	7	10	15	4	11	(000)
762.27571	0.4249	22	11	12	21	10	11	(000)
798.36530	0.2892	23	12	11	22	11	12	(000)
798.56397	0.1383	20	18	3	19	17	2	(010)
798.75874	0.2254	15	2	13	14	1	14	(000)
799.06573	0.1118	15	3	13	14	0	14	(000)
801.21981	0.3439	21	17	4	20	16	5	(000)
801.36109	0.2363	21	21	0	20	20	1	(000)
802.81730	0.3852	22	14	8	21	13	9	(000)
802.98999	0.1725	13	7	6	12	4	9	(000)
803.50603	0.2252	16	5	12	15	2	13	(010)
804.11311	0.3531	21	18	3	20	17	4	(000)
804.19000*	0.1302	21	14	7	20	13	8	(010)
804.42324	0.3070	21	20	1	20	19	2	(000)
804.58205*	0.1103	21	14	7	20	13	8	(010)
805.22471	0.3552	21	19	2	20	18	3	(000)
805.99389	0.2177	16	3	13	15	2	14	(000)
806.69581	0.4440	17	4	13	16	3	14	(000)
808.03805	0.4137	16	4	13	15	1	14	(000)
811.55952	0.4627	22	15	7	21	14	8	(000)
811.93309	0.2835	23	13	11	22	12	10	(000)
811.96458	0.3843	23	13	10	22	12	11	(000)
811.97965	0.1856	21	15	6	20	14	7	(010)
813.75067	0.2746	23	8	15	22	7	16	(000)
814.51706	0.1330	12	8	5	11	5	6	(000)
815.30059	0.4788	18	7	12	17	4	13	(000)
816.15525	0.1429	21	16	5	20	15	6	(010)
816.45026	0.2785	17	5	13	16	2	14	(000)
816.68703	0.2957	24	12	13	23	11	12	(000)
817.15695	0.1864	24	12	12	23	11	13	(000)
817.20881*	0.1125	21	20	1	20	19	2	(010)
818.42382	0.4359	22	16	6	21	15	7	(000)
819.93233*	0.2082	21	17	4	20	16	5	(010)
822.18246*	0.1162	21	19	2	20	18	3	(010)
822.26460*	0.1341	21	18	3	20	17	4	(010)
822.95571	0.2227	22	22	0	21	21	1	(000)
823.18909	0.3983	23	14	9	22	13	10	(000)
823.53731	0.3860	22	17	5	21	16	6	(000)
825.63552	0.1842	20	6	14	19	5	15	(000)
826.13343	0.1538	16	7	10	15	4	11	(010)
826.97402	0.3396	22	18	4	21	17	5	(000)
827.04029	0.2362	22	21	1	21	20	2	(000)
827.70865	0.4713	18	6	13	17	3	14	(000)
828.75481	0.2857	22	19	3	21	18	4	(000)
828.83165	0.2512	22	20	2	21	19	3	(000)
831.19402	0.2332	24	13	12	23	12	11	(000)
832.31968	0.3132	23	15	8	22	14	9	(000)
832.92807	0.2104	17	4	13	16	3	14	(010)
835.45046	0.1785	25	12	13	24	11	14	(000)

TABLE 1—*Continued*

Wavenumber	Intensity	J'	K_a'	K_c'	J	K_a	K_c	(0v0)
835.55331	0.1698	14	8	7	13	5	8	(000)
839.57208	0.2469	23	16	7	22	15	8	(000)
842.89688	0.1814	24	14	10	23	13	11	(000)
843.54665*	0.0990	23	23	0	22	22	1	(000)
845.10003	0.2290	23	17	6	22	16	7	(000)
845.73149	0.2045	16	8	9	15	5	10	(000)
848.57312	0.1310	23	22	1	22	21	2	(000)
849.00507	0.2276	23	18	5	22	17	6	(000)
849.63800	0.1830	19	7	13	18	4	14	(000)
849.89257	0.1712	25	13	12	24	12	13	(000)
850.81073	0.3964	19	5	14	18	4	15	(000)
850.97520	0.1951	16	4	13	15	1	14	(010)
851.24837	0.1203	15	2	13	14	1	14	(010)
851.25820	0.1511	23	21	2	22	20	3	(000)
851.34264	0.1973	23	19	4	22	18	5	(000)
851.62563	0.1010	17	8	10	16	5	11	(000)
852.11657	0.1721	23	20	3	22	19	4	(000)
852.41199	0.2496	24	15	9	23	14	10	(000)
852.48943	0.1386	13	8	5	12	5	8	(000)
852.75443	0.1181	16	2	14	15	1	15	(000)
852.91156	0.2601	16	3	14	15	0	15	(000)
858.54341	0.3281	17	3	14	16	2	15	(000)
859.66033	0.1621	17	4	14	16	1	15	(000)
859.91051	0.1718	18	4	14	17	3	15	(000)
860.02730	0.1827	24	16	8	23	15	9	(000)
860.83946	0.2427	18	8	11	17	5	12	(000)
861.96455	0.1274	25	14	11	24	13	12	(000)
864.04819	0.1623	18	6	14	17	3	14	(010)
864.62304*	0.1437	24	24	0	23	23	1	(000)
865.68669	0.3539	18	5	14	17	2	15	(000)
865.92987*	0.1614	24	17	7	23	16	8	(000)
866.17192*	0.1237	24	17	7	23	16	8	(000)
870.24464	0.1431	24	18	6	23	17	7	(000)
871.84116	0.1465	25	15	10	24	14	11	(000)
872.97092*	0.1659	19	6	14	18	3	15	(000)
872.97092*	0.1659	24	19	5	23	18	6	(000)
873.05353	0.1227	24	22	2	23	21	3	(000)
874.39734	0.1094	24	20	4	23	19	5	(000)
874.93458	0.1001	19	8	12	18	5	13	(000)
879.79967	0.1237	25	16	9	24	15	10	(000)
883.07297	0.1501	15	7	8	14	4	11	(000)
883.31545	0.2428	21	6	15	20	5	16	(000)
886.04332	0.1060	25	17	8	24	16	9	(000)
887.40891	0.2749	20	7	14	19	4	15	(000)
894.63740	0.2332	20	8	13	19	5	14	(000)
902.29342	0.1563	17	3	14	16	2	15	(010)
903.53332	0.1797	18	5	14	17	2	15	(010)
904.62103	0.1895	23	7	16	22	6	17	(000)
904.67827	0.1510	20	5	15	19	4	16	(000)
906.22841	0.2622	17	2	15	16	1	16	(000)
906.30980	0.1082	17	3	15	16	0	16	(000)
906.75378	0.1767	15	8	7	14	5	10	(000)
910.05108	0.1386	16	3	14	15	0	15	(010)
910.09980	0.1896	18	3	15	17	2	16	(000)
910.71027	0.4266	18	4	15	17	1	16	(000)
911.23428	0.4688	19	4	15	18	3	16	(000)
913.98373	0.1064	13	9	4	12	6	7	(000)
914.60786	0.2387	19	5	15	18	2	16	(000)
918.82257	0.4750	20	6	15	19	3	16	(000)
919.87598	0.1199	21	8	14	20	5	15	(000)
921.39854	0.1148	15	6	9	14	3	12	(000)

The strongest lines belong to the pure rotational spectrum of the ground (000) and first excited bending level (010). Except for some OH lines, the rest of the transitions belong to the pure rotational spectrum of higher excited vibrational levels such as (100), (020), (001) and to the rovibrational bands ν_2, $2\nu_2 - \nu_2$. About 250 lines belong to the pure rotational spectrum of water in the ground and (010) vibrational states. These lines have an intensity between 0.7 and 0.3 in relative units (r.u.). At least half of the approximately 1000 lines with an intensity between 0.3 and 0.1 also belong to these states. The lowest observable intensity was about 0.003 relative units. Some of the more than 3000 lines with intensity between 0.1 and 0.003 r.u. also belong to the ground and (010) states, but the majority of them are due to the pure rotational transitions of higher vibrational states and rovibrational bands.

Lines with J rotational quantum numbers between 9 and 13, which are quite strong in room temperature spectra, suffered from self absorption caused by cooler water at the ends of the cell, atmospheric water and trace amounts of water in the spectrometer. Because of the Doppler effect, the high temperature emission lines are broader than the cooler absorption lines. The cooler water thus removes the line center from the emission lines, resulting in doublet line artifacts. As a rule, the line centers of these doublets were found to be shifted to the right and to the left by approximately 0.005 cm^{-1} from the line center of the room temperature transition. For completeness they are listed in Table 1 and the weaker components of such artifact doublets are marked by the letters ''art.''

A comprehensive analysis of the present spectrum would require a reliable calculation of the energy levels for the first few vibrational states up to very high values of the rotational quantum numbers. This could be done using variational calculations, since this approach allows the simultaneous calculation of energy levels and intensities of the lines. The only problem is the accuracy of the potential energy and dipole moment surfaces. Recently (*34*) a potential energy surface good enough to reliably predict highly excited rotational states has been obtained. Reliable dipole moment surfaces are also available (*35*). Work on the comprehensive assignment of all the lines in the present spectrum is underway.

Nevertheless, the assignment of the strongest lines of the spectrum, belonging to the ground and (010) states, can be achieved using both the available experimental energy levels

TABLE 2

Energy Levels of Water (in cm^{-1}) Obtained from the Wavenumbers of the Hot Water Spectrum for the Ground Vibrational State

J	K_a	K_c	Position	
14	0	14	2073.5180	a
14	1	14	2073.5187	a
14	1	13	2327.8912	a
14	2	13	2327.9141	a
14	2	12	2550.8847	
14	3	12	2551.4857	
14	3	11	2739.4293	
14	4	11	2746.0276	
14	4	10	2880.8372	
14	5	10	2918.2482	
14	5	9	2983.3948	
14	6	9	3084.8380	
14	6	8	3101.4312	
14	7	8	3264.3393	
14	7	7	3266.5204	
14	8	7	3464.8864	
14	8	6	3465.0711	
14	9	6	3685.4075	
14	9	5	3685.4245	
14	10	5	3922.3192	
14	10	4	3922.3324	
14	11	4	4172.1503	c
14	11	3	4172.1503	c
14	12	3	4431.6326	c
14	12	2	4431.6326	c
14	13	2	4697.6622	c
14	13	1	4697.6622	c
14	14	1	4967.0541	c
14	14	0	4967.0541	c
15	0	15	2358.3044	a
15	1	15	2358.3047	a
15	1	14	2631.2718	a
15	2	14	2631.2816	a
15	2	13	2872.2774	
15	3	13	2872.5837	
15	3	12	3080.1792	
15	4	12	3083.8730	
15	4	11	3244.6032	
15	5	11	3269.5422	
15	5	10	3360.6047	
15	6	10	3443.1905	
15	6	9	3472.8835	
15	7	9	3624.1715	
15	7	8	3629.0981	
15	8	8	3824.5048	
15	8	7	3825.0000	
15	9	7	4045.2867	
15	9	6	4045.3208	
15	10	6	4283.3113	
15	10	5	4283.3132	
15	11	5	4534.9521	c
15	11	4	4534.9521	c
15	12	4	4796.9684	c
15	12	3	4796.9684	c
15	13	3	5066.2239	c
15	13	2	5066.2239	c
15	14	2	5339.6727	c
15	14	1	5339.6727	c
15	15	1	5614.1004	c
15	15	0	5614.1004	c
16	0	16	2660.9497	a
16	1	16	2660.9499	a
16	1	15	2952.3890	a
16	2	15	2952.3962	a
16	2	14	3211.0591	
16	3	14	3211.2160	
16	3	13	3437.2755	
16	4	13	3439.3099	
16	4	12	3623.7687	
16	5	12	3639.5413	
16	5	11	3758.4050	
16	6	11	3822.2508	
16	6	10	3870.2046	
16	7	10	4006.0755	
16	7	9	4016.1333	
16	8	9	4206.3336	
16	8	8	4207.5526	
16	9	8	4427.1244	
16	9	7	4427.2339	
16	10	7	4665.9732	
16	10	6	4665.9822	
16	11	6	4919.2577	c
16	11	5	4919.2577	c
16	12	5	5183.5801	c
16	12	4	5183.5801	c
16	13	4	5455.8871	c
16	13	3	5455.8871	c
16	14	3	5733.1485	c
16	14	2	5733.1485	c
16	15	2	6012.3464	c
16	15	1	6012.3464	c
16	16	1	6290.1968	c
16	16	0	6290.1968	c
17	0	17	2981.3630	a
17	1	17	2981.3631	a
17	1	16	3291.1485	a
17	2	16	3291.1522	a
17	2	15	3567.1783	
17	3	15	3567.2595	
17	3	14	3810.9396	
17	4	14	3812.0493	
17	4	13	4017.9118	
17	5	13	4027.5094	
17	5	12	4174.2910	
17	6	12	4221.0380	
17	6	11	4291.9110	
17	7	11	4409.3477	
17	7	10	4428.1191	
17	8	10	4610.0216	
17	8	9	4612.7933	
17	9	9	4830.6054	
17	9	8	4830.8966	
17	10	8	5070.0174	
17	10	7	5070.0350	
17	11	7	5324.6633	c
17	11	6	5324.6633	c
17	12	6	5591.1250	c
17	12	5	5591.1250	c
17	13	5	5866.2309	c
17	13	4	5866.2309	c
17	14	4	6147.0802	c
17	14	3	6147.0802	c
17	15	3	6430.7181	c
17	15	2	6430.7181	c
17	16	2	6714.1226	c
17	16	1	6714.1226	c
17	17	1	6993.8964	c
17	17	0	6993.8964	c
18	0	18	3319.4512	a
18	1	18	3319.4512	a
18	1	17	3647.4632	a
18	2	17	3647.4651	a
18	2	16	3940.5440	a
18	3	16	3940.5898	a
18	3	15	4201.2520	
18	4	15	4201.8588	
18	4	14	4427.1700	
18	5	14	4432.8650	
18	5	13	4606.1709	
18	6	13	4638.6487	
18	6	12	4735.8490	
18	7	12	4833.2126	
18	7	11	4865.2257	
18	8	11	5035.1322	
18	8	10	5040.8622	
18	9	10	5255.4518	
18	9	9	5256.1166	
18	10	9	5495.0933	
18	10	8	5495.1411	
18	11	8	5750.8534	
18	11	7	5750.8614	
18	12	7	6019.1794	c
18	12	6	6019.1794	c
18	13	6	6296.9014	c
18	13	5	6296.9014	c
18	14	5	6581.0464	c
18	14	4	6581.0464	c
18	15	4	6868.8312	c
18	15	3	6868.8312	c
18	16	3	7157.3474	c
18	16	2	7157.3474	c
18	17	2	7443.5386	c
18	17	1	7443.5386	c
18	18	1	7723.8438	c
18	18	0	7723.8438	c
19	0	19	3675.1160	a
19	1	19	3675.1160	a
19	1	18	4021.2177	a
19	2	18	4021.2187	a
19	2	17	4331.0723	a
19	3	17	4331.0930	a
19	3	16	4608.2251	a
19	4	16	4608.5572	d
19	4	15	4851.8241	
19	5	15	4855.1519	
19	5	14	5052.6696	
19	6	14	5074.2243	d
19	6	13	5199.6023	
19	7	13	5276.8065	d
19	7	12	5326.9873	
19	8	12	5481.1021	d
19	8	11	5492.0843	
19	9	11	5701.2826	d
19	9	10	5702.7871	
19	10	10	5940.8900	d
19	10	9	5941.0445	
19	11	9	6197.4474	
19	11	8	6197.4714	
19	12	8	6467.4088	c
19	12	7	6467.4088	c
19	13	7	6747.4635	c
19	13	6	6747.4635	c
19	14	6	7034.6919	c
19	14	5	7034.6919	c
19	15	5	7326.2778	c
19	15	4	7326.2778	c
19	16	4	7619.5258	c
19	16	3	7619.5258	c
19	17	3	7911.5480	c
19	17	2	7911.5480	c
19	18	2	8199.2217	c
19	18	1	8199.2217	c
19	19	1	8478.7676	c
19	19	0	8478.7676	c
20	0	20	4048.2524	a
20	1	20	4048.2524	a
20	1	19	4412.3168	a
20	2	19	4412.3173	a
20	2	18	4738.6237	a
20	3	18	4738.6359	a
20	3	17	5031.7959	d
20	4	17	5031.9799	
20	4	16	5292.1024	
20	5	16	5294.0407	
20	5	15	5513.2355	
20	6	15	5527.0467	
20	6	14	5680.7874	d
20	7	14	5739.2347	
20	7	13	5812.0743	d
20	8	13	5947.3100	
20	8	12	5966.8266	d
20	9	12	6167.7135	
20	9	11	6170.8317	
20	10	11	6407.0839	d
20	10	10	6407.4464	d
20	11	10	6664.1450	
20	11	9	6664.1731	
20	12	9	6935.4198	
20	12	8	6935.4301	
20	13	8	7217.5737	c
20	13	7	7217.5737	c
20	14	7	7507.5802	c
20	14	6	7507.5802	c
20	15	6	7802.7130	c
20	15	5	7802.7130	c
20	16	5	8100.2790	c
20	16	4	8100.2790	c
20	17	4	8397.6455	c
20	17	3	8397.6455	c
20	18	3	8691.9210	c
20	18	2	8691.9210	c
20	19	2	8979.8820	c
20	19	1	8979.8820	c
20	20	1	9257.4726	c
20	20	0	9257.4726	c
21	0	21	4438.7499	a
21	1	21	4438.7499	a
21	1	20	4820.6444	a
21	2	20	4820.6447	a
21	2	19	5163.0830	a
21	3	19	5163.0891	a
21	3	18	5471.8634	
21	4	18	5471.9684	d
21	4	17	5748.1247	
21	5	17	5749.2430	d
21	5	16	5987.8792	
21	6	16	5996.5192	d
21	6	15	6177.3580	
21	7	15	6219.6224	d
21	7	14	6318.5564	
21	8	14	6433.1124	d
21	8	13	6465.2352	d
21	9	13	6654.3026	d
21	9	12	6660.3621	d
21	10	12	6893.2154	d
21	10	11	6894.1131	d
21	11	11	7150.5698	d
21	11	10	7150.6609	d
21	12	10	7422.8833	c
21	12	9	7422.8858	c
21	13	9	7706.8290	c
21	13	8	7706.8290	c
21	14	8	7999.3671	c
21	14	7	7999.3671	c
21	15	7	8297.7086	c
21	15	6	8297.7086	c
21	16	6	8599.2846	c
21	16	5	8599.2846	c
21	17	5	8901.4988	c
21	17	4	8901.4988	c

TABLE 2—*Continued*

J	K_a	K_c	Position	
21	18	4	9201.7586	c
21	18	3	9201.7586	c
21	19	3	9497.1457	c,d
21	19	2	9497.1457	c,d
21	20	2	9784.3052	c,d
21	20	1	9784.3052	c,d
21	21	1	10058.8367	c,d
21	21	0	10058.8367	c,d
22	0	22	4846.4961	a
22	1	22	4846.4961	a
22	1	21	5246.0810	
22	2	21	5246.0810	
22	2	20	5604.3077	
22	3	20	5604.3119	
22	3	19	5928.3096	d
22	4	19	5928.3645	
22	4	18	6219.8886	
22	5	18	6220.5425	
22	5	17	6476.8335	d
22	6	17	6482.1609	d
22	6	16		
22	7	16	6717.1790	d
22	7	15		
22	8	15	6937.4118	d
22	8	14		
22	9	14	7160.5163	d
22	9	13	7171.5687	d
22	10	13	7399.2414	d
22	10	12	7400.8866	d
22	11	12	7656.3888	d
22	11	11	7656.4807	d
22	12	11	7929.4325	
22	12	10	7929.4562	
22	13	10	8214.8630	
22	13	9	8214.9012	
22	14	9	8509.6463	c
22	14	8	8509.6463	c
22	15	8	8810.9266	c
22	15	7	8810.9266	c
22	16	7	9116.1324	c
22	16	6	9116.1324	c
22	17	6	9422.8219	c
22	17	5	9422.8219	c
22	18	5	9728.4728	c
22	18	4	9728.4728	c
22	19	4	10030.5134	c,d
22	19	3	10030.5134	c,d
22	20	3	10325.9774	c,d
22	20	2	10325.9774	c,d
22	21	2	10611.3455	c,d
22	21	1	10611.3455	c,d
22	22	1	10881.7924	c,d
22	22	0	10881.7924	c,d
23	0	23	5271.3715	
23	1	23	5271.3715	
23	1	22	5688.5026	
23	2	22	5688.5026	
23	2	21	6062.1467	
23	3	21	6062.1467	
23	3	20	6400.9785	
23	4	20	6401.0138	d
23	4	19	6707.3426	
23	5	19	6707.7192	d
23	5	18	6980.3242	d
23	6	18	6983.5764	d
23	6	17	7211.3501	d
23	7	17		
23	7	16		
23	8	16		
23	8	15	7530.9297	d
23	9	15		
23	9	14	7704.7196	d
23	10	14	7924.4534	d
23	10	13	7927.6649	d
23	11	13		
23	11	12	8181.6850	d
23	12	12	8454.6036	d
23	12	11	8454.7541	d
23	13	11	8741.3893	d
23	13	10	8741.3971	d
23	14	10	9038.0521	c
23	14	9	9038.0521	c
23	15	9	9341.9660	c
23	15	8	9341.9660	c
23	16	8	9650.4987	c
23	16	7	9650.4987	c
23	17	7	9961.2324	c
23	17	6	9961.2324	c
23	18	6	10271.8270	c
23	18	5	10271.8270	c
23	19	5	10579.8154	c,d
23	19	4	10579.8154	c,d
23	20	4	10882.6300	c,d
23	20	3	10882.6300	c,d
23	21	3	11177.2356	c,d
23	21	2	11177.2356	c,d
23	22	2	11459.9186	c,d
23	22	1	11459.9186	c,d
23	23	1	11725.3390	c,d
23	23	0	11725.3390	c,d
24	0	24	5713.2512	
24	1	24	5713.2512	
24	1	23	6147.7603	
24	2	23	6147.7603	
24	2	22	6536.4428	
24	3	22	6536.4428	
24	3	21	6889.7206	d
24	4	21	6889.7365	
24	4	20	7210.3312	d
24	5	20	7210.5562	
24	5	19		
24	6	19		
24	6	18		
24	7	18		
24	7	17		
24	8	17		
24	8	16		
24	9	16		
24	9	15		
24	10	15	8468.5060	d
24	10	14		
24	11	14	8724.8531	d
24	11	13		
24	12	13	8998.3720	d
24	12	12		
24	13	12	9285.9481	d
24	13	11		
24	14	11	9584.2862	c
24	14	10	9584.2862	c
24	15	10	9890.4641	c
24	15	9	9890.4641	c
24	16	9	10201.9933	c
24	16	8	10201.9933	c
24	17	8	10516.4286	c,d
24	17	7	10516.4286	c,d
24	18	7	10831.4770	c,d
24	18	6	10831.4770	c,d
24	19	6	11144.7979	c,d
24	19	5	11144.7979	c,d
24	20	5	11454.2127	c,d

[a] Energy levels taken from Ref. *10.* [c] Energy levels obtained using unresolved doublets. [d] Energy levels which were not known previously.

(*10, 11*) and by extrapolation these levels and other available experimental data (*1–11*) using an effective Hamiltonian model.

In this work, the Padé–Borel (*4, 24*) method for the summation of the divergent perturbative effective Hamiltonian of the water molecule has been employed. A model with 30 parameters for fitting the available ground state data and 24 parameters for the (010) data was used. Recently very accurate fits to the available data on the ground and (010) states of water were achieved by Coudert (*27*). Accuracy close to the experimental error was obtained using a modified, exactly solvable model by Makarevicz (*38*) with 36 parameters for the (000) state and 31 for (010) state respectively. Our use of a 30 (000) and 24 (010) constant Padé–Borel model resulted in somewhat lower accuracy—up to a few wavenumbers for the calculation of the highest rotational quantum numbers levels obtained in this work. One of the reasons for this is the smaller number of fitted parameters. However, in most cases, this accuracy was enough for the assignment of the lines. Only in a few cases, involving the highest J and K_a quantum numbers, was the assignment ambiguous (see below). The transitions involving the rotational levels of the (000) and (010) vibrational states with rotational quantum numbers significantly higher than previously observed (*10, 11*) were assigned. In particular, transitions involving high J and high K_a ($\approx J$) were assigned up to $J = 25$ for the (000) state and for $J = 21$ for the (010) state. Levels up to $K_a = 20$ (000) and $K_a = 14$ (010) were previously known (*10, 11*). Some higher J, K_a transitions were also assigned; however, their intensities are lower than 0.1 r.u. and their assignment is less certain.

The measured values of the most intense (down to 0.1 r.u.) transition frequencies, together with their rotational quantum numbers, are presented in Table 1.[1] In a few cases, indicated by an asterisk, there is more than one candidate line for an assignment. More accurate variational calculations and/or the measurement of lines in other spectral regions will lead to the elimination of the ambiguity in the assignment as well as to the assignment of the weaker lines in the spectrum. The assignment of the lines of the (020) state and of the ν_2 vibration–rotation lines was made using the available literature data (*22*). These lines and the additional lines of the (000) and (010) levels weaker than 0.1 r.u. will be presented in a separate publication.

The water energy levels derived from the new transitions of Table 1 are presented in Tables 2 and 3. These energy levels were obtained from the observed lines by the addition of the lower state energy levels either taken from the work of Flaud *et al.* (*10*) for the 000 vibrational level and Camy-Peyret *et al.* (*11*) for the 010 level or, if available, from the energy levels obtained in this work. We do not list the lower J energy levels since they are

[1] The full line list is available from the Depository of Unpublished Data and from the authors on request.

TABLE 3

Energy Levels of Water (in cm^{-1}) Obtained from the Wavenumbers of the Hot Water Spectrum for the Excited Vibrational State (010)

J	K_a	K_c	Position	
12	0	12	3144.5732	a
12	1	12	3144.5794	a
12	1	11	3386.0534	a
12	2	11	3386.3820	a
12	2	10	3587.6693	a
12	3	10	3592.4256	
12	3	9	3738.5437	a
12	4	9	3770.8807	
12	4	8	3843.4063	
12	5	8	3940.5212	
12	5	7	3959.2550	
12	6	7	4123.2876	
12	6	6	4125.5965	
12	7	6	4329.3258	
12	7	5	4329.4988	
12	8	5	4557.5457	
12	8	4	4557.5585	
12	9	4	4803.8217	c
12	9	3	4803.8217	c
12	10	3	5064.1338	c
12	10	2	5064.1338	c
12	11	2	5334.8713	c
12	11	1	5334.8713	c
12	12	1	5612.4869	c
12	12	0	5612.4869	c
13	0	13	3391.1305	a
13	1	13	3391.1349	a
13	1	12	3654.0504	a
13	2	12	3654.2181	a
13	2	11	3877.0903	
13	3	11	3879.7199	a
13	3	10	4052.8140	
13	4	10	4074.0401	
13	4	9	4174.0408	
13	5	9	4252.4526	
13	5	8	4285.6493	
13	6	8	4437.4014	d
13	6	7	4442.7148	
13	7	7	4643.3781	
13	7	6	4643.8731	
13	8	6	4871.9516	
13	8	5	4871.9807	
13	9	5	5119.3779	c
13	9	4	5119.3779	c
13	10	4	5381.5546	c
13	10	3	5381.5546	c
13	11	3	5654.7733	c
13	11	2	5654.7733	c
13	12	2	5935.6106	c
13	12	1	5935.6106	c
13	13	1	6220.6209	c
13	13	0	6220.6209	c
14	0	14	3655.5180	a
14	1	14	3655.5187	a
14	1	13	3939.8912	a
14	2	13	3939.9141	a
14	2	12	4183.3919	a
14	3	12	4184.8360	
14	3	11	4382.7831	
14	4	11	4396.0533	
14	4	10	4525.2385	
14	5	10	4585.3512	
14	5	9	4638.3524	
14	6	9	4774.0460	
14	6	8	4785.0043	
14	7	8	4980.2250	
14	7	7	4981.4710	d
14	8	7	5208.8984	
14	8	6	5208.9907	
14	9	6	5457.2392	
14	9	5	5457.2464	
14	10	5	5721.1016	c
14	10	4	5721.1016	c
14	11	4	5996.6928	c
14	11	3	5996.6928	c
14	12	3	6280.5557	c
14	12	2	6280.5557	c
14	13	2	6569.4213	c,d
14	13	1	6569.4213	c,d
14	14	1	6859.8792	c
14	14	0	6859.8792	c
15	0	15	3937.5753	a
15	1	15	3937.5763	a
15	1	14	4243.1121	a
15	2	14	4243.1622	a
15	2	13	4506.7671	
15	3	13	4507.5223	a
15	3	12	4728.3037	
15	4	12		
15	4	11	4894.5909	
15	5	11	4938.2569	
15	5	10	5015.7065	
15	6	10	5132.5025	
15	6	9	5152.9667	
15	7	9	5339.4931	
15	7	8	5342.3487	
15	8	8	5568.0938	
15	8	7	5568.3568	
15	9	7	5817.0792	
15	9	6	5817.1001	
15	10	6	6082.4127	c
15	10	5	6082.4127	c
15	11	5	6360.2002	c
15	11	4	6360.2002	c
15	12	4	6646.9566	c
15	12	3	6646.9566	c
15	13	3	6939.4274	c,d
15	13	2	6939.4274	c,d
15	14	2	7234.4307	c,d
15	14	1	7234.4307	c,d
15	15	1	7528.5561	c,d
15	15	0	7528.5561	c,d
16	0	16	4237.3240	a
16	1	16	4237.3245	a
16	1	15	4564.0860	a
16	2	15	4564.1140	a
16	2	14	4847.1880	a
16	3	14	4847.6264	
16	3	13	5089.3832	a
16	4	13	5094.0873	
16	4	12	5280.0959	
16	5	12	5310.2731	
16	5	11		
16	6	11	5512.0169	
16	6	10	5546.7429	d
16	7	10	5720.7217	
16	7	9	5726.6901	
16	8	9	5949.2186	
16	8	8	5949.8748	
16	9	8	6198.5747	
16	9	7	6198.6277	
16	10	7	6465.1300	
16	10	6	6465.1314	
16	11	6	6744.9009	c
16	11	5	6744.9009	c
16	12	5	7034.3553	c
16	12	4	7034.3553	c
16	13	4	7330.2524	c,d
16	13	3	7330.2524	c,d
16	14	3	7629.4825	c,d
16	14	2	7629.4825	c,d
16	15	2	7928.9162	c,d
16	15	1	7928.9162	c,d
16	16	1	8225.0796	c,d
16	16	0	8225.0796	c,d
17	0	17	4554.6252	a
17	1	17	4554.6255	a
17	1	16	4902.6111	a
17	2	16	4902.6230	a
17	2	15	5204.7549	a
17	3	15	5204.9945	a
17	3	14	5466.4074	
17	4	14		
17	4	13	5680.5545	
17	5	13		
17	5	12	5835.2897	d
17	6	12		
17	6	11	5965.7487	
17	7	11	6123.4382	
17	7	10	6134.9017	
17	8	10	6351.8983	
17	8	9	6353.4060	d
17	9	9	6601.3836	d
17	9	8	6601.5198	d
17	10	8	6868.8823	
17	10	7	6868.8932	
17	11	7	7150.4108	c,d
17	11	6	7150.4108	c,d
17	12	6	7442.3418	c,d
17	12	5	7442.3418	c,d
17	13	5	7741.4383	c,d
17	13	4	7741.4383	c,d
17	14	4	8044.6529	c,d
17	14	3	8044.6529	c,d
17	15	3	8348.9761	c,d
17	15	2	8348.9761	c,d
17	16	2	8651.8329	c,d
17	16	1	8651.8329	c,d
17	17	1	8947.4517	c,d
17	17	0	8947.4517	c,d
18	0	18	4889.4911	a
18	1	18	4889.4912	a
18	1	17	5258.6278	a
18	2	17	5258.6339	a
18	2	16	5579.3641	a
18	3	16	5579.4993	a
18	3	15		
18	4	15	5861.2418	a
18	4	14	6095.5060	a
18	5	14		
18	5	13		
18	6	13	6330.4537	d
18	6	12		
18	7	12	6547.0014	d
18	7	11		
18	8	11	6775.7904	d
18	8	10		
18	9	10	7025.1588	d
18	9	9	7025.4749	d
18	10	9	7293.3108	d
18	10	8	7293.3432	d
18	11	8	7576.3363	d
18	11	7	7576.3395	d
18	12	7	7870.5134	c,d
18	12	6	7870.5134	c,d
18	13	6	8172.5650	c,d
18	13	5	8172.5650	c,d
18	14	5	8479.4880	c,d
18	14	4	8479.4880	c,d
18	15	4	8788.3794	c,d
18	15	3	8788.3794	c,d
18	16	3	9096.2919	c,d
18	16	2	9096.2919	c,d
18	17	2	9400.6200	c,d
18	17	1	9400.6200	c,d
18	18	1	9695.4142	c,d
18	18	0	9695.4142	c,d
19	0	19	5241.7443	a
19	1	19	5241.7443	a
19	1	18	5632.0440	a
19	2	18	5632.0475	a
19	2	17	5970.9398	a
19	3	17	5970.9971	a
19	3	16		
19	4	16		
19	4	15	6525.0581	a
19	5	15		
19	5	14		
19	6	14		
19	6	13		
19	7	13		
19	7	12	7023.9820	d
19	8	12		
19	8	11	7226.7763	d
19	9	11		
19	9	10		
19	10	10	7738.0462	d
19	10	9	7738.1306	d
19	11	9	8022.2966	d
19	11	8	8022.3013	d
19	12	8	8318.4672	c,d
19	12	7	8318.4672	c,d
19	13	7	8623.2247	c,d
19	13	6	8623.2247	c,d
19	14	6	8933.5679	c,d
19	14	5	8933.5679	c,d
19	15	5	9246.6922	c,d
19	15	4	9246.6922	c,d
19	16	4	9560.1332	c,d
19	16	3	9560.1332	c,d
19	17	3	9870.1257	c,d
19	17	2	9870.1257	c,d
19	18	2	10174.2585	c,d
19	18	1	10174.2585	c,d
19	19	1	10465.5004	c,d
19	19	0	10465.5004	c,d
20	0	20	5611.3316	a
20	1	20	5611.3316	a
20	1	19	6022.7991	a
20	2	19	6022.8011	a
20	2	18	6379.3666	a
20	3	18	6379.4036	a
20	3	17		
20	4	17		
20	4	16		
20	5	16		
20	5	15		
20	6	15		
20	6	14		
20	7	14		
20	7	13		
20	8	13		
20	8	12		
20	9	12		
20	9	11		
20	10	11		
20	10	10		
20	11	10	8487.9069	d
20	11	9	8487.9153	d
20	12	9	8785.7941	c,d
20	12	8	8785.7941	c,d
20	13	8	9092.9995	c,d
20	13	7	9092.9995	c,d
20	14	7	9406.7097	c,d

TABLE 3—*Continued*

J	K_a	K_c	Position	
20	14	6	9406.7097	c,d
20	15	6	9723.5135	c,d
20	15	5	9723.5135	c,d
20	16	5	10041.3674	c,d
20	16	4	10041.3674	c,d
20	17	4	10357.6841	c,d
20	17	3	10357.6841	c,d
20	18	3	10668.4944	c,d
20	18	2	10668.4944	c,d
20	19	2	10972.0620	c,d
20	19	1	10972.0620	c,d
20	20	1		
20	20	0		
21	0	21	5998.1661	a
21	1	21	5998.1661	a
21	1	20	6430.7950	a
21	2	20	6430.7950	a
21	2	19	6804.4702	a
21	3	19	6804.4900	a
21	3	18		
21	4	18		
21	4	17		
21	5	17		
21	5	16		
21	6	16		
21	6	15		
21	7	15		
21	7	14		
21	8	14		
21	8	13		
21	9	13		
21	9	12		
21	10	12		
21	10	11		
21	11	11		
21	11	10		
21	12	10		
21	12	9	9271.1998	d
21	13	9	9581.4895	c,d
21	13	8	9581.4895	c,d
21	14	8	9897.1895	c,d
21	14	7	9897.1895	c,d
21	15	7	10218.6894	c,d
21	15	6	10218.6894	c,d
21	16	6	10539.6687	c,d
21	16	5	10539.6687	c,d
21	17	5	10861.2997	c,d
21	17	4	10861.2997	c,d
21	18	4	11179.9487	c,d
21	18	3	11179.9487	c,d
21	19	3	11490.6769	c,d
21	19	2	11490.6769	c,d
21	20	2		
21	20	1		

[a] Energy levels taken from Ref. *11*.
[c] Energy levels obtained using unresolved doublets.
[d] Energy levels which were not known previously.

well known and, moreover, they are poorly determined from our emission spectra. For completeness we have added all known high J energy levels to Tables 2 and 3, even when our spectra do not provide new values. Note that possible confusion in the assignment of lines in Table 1 leads to ambiguities in the energy levels with the highest rotational quantum numbers of Tables 2 and 3.

IV. CONCLUSION

The emission spectrum of hot water (1550°C) was observed in the spectral region between 373 and 931 cm^{-1}. The wavenumbers of more than 4000 lines with an intensity from 0.7 down to 0.003 relative units were measured. More than 600 of the strongest lines belonging to the pure rotational spectrum in the ground (000) and first excited bending (010) vibrational levels were assigned. From the line positions, energy levels of the (000) and (010) states were derived with significantly higher rotational quantum numbers than previously available.

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