JOURNAL OF MOLECULAR SPECTROSCOPY **186,** 422–447 (1997)
ARTICLE NO. MS977449

High-Temperature Rotational Transitions of Water in Sunspot and Laboratory Spectra

Oleg L. Polyansky,*[,1] Nikolai F. Zobov,*[,1] Serena Viti,* Jonathan Tennyson,*
Peter F. Bernath,†[,2] and Lloyd Wallace‡

*Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom;
†Departments of Chemistry and Physics, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1;
and ‡National Optical Observatories, P.O. Box 26732, Tucson, Arizona 85732

Received August 22, 1997

Assignments are presented for spectra of hot water obtained in absorption in sunspots ($T \sim 3000$°C and $750 \leq \tilde{\nu} \leq 1010$ cm^{-1}) and in emission in the laboratory ($T \sim 1550$°C and $370 \leq \tilde{\nu} \leq 930$ cm^{-1}). These assignments are made using variational nuclear motion calculations based on a high-level *ab initio* electronic surface, with allowance for both adiabatic and nonadiabatic corrections to the Born–Oppenheimer approximation. Some 3000 of the 4700 transitions observed in the laboratory spectrum are assigned as well as 1687 transitions observed in the sunspot spectrum. All strong lines are now assigned in the sunspot measurements. These transitions involve mostly high-lying rotational levels within the (0,0,0), (0,1,0), (0,2,0), (1,0,0), and (0,0,1) vibrational states. Transitions within the (0,3,0), (0,4,0), (1,1,0), (0,1,1), (0,2,1), (1,1,1), (1,2,0), and (1,0,1) states are also assigned. For most bands the range of K_a values observed is significantly extended, usually doubled. New features observed include numerous cases where the closely degenerate levels $J_{K_aK_c}$ and $J_{K_aK_c+1}$ with high K_a are split by Coriolis interactions. Comparisons are made with the recent line list of Partridge and Schwenke (1997, *J. Chem. Phys.* **106,** 4618).

I. INTRODUCTION

The infrared spectrum of water is arguably the most important of all molecules because there are a multitude of applications. However, the spectrum of water is very complicated and the spectrum of hot water remains poorly understood. Detailed, line-by-line data on hot water are required for radiative transport models of many hot systems. Such systems include the spectra of oxygen-rich late-type stars (*1–3*) for which water vapor is the most important source of infrared opacity and substellar objects, such as brown dwarfs, for which water is the most abundant molecule after hydrogen (*4, 5*). Hot water is also one of the primary products of the combustion of hydrocarbons and has been detected in emission from forest fires (*6*) and from flames, for example, from an oxyacetylene torch (*7*). There are numerous military applications, including the simulation of rocket plumes (*8*) and the identification of ships, aircraft, helicopters, and tanks from their exhaust signatures.

Recently spectra of hot water have been observed in sunspots (*9–11*) and at lower temperatures in the laboratory (*12, 13*). The sunspot spectra were originally considered unassignable and only small portions of the laboratory spectra have been assigned on a case-by-case basis (*12–14*). However, in a recent paper (*15*), henceforth I, we demonstrated that by using a combination of high-level *ab initio* calculation and careful spectral analysis it was possible to assign a large number of new transitions in both these spectra. This assignment procedure represents a significant shift away from traditional, perturbation theory-based, methods of spectral assignment. In this paper we present full results of this analysis.

II. OBSERVED SPECTRA

Both the spectra under analysis have been published elsewhere and here we confine ourselves to brief details.

The sunspot spectrum was published in an atlas by Wallace *et al.* (*9–11*) in the wavenumber range $420 \leq \tilde{\nu} \leq 1233$ cm^{-1}. It was recorded using the 1-m Fourier transform spectrometer of the McMath–Pierce Solar Telescope of the National Solar Observatory on Kitt Peak at a resolution of about 0.005 cm^{-1}. At both ends of this spectrum there are significant gaps due to telluric absorption and some portions show many strong absorptions due to other molecules, such as SiO. However, the region $750 \leq \tilde{\nu} \leq 1010$ cm^{-1} is dominated by absorption due to water and we concentrated on this region.

The observed sunspot spectrum is highly congested with

Supplementary data for this article may be found on the journal home page (http://www.apnet.com/www/journal/ms.htm or http://www.europe.apnet.com/www/journal/ms.htm).

[1] Permanent address: Institute of Applied Physics, Russian Academy of Science, Uljanov Street 46, Nizhnii Novgorod, Russia 603024.

[2] Also: Department of Chemistry, University of Arizona, Tucson, AZ 85721.

0022-2852/97 $25.00

up to 50 lines per wavenumber. Prior to I, there were no assigned water transitions in the spectrum but many transitions could be attributed to water on the basis of a comparison with the laboratory spectrum described below. The assigned SiO vibration–rotation lines in the sunspot spectrum suggest a temperature of $T \sim 3200$ K (*9, 10*) and this temperature is assumed for the water lines.

The laboratory spectrum was obtained to confirm that the sunspot features were indeed due to water (*9*). The emission spectrum, details of which can be found in Polyansky *et al.* (*12*), was recorded using a Bruker Fourier transform spectrometer located at the University of Waterloo (*16*). It covers the wavenumber range $370 \leq \tilde{\nu} \leq 930$ cm^{-1} and was recorded at a temperature of 1550°C. This spectrum has a similar resolution ($\delta\tilde{\nu} \sim 0.01$ cm^{-1}) to the sunspot spectrum but is much less crowded because of the lower temperature. While many of the water lines in the sunspot spectrum are blended, the lines in the laboratory spectrum are nearly all resolved.

III. VARIATIONAL CALCULATIONS

Assignments were made using synthetic spectra generated from an *ab initio* line list. Comparisons could also be made with recently published line lists (*17–19*) based on calculations made with effective, spectroscopically determined potential energy surfaces. We note that, in general, these fitted potentials give line positions which have significantly smaller absolute errors than our *ab initio* line list, but that the errors in the *ab initio* line list are much more systematic. This smooth behavior of the errors proved to be crucial for making reliable assignments. The use of more than one line list is helpful for checking assignments. Similar remarks were made in the course of the recent analysis of the spectrum of H_3^+ (*20*); however, the spectroscopically determined H_3^+ line list reproduced the experimental data to much higher accuracy ($\sim$0.015 cm^{-1}) than any of the line lists available for water. A more detailed comparison of the line lists derived from fitted and *ab initio* potentials is given below.

Energy levels and wavefunctions were generated for our line list using a very high-quality *ab initio* (Born–Oppenheimer) potential energy surface due to Partridge and Schwenke (*21*). Allowance for non-Born–Oppenheimer effects was made by adding an *ab initio* mass-dependent adiabatic surface (*22*) and by adjusting the effective atomic masses to allow, in part, for nonadiabatic effects. Following Zobov *et al.* (*22*) we used an H atom mass of 1.007551 amu, midway between that of H and a proton, and an O atom of 15.990526 amu. Dipole transitions were calculated using the *ab initio* dipole surfaces of Gabriel *et al.* (*23*).

Calculations were performed using the DVR3D program suite (*24*) which was modified somewhat to improve performance for large calculations such as these. The calculations were performed using symmetrized Radau coordinates (r_1, r_2, θ) (*25*), which for water are close to, but more computationally convenient than, bond length–bond angle coordinates. We used a DVR grid of 40 points based on Gauss (-associated) Legendre polynomials in the θ coordinate. For the radial coordinates we used a DVR grid of 21 points with radial basis set parameters of $r_e = 2.06a_0$, $D_e = 0.14E_h$, and $\omega_e = 0.014E_h$, where r_e is the equilibrium radius, D_e is the dissociation energy, and ω_e is the fundamental frequency of the Morse oscillator-like functions upon which the DVR is based (*24*). This number of grid points is sufficient to obtain good convergence for low-lying vibrational levels (*26*).

In the first ''vibrational'' step we diagonalized a series of final secular problems of dimension 1000 from which we retained the lowest 500 eigenvalues and eigenvectors. For given J, the full rovibrational problem was solved using a basis of the $150 \times (J + 1)$ lowest solutions from the first step.

The number of eigenvalues obtained varied with J with no fixed rule. We computed eigenvalues with energies of up to at least 18 000 cm^{-1} for $J \leq 25$; for $J = 25$ this corresponds to the lowest 500 eigenvalues for each symmetry block. For $25 \leq J \leq 33$, eigenenergies up to 23 000 cm^{-1} were computed corresponding to 320 eigenvalues per symmetry block for $J = 33$. These criteria ensured that we covered all the energy levels belonging to the (000), (100), (010), (020), (001), and (030) vibrational states and of course, low K_a states of many higher vibrational bands are also included. Temperature-dependent spectra were generated using an adapted version of program SPECTRA (*27*) which uses full nuclear spin statistics and only rigorous dipole transition selection rules.

IV. SPECTRAL ANALYSIS

IV.1. Procedure

For both laboratory and sunspot spectra, assignments were made in a series of steps. First, all transitions between energy levels known from previous work (*7, 12, 13, 28–32*) were assigned. Such assignments, which we will call trivial, form only a minor part of both spectra. The next step was to use our line list to generate synthetic spectra at an appropriate temperature.

For the laboratory spectra, intensities were observed to vary from 0.7 to 0.003 in relative units (*12*). Synthetic spectra gave excellent line-by-line agreement in intensity over the entire dynamic range. This meant that intensities as well as line positions could be used as guides for assignment.

For the sunspot the situation is more complicated. Without implementing a detailed radiative transport model it is not possible to use the measured absorptions directly to give line intensities. Instead the sunspot spectrum was divided into four echelons on the basis of the strength of these absorptions. Strong transitions show 6–8% absorption, medium transitions show 4–6% absorption, weak ab-

TABLE 1

Assigned Line Frequencies (in cm^{-1}) of the Hot Water Spectrum Observed in Sunspots (Laboratory Frequencies Are Also Given where Observed)

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
722.04394	19	14	5	18	13	6	100	722.04435
722.77418	18	12	6	17	11	7	021	722.77494
722.91650	17	17	0	16	16	1	010	722.91670
723.28241	20	11	9	19	10	10	000	723.28313
723.41320	15	12	3	14	11	4	040	723.41290
724.48467	18	15	3	17	14	4	011	724.48594
726.00063	21	8	13	20	7	14	000	726.00050
726.07282	28	9	20	27	8	19	010	726.07234
726.40111	21	10	11	20	9	12	000	726.39964
726.52430	23	10	14	22	9	13	001	726.52496
726.62891	18	16	2	17	15	3	000	726.62928
727.45275	20	8	12	19	7	13	020	727.45297
727.54456	18	15	4	17	14	3	110	727.54527
727.86596	21	10	12	20	9	11	011	727.86725
728.99355	19	11	8	18	10	9	010	728.99050
729.05279	19	15	4	18	14	5	100	729.05455
731.07133	17	11	6	16	10	7	030	731.07147
732.44631	20	10	11	19	9	10	010	732.44626
732.51988	19	17	3	18	16	2	001	732.52150
732.54897	18	17	2	17	16	1	110	732.54934
732.57487	18	18	1	17	17	0	110	732.57392
733.57548	16	14	3	15	13	2	030	733.57691
733.69532	27	9	19	26	8	18	010	733.69445
733.99940	17	10	7	17	7	10	010	
734.29522	19	16	3	18	15	4	100	734.29504
735.87337	13	11	2	12	10	3	030-110	735.87369
738.45575	22	9	13	21	8	14	000	738.45629
738.52764	20	14	6	19	13	7	001	738.53003
738.54709	24	12	12	24	9	15	000	738.55265
738.78441	19	14	6	18	13	5	011	738.78398
738.87889	22	10	13	21	9	12	000	738.87926
740.12628	22	11	12	21	10	11	001	740.12682
740.21360	26	9	18	25	8	17	010	740.21165
743.12265	21	11	11	20	10	10	000	743.12339
743.34767	15	7	9	14	4	10	000	743.34735
744.58580	10	6	5	9	3	6	020	744.58153
746.38338	16	11	6	15	10	5	020-100	746.38438
746.40065	20	15	5	19	14	6	001	746.40038
746.58367	22	10	12	21	9	13	000	746.58395
747.31553	18	16	3	17	15	2	010	747.31583
747.91584	21	9	12	20	8	13	030-110	747.91872
748.78663	18	17	2	17	16	1	010	748.78707
749.01330	19	19	1	18	18	0	011	749.01292
749.16461	22	10	13	21	9	12	100-020	749.16205
749.25936	14	3	11	13	2	12	021	749.26107
749.35831	19	11	9	18	10	8	020	749.35865
749.46165	16	8	9	15	7	8	100-020	749.46501
750.32776	19	15	4	18	14	5	110	750.32796
750.69566	19	16	3	18	15	4	000	750.69458
750.76478	22	10	12	21	9	13	011	750.76684
750.95363	18	6	13	18	3	16	010	
751.72846	21	9	12	20	8	13	020	751.72929
752.00356	16	7	10	15	4	11	100	752.00330
752.02950	16	1	15	17	4	14	010-000	752.03059
752.09590	22	11	11	21	10	12	100	752.09679
752.53400	22	10	12	21	9	13	100-020	752.53469
753.26213	21	10	11	20	9	10	010	753.26375
753.45568	21	8	13	20	7	14	020	753.45813
753.69028	18	11	8	17	10	7	030	753.69071
753.71235	18	11	7	17	10	8	030	753.71269
753.73939	18	13	6	17	12	5	020	753.73943
754.82949	21	10	12	20	9	11	020-100	754.83005
754.86501	15	5	11	14	2	12	010	754.86499
754.92332	19	19	0	18	18	1	000	754.92380
755.18342	30	10	21	29	9	20	000	755.18262
755.28189	21	13	8	20	12	9	100	755.28166
755.33968	15	10	5	14	9	6	030	755.34075
756.19919	22	9	14	21	8	13	020	756.19878
756.23351	20	17	3	19	16	4	001	756.23340
756.36571	19	17	2	18	16	3	110	756.36592
756.46259	16	12	5	16	9	8	000	
756.50331	23	9	14	22	8	15	001	756.50303
756.56086	12	7	5	11	4	8	100	
756.63965	21	10	11	20	9	12	020-100	756.63928
756.73725	20	20	0	19	19	1	001	756.73764
756.76800	14	3	11	13	2	12	020	756.76801
756.80364	22	12	11	21	11	10	001	756.80479
756.88768	19	18	1	18	17	2	110	756.88726
756.93469	20	16	5	19	15	4	100	756.93530
756.96059	18	4	15	17	9	8	030-020	756.96015
756.99596	22	12	10	21	11	11	001	756.99519
757.01309	22	9	14	21	14	7	020-010	757.01390
758.34765	20	18	2	19	17	3	001	758.34803
758.47447	19	6	13	18	5	14	020	758.47437
758.61913	20	19	1	19	18	2	001	758.61822
758.90494	22	9	13	21	8	14	010	758.90567
759.29932	16	6	11	15	3	12	011	759.2998
759.51996	22	6	16	22	3	19	000	
759.53792	19	6	13	18	5	14	030	759.53683
759.68771	22	8	14	21	7	15	001	759.68663
759.88706	21	14	7	20	13	8	001	759.88585
759.91019	21	14	8	20	13	7	001	759.91124
760.01230	17	17	0	16	16	1	030	760.01046
760.11684	20	14	6	19	13	7	000	760.11674
760.18331	16	6	11	15	3	12	110	760.18640
760.41921	11	6	5	10	3	8	010	760.41834
760.59426	18	14	5	17	13	4	020	760.59492
760.82993	23	11	12	22	10	13	001	760.83306
760.91271	20	17	4	19	16	3	100	760.91264
761.00299	19	14	6	18	13	5	010	761.00294
761.35018	21	12	10	20	11	9	011	761.35092
761.44240	24	9	16	23	8	15	100-020	761.45104
761.47218	16	7	10	15	4	11	000	761.47289
761.57005	10	5	5	9	2	8	020	
762.03338	17	4	13	18	7	12	020-010	
762.22924	17	16	1	16	15	2	030	762.22937
762.27567	22	11	12	21	10	11	000	762.27571
762.52457	21	12	9	21	9	12	000	
763.49098	20	12	9	19	11	8	010	763.49275
763.50440	20	12	8	19	11	9	010	763.50310
763.64440	22	12	10	21	11	11	100	763.64369
763.67888	22	12	11	21	11	10	100	763.67879
763.72748	18	12	7	18	9	10	000	
763.78637	24	10	15	23	9	14	000	763.78639
763.90429	20	19	2	19	18	1	100	763.90529
764.24846	23	10	14	22	9	13	100-020	
764.48601	17	6	12	16	3	13	001	764.48728
764.63455	12	5	7	11	2	10	100	
764.94844	21	14	7	20	13	8	100	764.94825
765.05809	17	15	3	16	13	4	011-030	765.05776

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
765.45136	18	15	4	17	14	3	020	765.44731
765.48264	18	18	1	17	17	0	020	765.48272
765.77084	19	12	7	18	11	8	020	765.77063
765.79420	19	12	8	18	11	7	020	765.79491
766.40971	11	8	3	10	5	6	001	
766.43255	20	14	7	19	13	6	110	766.43329
766.73680	19	6	13	18	5	14	000	766.73727
767.14842	23	10	13	22	9	14	000	767.14864
767.20387	19	15	5	18	14	4	010	767.20415
767.23780	15	7	9	14	4	10	011	767.2405
767.26377	16	5	12	15	2	13	000	767.26388
767.30738	23	9	14	22	8	15	000	767.30775
767.32581	22	8	14	21	7	15	000	767.32519
767.44634	18	16	3	17	15	2	020	767.44652
767.65909	18	17	2	17	16	1	020	767.65948
767.80931	13	1	12	14	4	11	030-020	
768.00304	13	3	11	12	0	12	021	768.0043
768.02116	20	15	5	19	14	6	000	768.02110
768.21338	16	4	12	15	3	13	011	768.21439
768.23874	21	15	7	20	14	6	001	768.23903
768.40575	18	12	6	17	11	7	030	768.40527
768.43300	18	12	7	17	11	6	030	768.43331
768.75537	22	10	13	21	9	12	010	768.75525
769.18204	28	10	19	27	9	18	000	769.18219
769.56431	23	10	13	22	9	14	100-020	769.56922
769.86322	21	11	11	20	10	10	010	769.86391
769.88618	22	13	10	21	12	9	001	
769.90907	22	13	9	21	12	10	001	769.90835
770.27210	16	8	8	16	3	13	000	
770.37860	19	5	15	18	5	14	001-020	
770.44202							OH	
770.46018	22	8	14	21	7	15	010	770.46033
770.63230	20	11	9	19	10	10	020	770.63320
770.66756	20	11	10	19	10	9	020	770.66736
770.91114	25	10	16	24	9	15	000	770.91117
771.05243	20	15	5	19	14	6	011	771.05336
771.34220	24	10	14	23	9	15	001	771.34271
771.40893	21	13	8	20	12	9	000	771.40923
771.63397	20	20	0	19	19	1	011	
771.75369	19	19	1	18	18	0	010	771.75382
771.80062	15	6	10	14	3	11	021	771.7958
771.88944	17	2	15	18	5	14	010-000	771.88759
771.94510	10	7	4	9	4	5	010	771.94549
771.97154	13	7	6	12	4	9	001	771.97190
772.28027	17-	6	12	16	3	13	100	772.28082
772.36570	12	6	6	11	3	9	011	772.3534
772.42373	20	15	6	19	14	5	110	772.42559
772.57348	16	4	12	15	3	13	010	772.57363
772.78795	21	15	6	20	14	7	100	772.78810
772.84411	24	11	14	23	10	13	001	772.84444
772.99219	22	10	13	21	9	12	020-100	772.99249
773.10555	22	10	12	21	9	13	010	773.10508
773.14799	22	9	13	21	8	14	020	773.14823
773.20090	13	6	8	12	3	9	020	773.20064
773.29236	27	10	18	26	9	17	000	773.29125
773.63833	19	17	3	18	16	2	010	773.63854
773.75273	17	11	6	16	10	7	020-100	773.75240
773.83390	19	18	2	18	17	1	010	773.83385
773.92415	21	16	6	20	15	5	001	773.92430
774.00191	20	16	5	19	15	4	000	774.00120
774.20505	26	10	17	25	9	16	000	774.20495
774.25909	19	6	13	18	5	14	001	774.25956
774.53242	20	13	8	19	12	7	010	774.53229
774.84494	19	9	10	18	8	11	100-020	774.84229
774.90059	20	19	1	19	18	2	011	774.90252
775.10154	15	12	3	14	11	4	020-100	775.10170
775.42050	22	13	10	21	12	9	100	775.42340
775.43499	22	13	9	21	12	10	100	
775.64061	23	12	12	22	11	11	001	775.64073
775.81550	20	18	2	19	17	3	011	775.81394
776.10314	23	12	11	22	11	12	001	776.10266
776.21226	19	13	6	18	12	7	020	776.21226
776.74296	20	16	5	19	15	4	110	776.74231
777.33601	18	13	5	17	12	6	030	
777.35239	18	13	6	17	12	5	030	777.34851
777.40480	25	10	16	24	9	15	011	
777.46170	16	3	14	17	4	13	020-010	777.46195
777.72065	19	10	10	18	9	9	020	777.49800
777.86053	13	6	7	12	5	8	100-020	777.86055
777.89056	19	10	9	18	9	10	020	777.89044
778.11887	20	17	3	19	16	4	000	778.11966
778.32496	20	20	1	19	19	2	110	778.32466
778.70492	20	20	1	19	19	0	000	778.70499
778.77147	22	12	11	21	11	10	000	778.77158
778.88739	22	12	10	21	11	11	000	778.88644
778.90762	21	16	5	20	15	6	100	
779.10130	21	17	5	20	16	4	001	779.10062
779.39904	20	17	4	19	16	3	110	
779.43859	21	21	1	20	20	0	001	779.43876
779.47215	20	17	4	19	16	3	110	779.47200
779.64021	24	11	13	23	10	14	001	779.64051
779.96192	20	19	2	19	18	1	110	779.96324
780.14087	18	14	5	17	13	4	030	780.14082
780.37104	20	18	2	19	17	3	000	780.37298
780.38490	23	11	13	22	10	12	000	780.38396
780.44415	15	4	12	14	1	13	011	780.44477
780.46166	20	18	3	19	17	2	110	780.46346
780.56225	22	14	9	21	13	8	001	780.56326
780.57448	22	14	8	21	13	8	001	780.57369
780.65990	20	19	2	19	18	1	000	780.66034
780.87978	16	10	7	15	9	6	030	
781.30705	22	8	14	21	7	15	020	781.31340
781.79360	21	14	7	20	13	8	000	781.79343
781.87528	21	18	4	20	17	3	001	781.87806
781.89865							OH	
781.98434	15	2	13	14	1	14	001	781.9784
782.06317	21	14	8	20	13	7	011	782.06823
782.26594	21	20	2	20	19	1	001	782.26526
782.44253	23	11	12	22	10	13	000	782.44360
782.47326	23	12	12	22	11	11	100	
782.51471	18	18	1	17	17	0	030	782.51637
782.69163	23	12	11	22	11	12	100	782.69271
782.78082	20	15	6	19	15	5	020-001	782.78154
782.79769	15	3	13	14	0	14	001	782.79809
782.94170	23	9	14	22	8	15	010	782.94183
782.99864	21	19	3	20	18	2	001	782.99913
783.09899	16	7	10	15	4	11	011	783.0931
783.21376	14	1	14	15	2	13	010-000	783.21412
783.26301	20	14	6	19	13	7	010	783.26340
783.29325	20	14	7	19	13	6	010	783.29377
783.31467	21	17	4	20	16	5	100	783.31438
783.48484	19	14	5	18	13	6	020	783.48504

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
783.71408	15	8	8	14	5	9	001	
783.76240	17	6	12	16	3	13	000	783.76246
783.79257	16	6	11	15	3	12	010	783.79347
783.82498	15	2	13	14	1	14	100	783.82489
783.87335	14	4	11	13	1	12	020	783.87350
784.18795	21	12	10	20	11	9	010	784.18819
784.21321	21	12	9	20	11	10	010	784.21363
785.34103	16	4	12	15	3	13	020	785.34123
785.39401	18	5	14	18	2	17	000	785.39727
785.45829	22	14	8	21	13	9	100	785.45718
785.51816	22	14	9	21	13	8	100	785.51393
785.57986	17	7	11	16	4	12	000	785.57960
785.62223	21	7	14	20	6	15	010	785.62270
785.67794	21	21	0	20	20	1	100	785.67786
786.02901	21	7	14	20	6	15	100	
786.05212	18	17	2	17	16	1	030	786.05192
786.10983	21	18	3	20	17	4	100	786.11138
786.12582	21	7	14	20	6	15	100	786.12449
786.21282	25	11	15	24	10	14	001	786.21309
786.50895	13	8	6	12	5	7	001	786.50889
787.02775	21	20	1	20	19	2	100	787.02754
787.05862	18	16	3	17	15	2	030	
787.20550	20	12	9	19	11	8	020	787.20706
787.22271	20	12	8	19	11	9	020	787.22315
787.32271	21	19	2	20	18	3	100	787.32170
787.44465	21	14	7	20	13	8	110	787.44401
787.67098	16	5	12	15	2	13	011	787.6690
788.05391	19	19	0	18	18	1	020	788.05403
788.35670	24	11	13	23	10	14	100	788.36403
788.38964	15	3	12	14	2	13	010	788.38963
788.73465	24	10	14	23	9	15	000	788.73499
788.96800	19	15	4	18	14	5	020	788.96804
789.01446	18	15	4	17	14	3	030	
789.09005	16	3	13	15	2	14	100	789.09758
789.11385	18	15	4	17	14	3	030	789.11480
789.15382	22	11	12	21	10	11	010	789.15380
789.34477	22	15	7	21	14	8	001	789.34438
789.37140	22	15	8	21	14	7	001	789.37142
789.42442	23	13	11	22	12	10	001	789.42351
789.44217							OH	
789.46773	23	13	10	22	12	11	001	789.46841
789.51115	21	16	6	20	15	5	011	
789.52924	22	12	11	21	11	10	110	789.52827
789.71924	22	11	11	21	10	12	010	789.71889
789.94533	20	15	6	19	14	5	010	789.94558
789.96854	21	10	11	20	9	12	030	789.96966
790.05372							OH	
790.12834	21	15	6	20	14	7	000	790.12837
790.15660	17	4	13	16	3	14	100	790.15735
790.32220	14	6	9	13	3	10	020	790.32306
790.43318	19	12	7	18	11	8	030	790.43147
790.47039	19	12	8	18	11	7	030	790.46925
790.68284							OH	
790.72645	24	10	14	23	9	15	011	
791.01890	18	5	13	17	4	14	001	791.01922
791.16411	21	11	10	20	10	11	020	791.16186
791.28540							OH	
792.01478	22	13	10	21	12	9	000	792.01535
792.18520	24	9	15	23	8	16	001	792.18438
792.25865	14	2	12	13	1	13	010	792.25842
792.44842	11	0	11	12	3	10	030-020	792.4468
792.53057	19	17	2	18	16	3	020	792.53110
792.79343	16	3	13	15	2	14	001	792.79352
792.82324	21	15	7	20	14	6	011	
793.12875	22	13	9	21	12	10	011	
793.28141	21	21	1	20	20	0	011	
793.45396	12	7	6	11	4	7	010	793.45427
793.61145	24	12	13	23	11	12	001	793.61085
793.68449	22	15	8	21	14	7	100	793.68515
793.70548	14	3	12	13	0	13	010	793.70547
793.83633	21	15	6	20	14	7	110	793.83569
794.01530	16	4	13	15	1	14	100	794.01651
794.12174	18	5	13	17	4	14	000	794.12159
794.37451	20	20	1	19	19	0	010	794.37417
794.55860	24	12	12	23	11	13	001	794.55827
794.67515	20	16	5	19	15	4	010	794.67518
794.81473	14	2	13	15	3	12	020-010	794.8163
794.88343	23	13	10	22	12	11	100	794.88572
794.93769	23	13	11	22	12	10	100	794.93806
794.96222	21	7	14	20	6	15	030	794.96263
795.42817	23	10	13	22	9	14	020-100	795.42857
795.47285	22	16	6	21	15	5	001	795.47233
795.68121	21	13	9	20	12	8	010	795.68433
795.69561	21	13	8	20	12	9	010	795.69543
796.27020	23	9	14	22	8	15	020	796.27001
796.49503	15	4	12	14	1	13	010	796.49525
796.57142	21	16	5	20	15	6	000	796.57162
796.65903	20	11	9	19	10	10	030	796.66157
796.94212	20	11	10	19	10	9	030	796.94069
797.01150	20	5	16	21	6	15	010-000	797.01197
797.13680	18	7	12	17	4	13	100	797.13704
797.18841	24	11	14	23	10	13	000	797.18824
797.42218	21	20	2	20	19	1	011	797.42458
797.54970	20	17	4	19	16	3	010	797.55087
797.60796	20	19	2	19	18	1	010	797.60820
797.76720	21	17	5	20	16	4	011	797.76833
797.96376	20	13	8	19	12	7	020	797.96434
797.98326	20	13	7	19	12	8	020	797.98347
798.12276	23	12	12	22	11	11	000	798.12288
798.36493	23	12	11	22	11	12	000	798.36530
799.33689	21	19	3	20	18	2	011	
799.37517	22	13	10	21	12	9	110	799.37712
799.39011	21	18	4	20	17	3	011	
799.61875	21	21	0	20	20	1	110	
799.69816	19	13	6	18	12	7	030	799.69804
799.72716	19	13	7	18	12	6	030	
799.91958	23	12	12	22	11	11	011	
799.97152	13	7	7	12	4	8	010	799.96988
800.11946	17	6	12	16	3	13	011	800.11832
800.16980	22	16	7	21	15	6	100	800.16902
800.28193	24	9	15	23	8	16	000	800.28147
800.44417	25	11	15	24	10	14	100	
800.48075	10	6	4	9	3	7	020	800.48144
800.54929	24	12	13	23	11	12	100	800.55166
800.56373	23	14	10	22	13	9	001	
801.04878	24	12	12	23	11	13	100	
801.13174	22	17	5	21	16	6	001	801.13258
801.15934	22	22	0	21	21	1	001	801.15874
801.18627	17	5	13	16	2	14	001	801.18778
801.21987	21	17	4	20	16	5	000	801.21981
801.25258	24	11	13	23	10	14	000	801.25294
801.36149	21	21	0	20	20	1	000	801.36109

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
801.69371	21	17	4	20	16	5	110	801.69304
801.82800	21	20	1	20	19	2	110	
801.95782	17	8	10	16	5	11	001	801.95749
802.09369	24	10	15	23	9	14	020-100	802.09418
802.32973	12	6	6	11	3	9	010	802.32947
802.43038	19	14	5	18	13	6	030	
802.64542	17	5	13	16	2	14	100	802.64531
802.81738	22	14	8	21	13	9	000	802.81730
802.86666	22	14	8	21	13	9	011	
803.23299	21	19	2	20	18	3	110	
803.24748	21	18	3	20	17	4	110	
803.26638	15	2	13	16	5	12	020-010	803.27136
803.43721	18	5	13	17	4	14	020	803.43792
803.82219	19	19	0	18	18	1	030	803.82139
803.86823							OH	
804.11271	21	18	3	20	17	4	000	804.11311
804.18994	22	12	11	21	11	10	010	804.19000
804.24284	12	5	7	11	2	10	011	804.2391
804.27371	22	12	10	21	11	11	010	804.27309
804.32565	27	11	17	26	10	16	001	
804.42306	21	20	1	20	19	2	000	804.42324
804.50108	22	18	4	21	17	5	001	804.50061
804.58208	21	14	7	20	13	8	010	804.58205
804.68572	17	7	11	16	4	12	011	804.68462
804.84895	22	21	1	21	20	2	001	804.85601
804.86575	21	14	8	20	13	7	010	804.86734
804.99905							OH	
805.22490	21	19	2	20	18	3	000	805.22471
805.26089	17	10	7	16	9	8	030	805.26104
805.33666	23	14	9	22	13	10	100	805.33432
805.40350	22	10	13	21	9	12	030	
805.43141	21	8	13	20	13	8	020-010	805.43159
805.50091	24	9	15	23	8	16	100	805.50111
805.63651	20	14	7	19	13	6	020	805.63673
805.82438	25	11	14	24	10	15	100	805.82327
805.99295	16	3	13	15	2	14	000	805.99389
806.18411	14	7	8	13	4	9	010	806.18463
806.24357	18	5	13	17	4	14	011	806.24467
806.31892	22	19	3	21	18	4	001	806.31828
806.48844	22	20	2	21	19	3	001	806.48805
806.69561	17	4	13	16	3	14	000	806.69581
807.10164	22	22	1	21	21	0	100	807.10139
807.52346	23	11	13	22	10	12	010	807.52327
807.68688	22	14	9	21	13	8	110	
807.71630	22	14	8	21	13	9	110	
807.93186	21	12	10	20	11	9	020	807.93053
808.09090	21	12	9	20	11	10	020	808.08987
808.21037	24	13	12	23	12	11	001	
808.24222	22	18	5	21	17	4	100	808.24286
808.38471	24	13	11	23	12	12	001	808.38492
808.50508	19	18	1	18	17	2	030	808.50470
808.56581	18	4	15	19	5	14	010-000	808.57048
808.63193	23	11	12	22	10	13	010	808.63210
808.67593	23	12	11	22	11	12	110	808.67637
808.85085	23	8	15	22	7	16	110	
808.96588	22	21	2	21	20	1	100	808.96472
809.31904	25	10	16	24	9	15	010	809.31777
809.48170	20	20	1	19	19	0	020	809.48420
809.49536	23	9	14	22	8	15	030	
809.65744	23	8	15	22	7	16	010	809.65816
809.67575	24	9	15	23	8	16	010	809.67632
809.81222	23	15	9	22	14	8	001	809.81221
809.94741	22	19	4	21	18	3	100	809.94573
810.15138	22	20	3	21	19	2	100	810.15157
810.20353	15	6	10	14	3	11	020	810.20368
810.56403	25	12	14	24	11	13	001	810.55802
810.78939	22	11	12	21	10	11	020	810.78934
810.84470	19	17	2	18	16	3	030	
810.88538	22	11	11	21	10	12	020	810.88625
811.17614	19	16	3	18	15	4	030	811.17606
811.48203	24	10	14	23	9	15	010	811.48118
811.55875	22	15	7	21	14	8	000	811.55952
811.68991	20	15	6	19	14	5	020	811.69025
811.73307	20	12	8	19	11	9	030	811.73328
811.76875	20	12	9	19	11	8	030	811.76847
811.93316	21	15	6	20	14	7	010	811.93309
811.96329	23	13	10	22	12	11	000	811.96458
811.98065	21	15	6	20	14	7	010	811.97965
812.28964	23	13	11	22	12	10	011	
812.32022	25	11	15	24	10	14	000	812.31949
812.48061	25	12	13	24	11	14	001	
813.33012	19	15	4	18	14	5	030	813.32896
813.62951	26	11	16	25	10	15	100	813.62951
813.69021	24	13	12	23	12	11	100	813.69162
813.74952	23	8	15	22	7	16	000	813.75067
813.77430	18	6	13	17	3	14	100	813.77409
813.93685	23	15	8	22	14	9	100	813.93737
813.97536	20	19	2	19	18	1	020	813.97521
814.04293	22	22	0	21	21	1	011	
814.24929	15	7	9	14	4	10	010	814.24940
814.57264	22	15	8	21	14	7	110	814.57262
814.67519	20	16	5	19	15	4	020	814.67491
815.06103	17	6	11	16	3	14	020-100	815.0621
815.29939	18	7	12	17	4	13	000	815.30059
815.34041	20	6	14	19	5	15	020	815.34085
815.37386	13	8	5	12	5	8	001	
815.89689	21	21	0	20	20	1	010	815.89698
816.15377	22	13	10	21	12	9	010	816.15525
816.16776	20	18	3	19	17	2	020	816.16707
816.18535	22	13	9	21	12	10	010	816.18551
816.23067	23	16	8	22	15	7	001	816.23153
816.38474	20	17	4	19	16	3	020	816.38383
816.45021	17	5	13	16	2	14	000	816.45026
816.68719	24	12	13	23	11	12	000	816.68703
816.78575	26	10	17	25	9	16	010	816.78548
817.11452	12	0	12	13	3	11	020-010	817.1233
817.15644	21	16	5	20	15	6	010	817.15695
817.20830	24	12	12	23	11	13	000	817.20881
817.50472	20	6	14	19	5	15	100	
817.66308	21	10	12	20	9	11	020	
817.72043	25	12	14	24	11	13	100	
818.23392	26	11	15	25	10	16	001	818.23432
818.28099	14	8	7	13	5	8	100	818.28080
818.42443	22	16	6	21	15	7	000	818.42382
818.63497	25	12	13	24	11	14	100	818.63492
818.97908	22	21	1	21	20	2	011	
819.04725	21	13	8	20	12	9	020	819.04574
819.17057	21	10	11	20	9	12	020	819.16978
819.35247	21	13	9	20	12	8	020	819.3525
819.41328	15	2	14	14	2	13	001-020	819.41052
819.64970	22	17	5	21	16	6	011	
819.77699	12	1	12	13	2	11	020-010	819.77713

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
819.88919	24	14	11	23	13	10	001	
819.90783	24	14	10	23	13	11	001	819.90925
819.93223	25	11	14	24	10	15	000	819.93233
819.95860	22	22	1	21	21	0	110	
820.04700	16	2	14	15	1	15	101	820.0444
820.19005	21	20	1	20	19	2	010	820.19016
820.35515	11	7	5	10	4	6	021	820.3619
820.56021	8	7	2	7	4	3	020	
820.58010	21	17	5	20	16	5	010	820.58322
820.68036	27	10	18	26	9	17	010	820.68000
820.78257	23	16	7	22	15	8	100	820.78188
821.31672	20	13	7	19	12	8	030	
821.35932	20	13	8	19	12	7	030	821.35883
821.71994	22	20	2	21	19	3	011	
821.93908	22	18	4	21	17	5	011	
822.01486	23	23	1	22	22	0	001	822.01527
822.18211	21	19	2	20	18	3	010	822.18246
822.26491	21	18	3	20	17	4	010	822.26460
822.29253	17	6	12	16	3	13	010	822.29260
822.43895	23	17	7	22	16	6	001	
822.50898	22	21	2	21	20	1	110	
822.64497	22	19	3	21	18	4	011	
822.80512	15	3	12	14	2	13	020	822.80518
822.83806	12	5	7	11	2	10	010	822.84194
822.95584	22	22	1	21	21	0	000	822.95571
823.18929	23	14	9	22	13	10	000	823.18909
823.39840	23	12	12	22	11	11	010	823.39754
823.53729	22	17	6	21	16	5	000	823.53731
823.64008	23	12	11	22	11	12	010	823.64008
823.98641	20	6	14	19	5	15	010	823.98649
824.02840	20	20	1	19	19	0	030	
824.15148	20	14	7	19	13	6	030	
824.56435	24	14	11	23	13	10	100	824.56639
824.57913	24	14	10	23	13	11	100	
824.66604	24	11	14	23	10	13	010	824.66618
824.74165	19	7	13	18	4	14	001	824.74177
824.77501	22	20	3	21	19	2	110	
824.99584	17	4	13	16	3	14	011	825.0039
825.06590	22	14	8	21	13	9	010	825.06640
825.15427							OH	
825.26858	26	11	16	25	10	15	000	825.26774
825.50226							OH	
825.55455	26	10	16	25	9	17	001	
825.63587	20	6	14	19	5	15	000	825.63552
825.71921	22	19	4	21	18	3	110	
825.76677	22	14	9	21	13	8	010	825.76670
825.92934	25	13	13	24	12	12	001	
825.98089	23	17	6	22	16	7	100	825.97962
826.00433	25	13	13	24	12	12	001	826.00334
826.12955	16	7	10	15	4	11	010	826.13343
826.26700	23	18	6	22	17	5	001	826.26887
826.46602	23	22	2	22	21	1	001	826.46566
826.61216							OH	
826.97418	22	18	5	21	17	4	000	826.97402
827.03989	22	21	1	21	20	2	000	827.04029
827.05950	21	14	8	20	13	7	020	
827.07523	21	14	7	20	13	8	020	827.07384
827.11828	13	8	6	12	5	7	000	827.11815
827.32954	22	12	10	21	11	11	020	
827.44106	22	12	10	21	11	11	020	
827.47808							OH	
827.58848	23	23	0	22	22	1	100	827.59694
827.64404	17	3	14	16	2	15	101	827.6558
827.70829	18	6	13	17	3	14	000	827.70865
827.78371							OH	
827.93677	22	12	11	21	11	10	020	827.93654
828.29447	17	4	14	16	1	15	101	828.3064
828.55522	20	6	14	19	5	15	001	828.55489
828.66557	23	19	5	22	18	4	001	828.66516
828.71926	18	10	9	17	9	8	030	
828.75555	22	19	4	21	18	3	000	828.75481
828.83148	22	20	3	21	19	2	000	828.83165
828.87795	23	21	3	22	20	2	001	
828.91506	24	11	13	23	10	14	010	
829.14050	23	8	15	22	7	16	030	829.14066
829.39529	22	7	15	21	6	16	030	
829.52470	23	11	13	22	10	12	020	829.52570
829.55698	24	11	13	23	10	12	010	
829.57890	23	20	4	22	19	3	001	829.57665
829.60308	24	15	9	23	14	10	001	
829.62691	23	18	5	22	17	6	100	829.62712
829.71383	16	3	14	17	4	13	010-000	829.71457
829.73324	20	19	2	19	18	1	030	
829.75541	23	22	1	22	21	2	100	
829.82225	23	11	12	22	10	13	020	829.82241
829.84929	21	21	0	20	20	1	020	829.84958
829.99263	26	12	14	25	11	15	001	
830.73070	16	3	13	15	2	14	011	830.73105
830.80590	16	8	9	15	5	10	100	830.80668
830.91807	14	4	11	13	1	12	030	830.92025
831.07948	24	13	11	23	12	12	011	
831.19419	24	13	12	23	12	11	000	831.19402
831.25763	24	13	11	23	12	12	000	831.25789
831.32881	21	12	9	20	11	10	030	
831.63867	25	10	15	24	9	16	010	831.63877
831.73861	25	13	13	24	12	12	100	
831.75503	23	21	2	22	20	3	100	
831.77567	23	19	4	22	18	5	100	
831.79169	21	12	9	20	11	10	030	
831.85890	25	13	12	24	12	13	100	831.86113
832.26496	21	12	10	20	11	9	030	
832.32006	23	15	8	22	14	9	000	832.31968
832.47326	23	20	3	22	19	4	100	832.47484
832.59071	19	7	13	18	4	14	100	832.59066
832.67120	22	15	8	21	8	13	010-020	832.67118
832.92846	17	4	13	16	3	14	010	832.92807
833.14719	20	18	3	19	17	2	030	
833.23293	22	15	7	21	14	8	010	833.23378
833.52173	22	15	8	21	14	7	010	833.52166
833.54635	24	15	10	23	14	9	100	833.54674
833.62673	21	15	6	20	14	7	020	833.62666
833.89909	26	12	15	25	11	14	100	833.90045
833.99995	23	23	1	22	22	0	011	833.99855
834.19619	20	16	5	19	15	4	030	834.19661
834.37628	25	12	14	24	11	13	000	834.37582
834.61446	20	17	4	19	16	3	030	834.61421
834.83345	15	3	13	14	0	14	011	834.8327
834.92144	15	13	2	14	12	3	020-100	
835.05548	15	2	13	14	1	14	011	835.0646
835.14342	28	11	18	27	10	17	100	
835.33456	21	20	1	20	19	2	020	835.33433
835.36777	27	11	17	26	10	16	000	835.36950

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
835.45049	25	12	13	24	11	14	000	835.45046
835.53109	22	10	13	21	9	12	020	
835.55317	14	8	7	13	5	8	000	835.55331
835.68556	17	12	5	16	11	6	020-100	
835.88178	22	11	12	21	10	11	030	
835.89197	23	13	11	22	12	10	010	835.89141
835.97829	26	10	16	25	9	17	011	
836.00416	23	13	10	22	12	11	010	836.00367
836.32889	20	15	6	19	14	5	030	
836.38897	22	22	1	21	21	0	010	836.38869
836.41874	24	16	8	23	15	9	001	
837.00829	21	16	5	20	15	6	020	837.00805
837.06445	15	7	9	14	4	10	021	837.0633
837.08209	24	13	12	23	12	11	110	
837.21107	16	2	14	15	1	15	100	837.2069
837.29665	17	5	13	16	2	14	011	837.29594
837.46412	16	3	14	15	0	15	100	837.46418
837.84516	17	8	10	16	5	11	100	
837.98642	26	10	16	25	9	15	000	837.98670
838.08557	25	9	16	24	8	15	000	838.08589
838.48427	19	5	14	18	4	15	100	838.47388
838.50283	21	19	2	20	18	3	020	838.49973
838.54612	25	14	11	24	13	12	001	
838.77843	22	7	15	21	6	16	010	
838.80561	26	11	15	25	10	16	000	838.80594
838.87073	22	16	7	21	15	6	010	838.87129
839.27427	22	13	10	21	12	9	020	839.27451
839.30558	21	17	4	20	16	5	020	839.30593
839.38941	23	23	0	22	22	1	110	
839.40404	22	13	9	21	12	10	020	839.40287
839.49735	23	22	2	22	21	1	011	
839.51716								
839.57206	23	16	7	22	15	8	000	839.57208
839.69711							OH	
839.72368	25	9	16	24	8	17	100	839.72336
839.74831								
839.78004	21	18	3	20	17	4	020	839.78338
839.99249	25	9	16	24	8	17	010	839.99224
840.31878	14	7	7	13	4	10	000	840.31805
840.45325	27	12	16	26	11	15	001	
840.73376	24	16	9	23	15	8	100	840.73397
841.10250	15	8	8	14	5	9	000	841.10235
841.64853	22	21	2	21	20	1	010	841.64931
841.75107	25	11	15	24	10	14	010	841.75042
841.92194	24	12	13	23	11	12	010	841.92191
842.08337	23	22	1	22	21	2	110	
842.12925	24	24	0	23	23	1	001	
842.19604	21	13	8	20	12	9	030	842.19674
842.25750	21	13	9	20	12	8	030	
842.36490	24	12	12	23	11	13	010	842.36512
842.77040	22	17	6	21	16	5	010	842.77028
842.89530	24	14	11	23	13	10	000	842.89688
842.90826	24	14	10	23	13	11	000	842.90634
842.93033	17	3	14	16	2	15	001	
842.96116	28	11	18	27	10	17	000	842.96132
843.02101	23	21	3	22	20	2	011	
843.16148	21	21	0	20	20	1	030	
843.17932	25	14	11	24	13	12	100	843.17956
843.26400	17	7	11	16	4	12	010	843.26222
843.30268	17	3	14	16	2	15	100	843.30208
843.45889	23	18	6	22	17	5	011	
843.49623	26	13	14	25	12	13	001	
843.54660	23	23	0	22	22	1	000	
843.60629	16	5	12	15	2	13	020	843.60700
843.62570	17	4	14	16	1	15	001	843.62567
844.05109	26	13	13	25	12	14	001	
844.56254	30	11	20	29	10	19	000	844.56388
844.57987	22	20	3	21	19	2	010	844.58030
844.68984	25	11	14	24	10	15	010	844.69001
844.72524	23	20	4	22	19	3	011	
844.75294	17	4	14	16	1	15	100	844.75158
844.82947	19	5	14	18	4	15	001	844.82912
844.88353	23	19	5	22	18	4	011	
844.95293	18	4	14	17	3	15	100	844.95302
845.01699	22	18	5	21	17	4	010	845.01762
845.10071	23	17	6	22	16	7	000	845.10003
845.23069	14	2	12	13	1	13	020	845.23004
845.49714	21	14	7	20	13	8	030	845.49757
845.63516	22	19	4	21	18	3	010	845.63559
845.67480	23	14	9	22	13	10	010	845.67541
845.73083	16	8	9	15	5	10	000	845.73149
845.98615	23	14	10	22	13	9	010	845.98638
846.03430	15	3	12	14	2	13	030	846.03477
846.18627	16	3	13	15	2	14	010	846.18318
846.27880	24	17	8	23	16	7	100	846.27850
846.81158	23	12	11	22	11	12	020	846.81237
846.91681	23	20	3	22	19	4	110	
847.14529	24	23	1	23	22	2	001	
847.19851	24	18	6	23	17	7	001	847.20060
847.21712	24	24	1	23	23	0	100	847.21657
847.25876	24	11	14	23	10	13	020	847.25968
847.31549	18	4	14	17	3	15	001	847.31595
847.34583	17	4	13	18	7	12	010-000	847.34340
847.42854	22	14	8	21	13	9	020	847.42998
847.50714	27	12	15	26	11	16	001	
847.65832	22	7	15	21	6	16	000	847.65868
847.76823	22	14	9	21	13	8	020	847.76879
847.84428	9	7	2	8	4	5	020	
847.98607	25	9	16	24	8	17	020	847.98639
848.57305	23	22	1	22	21	2	000	848.57312
848.60420	25	15	11	24	14	10	001	848.60567
848.82697	14	3	12	13	0	13	020	848.82641
848.92558	12	9	3	11	6	6	001	
849.00492	23	18	5	22	17	6	000	849.00507
849.05749	26	13	14	25	12	13	100	849.05833
849.22365	22	22	1	21	21	0	020	849.22314
849.43224	24	23	2	23	22	1	100	
849.47190	27	12	16	26	11	15	100	
849.63800	19	7	13	18	4	14	000	849.63800
849.75544	25	13	13	24	12	12	000	849.75545
849.83199	21	20	1	20	19	2	030	
849.89256	25	13	12	24	12	13	000	849.89257
850.06047	18	5	14	17	2	15	001	850.06278
850.10453	24	19	5	23	18	6	001	850.10554
850.22313	24	22	2	23	21	3	001	
850.28598	24	18	7	23	17	6	100	850.28891
850.75836	17	4	13	16	3	14	020	850.75843
850.81056	19	5	14	18	4	15	000	850.81073
850.97509	16	4	13	15	1	14	010	850.97520
851.04881	26	12	15	25	11	14	000	851.04911
851.25927	23	21	2	22	20	3	000	851.25820
851.28095	18	5	14	17	2	15	100	851.28163

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
851.34245	23	19	4	22	18	5	000	851.34264
851.39046	23	10	14	22	9	13	020	
851.50474	19	10	9	18	9	10	030	
851.58658	24	20	4	23	19	3	001	851.58703
851.62643	17	8	10	16	5	11	000	851.62563
851.64892	24	21	3	23	20	4	001	
851.88506	19	5	14	18	4	15	110	851.88446
851.92108	22	12	10	21	11	11	030	
852.03584	15	3	13	14	0	14	010	852.03999
852.11736	23	20	3	22	19	4	000	852.11657
852.14389	22	12	11	21	11	10	030	852.14549
852.17556	24	22	3	23	21	2	100	
852.33805	27	12	15	26	11	16	100	
852.52188	25	15	10	24	14	11	100	852.52099
852.75346	16	2	14	15	1	15	000	852.75443
852.83446	24	19	6	23	18	5	100	852.83542
853.16239	26	12	14	25	11	15	000	853.16257
853.22534	26	10	16	25	9	17	010	853.22615
853.24330	24	24	0	23	23	1	011	
853.29333	17	7	11	16	4	12	010	853.29350
853.37688	14	6	8	13	3	11	000	853.37679
853.75044	24	21	4	23	20	3	100	
853.81716	23	15	8	22	14	9	010	853.81702
853.98022	24	20	5	23	19	4	100	
854.14343	21	19	2	20	18	3	030	
854.52078	23	15	7	22	14	8	010	
854.74760	24	13	12	23	12	11	010	854.74763
854.78887	22	15	8	21	14	7	020	854.78903
854.83587	11	4	7	10	3	8	100-020	
855.15951	24	13	11	23	12	12	010	855.15750
855.31488	23	10	13	22	9	14	020	
855.42010	24	8	16	23	7	17	010	
855.45942	25	13	12	24	12	13	110	855.45814
855.60278	22	21	2	21	20	1	020	855.60171
855.68035	19	6	14	18	3	15	001	855.68008
855.80917	25	16	10	24	15	9	001	
855.90674	23	23	0	22	22	1	010	855.90615
856.06938	26	11	16	25	10	15	010	856.06976
856.20289	14	14	1	13	13	0	020-100	
856.33105	21	16	5	20	15	6	030	
856.58555	21	18	3	20	17	4	030	
856.86270	26	14	12	25	13	13	001	856.86180
857.13337	17	4	13	16	3	14	030	857.13353
857.33814	21	17	4	20	16	5	030	
857.67657	20	8	13	19	5	14	001	
857.98416	24	24	1	23	23	0	110	
858.28118	27	11	16	26	10	17	000	858.28109
858.44349	21	15	6	20	14	7	030	
858.52043	22	16	7	21	15	6	020	858.52206
858.54303	17	3	14	16	2	15	000	858.54341
858.60674	19	6	14	18	3	15	100	858.61169
858.94059	25	12	14	24	11	13	010	858.94060
859.05380	23	13	10	22	12	11	020	859.05441
859.27292	24	23	1	23	22	2	011	
859.31010	24	8	16	23	7	17	100	
859.60417	23	13	11	22	12	10	020	
859.63374	22	20	3	21	19	2	020	
859.65906	17	4	14	16	1	15	000	859.66033
859.83993	23	16	7	22	15	8	010	859.83868
859.90949	18	4	14	17	3	15	000	859.91051
859.98874	27	13	15	26	12	14	001	
860.02601	24	16	8	23	15	9	000	860.02730
860.04071	25	16	9	24	15	10	100	
860.45528	25	16	9	24	15	10	100	
860.53326	24	23	2	23	22	1	110	
860.57876	26	14	13	25	13	12	100	
860.63639	25	12	13	24	11	14	010	860.63700
860.70475	14	3	11	15	6	10	020-010	860.6975
860.83931	18	8	11	17	5	12	000	860.83946
861.11572	26	14	13	25	13	12	100	
861.31456	22	17	6	21	16	5	020	861.31445
861.45115	22	22	1	21	21	0	030	
861.55172	25	25	1	24	24	0	001	
861.82306	22	19	4	21	18	3	020	861.82290
861.94242	25	14	12	24	13	11	000	861.94350
861.96468	25	14	11	24	13	12	000	861.96455
862.03501							OH	
862.04894	23	22	1	22	21	2	010	862.04925
862.23826	26	11	15	25	10	16	010	862.23640
862.31983	12	8	4	11	5	7	011	862.3231
862.35646	22	18	5	21	17	4	020	862.35590
862.71615	22	7	15	21	6	16	001	
862.74838	25	17	9	24	16	8	001	862.74933
863.01789	17	4	14	18	5	13	010-000	863.01927
863.05124	12	2	11	13	3	10	030-020	863.05226
863.07803	28	12	17	27	11	16	100	
863.18580	24	24	1	23	23	0	000	863.18595
863.31667	24	22	2	23	21	3	011	
863.71724	28	12	17	27	11	16	100	
864.04884	18	6	13	17	3	14	010	864.04819
864.15512	23	17	6	22	16	7	010	864.15518
864.25667	24	22	3	23	21	2	110	864.25890
864.33640	24	8	16	23	7	17	000	864.33691
864.57958	19	7	13	18	4	14	010	864.58302
864.60416	18	12	7	17	11	6	020-100	
864.62284	19	5	14	18	4	15	010	864.62304
864.95106	24	10	15	23	9	14	020	864.96001
865.36426	24	14	10	23	13	11	010	865.36453
865.46788	25	11	14	24	10	15	020	865.46927
865.52629	24	14	11	23	13	10	010	865.52623
865.63245	24	12	13	23	11	12	020	865.63409
865.68640	18	5	14	17	2	15	000	865.68669
865.73730	24	21	3	23	20	4	011	
865.80152	23	21	2	22	20	3	010	865.80141
865.90048	25	17	9	24	16	8	100	865.90170
865.92982	24	17	8	23	16	7	000	865.92987
865.98967	24	19	5	23	18	6	011	
866.00894	25	25	0	24	24	1	100	
866.12399	22	14	9	21	13	8	030	
866.17177	18	7	12	17	4	13	010	866.17192
866.36953	27	13	14	26	12	15	100	
866.42113	25	17	9	24	16	8	100	
866.47582	19	5	14	18	4	15	020	866.47763
866.49172	27	12	16	26	11	15	000	866.49155
866.56172							OH	
866.83452	26	15	12	25	14	11	001	
866.85385	26	15	11	25	14	12	001	
866.88022	23	18	5	22	17	6	010	866.87971
866.92587	27	13	14	26	12	15	100	
866.95308							OH	
866.97107	25	24	2	24	23	1	001	866.96425
867.19649	15	2	13	16	5	12	010-000	867.19648

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
867.33911	13	9	5	12	6	6	001	
867.38053	25	18	8	24	17	7	001	867.38007
867.56777	27	10	17	26	9	18	000	867.57346
867.58698	26	13	14	25	12	13	000	867.58626
867.64769	23	23	0	22	22	1	020	
867.70668	23	14	9	22	13	10	020	867.70740
867.74775	23	20	3	22	19	4	010	867.74877
867.78073	23	14	10	22	13	9	020	
867.87225	26	13	13	25	12	14	000	867.87310
868.02371	25	24	1	24	23	2	100	
868.10031	23	19	4	22	18	5	010	868.10065
868.29269	16	3	13	17	6	12	010-000	868.29597
868.79047	27	11	17	26	10	16	010	868.79056
868.87412	22	21	2	21	20	1	030	
869.07775	24	23	2	23	22	1	000	869.07782
869.64087	16	3	13	15	2	14	021	869.6407
870.24309	24	18	6	23	17	7	000	870.24464
870.31942	15	8	7	14	5	10	001	
870.47559	27	12	15	26	11	16	000	870.47552
870.57138	25	23	3	24	22	2	001	
870.68887	25	19	7	24	18	6	001	
870.87775	26	15	12	25	14	11	100	
871.10842	15	7	8	14	4	11	100	871.10644
871.17562	14	7	7	13	4	10	011	871.1736
871.40712	26	15	12	25	14	11	100	
871.46239	25	23	2	24	22	3	100	
871.84085	25	15	10	24	14	11	000	871.84116
871.94260	11	2	9	12	5	8	030-020	871.9381
872.45883	13	9	4	12	6	7	001	
872.56574	24	22	3	23	21	2	000	872.56591
872.64221	25	22	4	24	21	3	001	
872.65974	25	20	6	24	19	5	001	
872.96932	19	6	14	18	3	15	000	872.97092
873.00379	13	7	6	12	4	9	010	872.99250
873.05347	24	19	5	23	18	6	000	873.05353
873.14273	25	19	6	24	18	7	100	873.14199
873.16714	17	8	10	16	5	11	011	873.1673
873.31424	25	21	5	24	20	4	001	873.31523
873.40113	21	6	15	20	5	16	100	873.40184
873.69148	25	13	12	24	12	11	010	873.69140
873.73439	27	14	14	26	13	13	001	
873.82692	25	22	3	24	21	4	100	
873.94801	22	20	3	21	19	2	030	
873.98203	27	14	13	26	13	14	001	
874.02869	24	15	10	23	14	9	010	874.02943
874.24888	21	6	15	20	5	16	020	874.25194
874.26366	24	21	4	23	20	3	000	874.26301
874.39801	24	20	5	23	19	4	000	874.39734
874.50299	24	24	1	23	23	0	010	874.50290
874.53666	25	13	13	24	12	12	010	874.53705
874.68857	25	20	5	24	19	6	100	
874.84563	23	22	1	22	21	2	020	
874.91068	25	21	4	24	20	5	100	
874.93460	19	8	12	18	5	13	000	874.93458
874.96306	11	10	2	10	7	3	001	
875.00196	11	10	1	10	7	4	001	
875.08268	12	7	5	11	4	8	021	875.0910
875.18330	23	15	8	22	14	9	020	875.18236
876.55069	27	10	17	26	9	18	010	876.55091
877.02263	11	7	5	10	4	6	020	877.02199
877.09643	26	12	14	25	11	15	010	877.09541
877.20449	23	16	7	22	15	8	020	879.20856
877.33948	28	13	15	27	12	16	001	
877.80449	18	3	15	17	2	16	101	877.8084
877.89998	26	12	15	25	11	14	010	877.90128
878.08500							OH	
878.12633	25	24	2	24	23	1	011	
878.42485	24	13	12	23	12	11	020	878.42458
878.52768	27	14	13	26	13	14	100	
878.54271	14	8	6	13	5	9	000	878.54005
878.68913	26	16	11	25	15	10	100	878.69137
878.78670	23	23	0	22	22	1	030	
878.81115	15	8	8	14	5	9	011	878.8098
879.20844	23	16	7	22	15	8	020	879.20856
879.31790	28	11	17	27	10	18	000	879.31731
879.43579	28	11	18	27	10	17	010	879.43587
879.63224	23	21	2	22	20	3	020	
879.64251	23	7	16	22	6	17	020	879.64024
879.78078	26	11	16	25	10	15	020	
879.80042	25	16	9	24	15	10	000	879.79967
879.98818	27	11	16	26	10	17	010	879.98784
880.04384	12	5	7	11	2	10	020	
880.07123	24	16	9	23	15	8	010	880.07163
880.31793	26	14	13	25	13	12	000	880.31812
880.34999	26	14	12	25	13	13	000	
880.37742	28	12	17	27	11	16	000	880.37104
880.37742	28	12	17	27	11	16	000	880.37104
880.72524	13	3	10	14	6	9	020-010	880.71940
880.74058	26	9	17	25	8	18	000	880.73973
881.34371	28	13	16	27	12	15	100	
881.40025	18	4	14	17	3	15	011	881.40734
881.45021	24	23	2	23	22	1	010	881.45056
881.81378	26	17	9	25	16	10	001	
881.92274	25	25	0	24	24	1	000	881.92126
882.12357	11	1	11	12	2	10	020-010	882.1273
882.30909	25	23	2	24	22	3	110	
882.47276	23	17	6	22	16	7	020	882.47289
882.58050	25	23	3	24	22	2	011	
882.62575	23	20	3	22	19	4	020	882.62876
882.71612	11	8	3	10	5	6	010	882.71096
882.75803	29	12	17	28	11	18	100	
882.86571							OH	
882.98233	25	12	13	24	11	14	020	882.98351
883.07198	15	7	8	14	4	11	000	883.07297
883.31529	21	6	15	20	5	16	000	883.31545
883.94338	11	4	7	10	1	10	020	
883.99456	23	18	5	22	17	6	020	883.99550
884.01692	21	6	15	20	5	16	010	884.01610
884.05458	23	19	4	22	18	5	020	884.05442
884.21701	16	3	13	15	2	14	020	884.21715
884.33348							OH	
884.36677							OH	
884.47957	14	9	6	13	6	7	001	
884.49843	25	14	11	24	13	12	010	884.49870
884.61978	27	15	13	26	14	12	001	
884.63467	27	13	15	26	12	14	000	884.63434
884.75878	24	17	8	23	16	7	010	884.75992
884.85313	26	17	10	25	16	9	100	
885.19710	24	24	1	23	23	0	020	
885.21661	27	13	14	26	12	15	000	885.21684
885.48899	25	22	4	24	21	3	011	
885.55460	26	25	2	25	24	1	100	

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
885.70715	25	22	3	24	21	4	110	
885.78545	18	5	14	19	6	13	020-010	885.78812
885.91755	26	25	1	25	24	2	001	
885.94514	24	22	3	23	21	2	010	885.94514
886.04313	25	17	8	24	16	9	000	886.04332
886.22311	17	9	9	16	6	10	020-100	
886.78549	26	18	8	25	17	9	001	
886.84488	29	11	19	28	10	18	010	886.84688
886.92796	23	22	1	22	21	2	030	
887.00986	24	14	10	23	13	11	020	
887.05195	24	14	11	23	13	10	020	
887.17809	25	21	5	24	20	4	011	
887.40866	20	7	14	19	4	15	000	887.40891
887.64470	28	12	16	27	11	17	000	887.64457
887.67249	12	7	6	11	4	7	020	
887.73055	17	3	15	16	0	16	001	887.72955
887.75525	17	2	15	16	1	16	001	887.75319
887.88309	24	18	7	23	17	6	010	887.88330
888.51327	15	4	11	16	7	10	010-000	888.51230
888.57590	27	15	12	26	14	13	100	
888.60374	25	24	1	24	23	2	000	888.60458
888.65534	24	21	4	23	20	3	010	888.65413
889.39202	19	6	14	18	3	15	011	889.38886
889.50271	26	18	9	25	17	8	100	889.50141
889.59678	24	19	6	23	18	5	010	889.59684
889.65766	26	24	3	25	23	2	100	
889.80164	17	2	15	16	1	16	100	889.80307
889.81996	24	20	5	23	19	4	010	889.81981
889.87450	17	3	15	16	0	16	100	
889.96114	26	24	2	25	23	3	001	
890.11044	12	9	3	11	6	6	000	890.09269
890.37451	16	2	14	15	1	15	011	890.3703
890.45791	26	19	7	25	18	8	001	
890.52684	18	4	14	17	3	15	010	890.52613
890.59825	26	15	10	25	14	11	000	890.59953
890.61315	26	15	11	25	14	12	000	890.60987
890.72317	25	18	7	24	17	8	000	890.72410
890.93810	20	5	15	19	4	16	100	890.93649
891.50309	25	8	17	24	7	18	020	891.50375
891.62630	26	13	14	25	12	13	010	891.62593
891.65530	30	11	20	29	10	19	010	891.65698
891.67144	15	9	6	14	6	9	020-100	
892.18901	26	13	13	25	12	14	010	
892.22826	25	25	0	24	24	1	010	892.22866
892.28665	29	12	18	27	11	17	000	892.28689
892.34399	17	5	13	16	2	14	020	892.34411
892.57787	26	23	3	25	22	4	001	
892.63243	27	16	12	26	15	11	001	892.63398
892.72509	26	19	8	25	18	7	100	
892.75965	26	23	4	25	22	3	100	
892.80478	25	23	2	24	22	1	000	892.80531
892.83958	26	20	6	25	19	7	001	892.83794
892.88868	25	15	10	24	14	11	010	892.89061
893.03435	18	4	15	17	1	16	001	893.03497
893.11572	24	23	2	23	22	1	020	893.11458
893.16560	18	3	15	17	2	16	001	893.16621
893.29588	27	12	16	26	11	15	010	893.29763
893.89496	26	22	4	25	21	5	001	
893.93772	25	19	6	24	18	7	000	893.93793
893.97686	26	21	5	25	20	6	001	
894.21263	27	12	15	26	11	16	010	894.21369
894.24598	26	25	2	25	24	1	110	
894.48352	19	7	13	18	4	14	010	894.4762
894.58257	26	22	5	25	21	4	100	
894.62073	26	20	7	25	19	6	100	
894.63767	20	8	13	19	5	14	000	894.63740
894.74745	23	7	16	22	6	17	010	894.74765
894.80309	24	15	10	23	14	9	020	894.80644
894.92353	18	4	15	17	1	16	100	894.92463
894.94108	28	14	15	27	13	14	100	
894.98669	24	8	17	25	9	16	010-000	
895.20466	26	21	6	25	20	5	100	
895.25013	25	22	3	24	21	4	000	895.25138
895.27252	24	24	1	23	23	0	030	
895.56043	14	9	5	13	6	8	001	
895.67888	16	4	13	15	1	14	020	895.67851
895.76498	25	20	5	24	19	6	000	895.76521
895.84678	14	3	12	15	4	11	020-010	895.84752
895.93081	19	4	15	18	3	16	100	895.93001
896.15050	26	25	1	25	24	2	011	
896.19989	25	21	4	24	20	5	000	896.20043
896.40010	25	13	12	24	12	13	020	896.40106
896.69987	19	4	15	18	3	16	001	896.70211
896.73641	27	16	11	26	15	12	100	
896.82915	23	20	3	22	19	4	030	
897.43433	15	9	7	14	6	8	001	897.44509
897.64192	12	8	5	11	5	6	010	897.64249
897.69477	12	1	12	13	2	11	010-000	897.69437
897.79857	23	16	7	22	15	8	030	
897.83237	28	11	17	27	10	18	010	
897.90896	11	9	3	10	6	4	011	897.9191
898.00849	27	14	14	26	13	13	000	898.00960
898.10463	27	14	13	26	13	14	000	898.10421
898.56121	24	22	3	23	21	2	020	898.55620
898.59301	27	27	1	26	26	0	001	
898.89326	26	16	11	25	15	10	000	898.89341
899.01450	17	13	4	16	12	3	020-100	
899.16172	19	5	15	18	2	16	001	899.16199
899.25420	23	15	8	22	14	9	030	
899.27087	13	5	8	12	2	11	010	899.26851
899.29015	26	24	3	25	23	2	110	
899.45635	19	5	15	18	2	16	100	899.45750
899.47346	23	18	5	22	17	6	030	
899.58296	25	16	9	24	15	10	010	899.58274
899.60721	25	16	10	24	15	9	010	
899.62489	23	19	4	22	18	5	030	
899.68702	23	17	6	22	16	7	030	
899.77164	14	7	8	13	4	9	020	
899.79752	26	26	1	25	25	0	000	899.79648
899.89856	25	24	1	24	23	2	010	899.89917
900.17199	27	17	11	26	16	10	001	
900.19498	19	9	11	18	6	12	001	900.18844
900.60666	22	7	16	23	8	15	010-000	900.59889
900.82373	28	13	16	27	12	15	000	900.82370
900.85180	12	10	3	11	7	4	001	
900.93298	26	12	15	25	11	14	020	900.93217
900.96369	26	24	2	25	23	3	011	
901.24113	26	14	12	25	13	13	010	
901.33897	27	27	0	26	26	1	100	
901.42309	28	10	18	27	9	19	000	
901.60665	28	15	14	27	14	13	001	
901.64917	28	15	13	27	14	14	001	

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1 v_2 v_3$	ν_{lab}
901.90233	25	25	0	24	24	1	020	
901.96113	28	13	15	27	12	16	000	901.96151
902.06403	27	26	1	26	25	2	100	
902.29322	17	3	14	16	2	15	010	902.29342
902.43531	29	11	18	28	10	19	000	902.43646
902.45272	16	8	8	15	5	11	001	
902.50154	26	14	13	25	13	12	010	902.50199
902.82639	24	17	8	23	16	7	020	902.82705
903.08861	27	17	11	26	16	10	100	
903.12090	27	17	10	26	16	11	100	
903.41215	15	6	9	14	3	12	001	903.4084
903.53547	18	5	14	17	2	15	010	903.53332
903.70169	20	6	15	21	7	14	010-000	903.70357
904.04107	20	6	15	19	3	16	100	904.04207
904.08035	27	26	2	26	25	1	001	
904.11840	29	12	17	28	11	18	000	904.11796
904.33290	26	23	3	25	22	4	011	
904.45770	24	20	5	23	19	4	020	
904.60123	25	17	8	24	16	9	010	904.60350
904.62111	23	7	16	22	6	17	000	904.62103
904.67808	20	5	15	19	4	16	000	904.67827
904.72041	24	18	7	23	17	6	020	904.72129
905.02545	25	23	2	24	22	3	010	905.02639
905.09761	17	4	14	16	1	15	010	905.09834
905.27412	24	19	6	23	18	5	020	905.27804
905.45140	27	18	10	26	17	9	001	
905.49039	28	15	14	27	14	13	100	
905.51803	26	17	10	25	16	9	000	905.51850
905.58221	26	17	9	25	16	10	000	905.58447
905.61826	25	14	11	24	13	12	020	905.62181
905.64991	25	14	12	24	13	11	020	
905.70183	29	14	16	28	13	15	001	
906.22719	17	2	15	16	1	16	000	906.22841
906.31034	17	3	15	16	0	16	000	906.30980
906.34564	21	7	15	20	4	16	001	
906.48555	26	22	4	25	21	5	011	
906.72128	18	6	13	17	3	14	020	906.72193
906.75448	15	8	7	14	5	10	000	906.75378
906.81007	27	25	2	26	24	3	100	
907.19677	26	25	2	25	24	1	000	907.19783
907.34142	16	7	9	15	4	12	001	907.33890
907.42458	14	7	7	13	4	10	010	907.43069
907.87536	28	12	17	27	11	16	010	907.87562
907.98148	19	6	14	18	3	15	010	907.98190
908.02539	13	1	12	14	4	11	010-000	908.02577
908.10097	27	18	9	26	17	10	100	908.09910
908.24696	20	9	12	19	6	13	001	
908.41260	27	25	3	26	24	2	001	
908.42685	25	22	3	24	21	4	010	
908.43994	25	18	7	24	17	8	010	908.43485
908.65231	27	13	15	26	12	14	010	
908.69298	27	15	13	26	14	12	000	908.69202
908.71958	27	15	12	26	14	13	000	908.71947
909.11884	26	26	1	25	25	0	010	909.12008
909.36558	16	7	10	15	4	11	020	909.36559
909.44638	27	19	9	26	18	8	001	
909.49227	15	2	13	14	1	14	020	909.49330
909.61689	16	2	14	15	1	15	010	909.61688
909.70144	13	4	9	14	7	8	010-000	909.70200
910.05026	16	3	14	15	0	15	010	910.05108
910.09779	18	3	15	17	2	16	000	910.09980
910.23926	25	19	6	24	18	7	010	910.24099
910.28034	13	9	5	12	6	6	000	910.27880
910.33357	24	22	3	23	21	2	030	
910.36264	25	21	4	24	20	5	010	910.36184
910.45153	25	24	1	24	23	2	020	
910.46975	26	14	9	25	13	8	000	910.46875
910.50683	28	12	16	27	11	17	010	910.50573
910.59877	27	24	3	26	23	4	100	
910.70994	18	4	15	17	1	16	000	910.71027
910.77951	25	25	0	24	24	1	030	
910.94010	25	20	5	24	19	6	010	910.93890
911.23435	19	4	15	18	3	16	000	911.23428
911.43074	25	8	17	24	7	18	100	911.43168
911.46557	26	15	11	25	14	12	010	911.46901
911.48310	27	24	4	26	23	3	001	
911.57210	26	15	12	25	14	11	010	911.56131
911.59640	27	19	8	26	18	9	100	911.59494
911.64930	15	3	13	14	0	14	020	911.6570
912.02369	26	24	3	25	23	2	000	912.02364
912.17727	27	20	8	26	19	7	001	
912.25720	15	7	8	14	4	11	011	912.2558
912.38673	14	8	6	13	5	9	011	912.3831
912.70949	13	8	6	12	5	7	010	912.69503
913.16167	18	4	14	17	3	15	020	913.16329
913.18244	27	23	4	26	22	5	100	
913.36346	27	23	5	26	22	4	001	
913.37968	27	26	2	26	25	1	011	
913.61034	17	9	9	16	6	10	001	913.61094
913.64626	25	15	11	24	14	10	020	
913.66891	25	15	10	24	14	11	020	
913.71274	27	21	7	26	20	6	001	
913.81857	27	20	7	26	19	8	100	
913.85069	14	2	12	15	5	11	010-000	913.85009
913.94730	23	7	16	22	6	17	001	
913.98247	13	9	4	12	6	7	000	913.98373
914.03162	26	19	8	25	18	7	000	914.03193
914.09910	27	22	6	26	21	5	001	
914.45636	26	13	14	25	12	13	020	914.45748
914.56875	27	22	5	26	21	6	100	
914.60807	19	5	15	18	2	16	000	914.60786
914.68198	12	2	11	13	3	10	020-010	914.68015
914.70509	16	3	13	15	2	14	030	914.70529
914.79818	27	21	6	26	20	7	100	
914.92193	24	21	4	23	20	3	030	
914.99737	28	14	15	27	13	14	000	914.99764
915.13350	26	23	4	25	22	3	000	915.13395
915.19065	28	14	14	27	13	15	000	915.19039
915.21523	14	9	6	13	6	7	100	
915.50419	9	2	7	10	5	6	030-020	915.4978
915.77274	27	12	15	26	11	16	020	915.77217
916.02252	29	13	17	28	12	16	000	916.02263
916.25027	26	20	7	25	19	6	000	916.25124
916.31688	28	28	0	27	27	1	001	
916.47109	25	23	2	24	22	3	020	
916.62661	29	11	18	28	10	19	010	916.62741
916.81048	26	22	5	25	21	4	000	916.81106
916.84935	27	27	0	26	26	1	000	916.85178
916.91909	24	16	9	23	15	8	030	
917.03002	27	9	18	26	8	19	010	917.03139
917.16578	26	21	6	25	20	5	000	917.16603
917.30710	27	16	12	26	15	11	000	917.31016

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
917.32368	27	16	11	26	15	12	000	917.32295
917.43901	26	25	2	25	24	1	010	
917.58453	13	6	7	12	3	10	020	917.58644
917.60185	28	27	2	27	26	1	100	
917.80222	26	26	1	25	25	0	020	
917.83412	28	17	11	27	16	12	001	
917.90042	25	8	17	24	7	18	000	
917.91864	24	20	5	23	19	4	030	
917.97437	29	15	15	28	14	14	001	
918.00535	28	28	1	27	27	0	100	
918.19123	29	13	16	28	12	17	000	918.19135
918.36862	26	16	11	25	15	10	010	918.37115
918.63641	25	16	9	24	15	10	020	918.63802
918.65444	25	16	10	24	15	9	020	
918.72690	15	9	6	14	6	9	001	
918.82314	20	6	15	19	3	16	000	918.82257
919.35562	27	14	13	26	13	14	010	919.35543
919.68284	17	7	11	16	4	12	020	919.68318
919.79604	16	4	13	17	5	12	010-000	919.79786
919.87549	21	8	14	20	5	15	000	919.87598
919.92174	22	8	15	21	5	16	001	919.92942
920.20642	27	14	14	26	13	13	010	920.20647
920.25658	25	24	1	24	23	2	030	
920.76431	25	22	3	24	21	4	020	
921.05345	28	17	12	27	16	11	100	
921.15909	28	17	12	27	16	11	100	921.15884
921.30750	24	19	6	23	18	5	030	
921.39858	15	6	9	14	3	12	000	921.39854
921.45140	28	27	1	27	26	2	001	
921.71427	29	12	18	28	11	17	010	
922.04996	27	24	4	26	23	3	011	
922.07671	30	12	18	29	11	19	000	922.07740
922.17861	29	15	14	28	14	15	100	
922.97734	28	26	3	27	25	2	100	
923.12574	26	24	3	25	23	2	010	
923.21164	20	5	15	19	4	16	010	923.21319
923.24610	14	8	7	13	5	8	010	923.24923
923.33259	12	9	3	11	6	6	011	923.3334
923.48427	26	14	13	25	13	12	020	
923.61906	25	21	4	24	20	5	020	
923.69771	26	17	10	25	16	9	010	923.69563
924.22190	27	17	10	26	16	11	000	924.22189
924.25113	28	13	15	27	12	16	010	
924.55805	25	18	7	24	17	8	020	924.55891
924.75654	28	13	16	27	12	15	010	924.75827
924.89474	27	26	1	26	25	2	000	924.89584
925.18843	25	20	5	24	19	6	020	
925.21586	27	27	0	26	26	1	010	
925.40996	16	14	3	15	13	2	020-100	
925.51305	25	19	6	24	18	7	020	
925.59968	13	10	4	12	7	5	001	
926.05714	13	10	3	12	7	6	001	
926.10280	28	18	11	27	17	10	100	
926.11716	28	15	14	27	14	13	000	926.11527
926.17194	28	15	13	27	14	14	000	926.17148
926.46915	12	7	5	11	4	8	020	
926.93025	26	25	2	25	24	1	020	
927.04458	25	23	2	24	22	3	030	
927.11424	26	23	4	25	22	3	010	
927.40202	28	25	4	27	24	3	100	
927.47571	20	7	14	19	4	15	010	927.47631
927.51948	21	7	15	20	4	16	000	927.52004
927.60305	27	9	18	26	8	19	000	927.60310
927.63806	26	18	9	25	17	8	010	927.63711
927.67998	28	19	9	27	18	10	001	
928.85425	20	5	15	19	4	16	020	928.85442
928.99419	14	9	6	13	5	7	000	928.99392
929.36874	27	18	9	26	17	10	000	
929.42108	28	25	3	27	24	4	001	
929.50972	22	8	15	21	5	16	100	
929.66077	12	2	10	13	5	9	020-010	929.6505
929.68554	26	19	8	25	18	7	010	
929.71031	26	22	5	25	21	4	010	
929.74176	15	8	8	14	5	9	010	
929.79956	28	19	10	27	18	9	100	
929.86796	30	13	18	29	12	17	000	
930.10054	27	18	9	26	17	10	000	
930.26187	27	25	2	26	24	3	000	
930.59456	27	13	14	26	12	15	020	
930.64005	28	24	5	27	23	4	100	
930.71222	28	20	8	27	19	9	001	
930.95450	29	16	13	28	15	14	100	
931.03557	26	21	6	25	20	5	010	
931.12749	26	20	7	25	19	6	010	
931.25023	29	14	16	28	13	15	000	
931.46009	13	8	5	12	5	8	010	931.46156
931.63349	29	14	15	28	13	16	000	931.63225
931.70695	26	15	12	25	14	11	020	
931.76469	28	24	4	27	23	5	001	
932.20187	25	22	3	24	21	4	030	
932.27079	16	7	9	15	4	12	000	932.26986
932.29304	28	20	9	27	19	8	100	
932.57697	28	21	7	27	20	8	001	
932.70700	28	23	6	27	22	5	100	
932.93174	27	27	0	26	26	1	020	
933.02761	19	4	15	18	3	16	011	933.0261
933.06676	28	23	5	27	22	6	001	
933.11495	28	28	1	27	27	0	000	
933.25765	19	6	14	20	7	13	020-010	933.2640
933.34959	28	22	6	27	21	7	001	
933.36712	27	19	8	26	18	9	000	933.36858
933.39365	26	24	3	25	23	2	020	
933.51251	16	8	9	15	5	10	010	933.51337
933.57193	30	12	19	29	11	18	010	
933.58697	28	21	8	27	20	7	100	
933.62108	18	7	12	17	4	13	020	933.62255
933.72746	28	22	7	27	21	6	100	
933.95650	27	24	3	26	23	4	000	
934.09355	30	13	17	29	12	18	000	
934.10703	27	26	1	26	25	2	010	
934.61320	22	6	16	21	5	17	001	
934.80180	29	17	13	28	16	12	001	
935.03821	28	16	13	27	15	12	000	
935.08518	28	16	12	27	15	13	000	
935.62141	26	25	2	25	24	1	030	
935.93040	27	20	7	26	19	8	000	
935.95329	25	21	4	24	20	5	030	
935.99585	28	14	14	27	13	15	010	
936.27936	27	23	4	26	22	5	000	
936.46977	27	16	11	26	15	12	010	
937.00193	28	14	15	27	13	14	010	
937.01772	26	16	11	25	15	10	020	

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
937.10520	30	11	19	29	10	20	010	
937.24875	27	21	6	26	20	7	000	
937.31946	14	9	5	13	6	8	000	
937.36525	27	22	5	26	21	6	000	
938.00981	16	8	8	15	5	11	000	938.0093
938.02285	16	8	8	15	5	11	000	
938.23029	26	23	4	25	22	3	020	
938.43302	25	20	5	24	19	6	030	
938.58500	21	6	16	20	5	15	000	
939.44905	25	19	6	24	18	7	030	
939.54024	18	2	16	17	1	17	001	
939.58695	14	3	11	15	6	10	010-000	939.5926
939.63552	15	8	7	14	5	10	011	939.6315
939.71402	18	3	15	17	2	16	011	939.7070
939.85907	29	10	19	28	9	20	000	
940.11616	29	13	16	28	12	17	010	
940.23049	14	3	12	15	4	11	010-000	940.2328
940.25472	27	25	2	26	24	3	010	
940.45597	29	13	17	28	12	16	010	
940.50049	18	8	11	17	5	12	010	
940.54817	28	28	1	27	27	0	010	
940.57991	29	10	19	28	9	20	100	
940.59850	27	14	14	26	13	13	020	
940.62604	29	18	12	28	17	11	001	
940.65896	17	5	13	18	6	12	020-010	940.6507
940.74479	26	17	9	25	16	10	020	
940.76402	26	17	10	25	16	9	020	
941.03721	27	14	13	26	13	14	020	
941.05908	21	5	16	20	4	17	100	
941.38493	14	5	9	13	2	12	001	941.3835
941.65255	30	12	18	29	11	19	010	
941.73693	28	27	2	27	26	1	000	
941.80458	26	22	5	25	21	4	020	
941.85748	18	2	16	17	1	17	100	
941.88964	18	3	16	17	0	17	100	
942.02877	18	5	14	17	2	15	020	
942.04416	27	17	10	26	16	11	010	
942.27937	28	17	12	27	16	11	000	
942.29486	28	17	11	27	16	12	000	
942.42533	16	9	7	15	6	10	001	942.4235
942.52214	27	26	1	26	25	2	020	
942.65041	19	3	16	18	2	17	001	942.6574
942.67552	19	4	16	18	1	17	001	942.6666
942.73060	30	16	14	29	15	15	001	
942.79129							OH	
942.85583	29	15	15	28	14	14	000	
942.89502	25	18	7	24	17	8	030	
942.93325	14	10	5	13	7	6	100	
942.97525	29	15	14	28	14	15	000	
942.99959	9	1	9	10	2	8	030-020	943.0009
943.16460	22	6	16	21	5	17	010	
943.41148	16	9	8	15	6	9	100	
943.47110	14	10	4	13	7	7	100	
943.49205	26	18	9	25	17	8	020	
943.69131	21	5	16	20	4	17	001	
943.94053	11	1	10	12	4	9	020-010	943.9382
944.07427	17	3	14	16	2	15	020	
944.14401	26	20	7	25	19	6	020	
944.20138	12	11	1	11	8	4	001	944.2108
944.36588	26	21	6	25	20	5	020	
944.38117	19	4	16	18	1	17	100	
944.68118	26	19	8	25	18	7	020	
944.76208	27	24	3	26	23	4	010	
944.87231	20	4	16	19	3	17	001	944.8731
945.01319	10	8	2	9	5	5	020	
945.05978	20	4	16	19	3	17	100	
945.18941	29	19	11	28	18	10	001	
945.36047	20	5	16	19	2	17	001	945.3532
945.56251	19	4	15	18	3	16	010	
945.60949	10	1	10	11	2	9	020-010	945.6100
945.96140	17	3	15	16	0	16	011	945.9657
946.02356	28	15	13	27	14	14	010	
946.19741	11	9	2	10	6	5	010	946.1970
946.26096	29	26	4	28	25	3	001	
946.29657	15	7	8	14	4	11	010	
946.32135	27	18	9	26	17	10	010	
946.60508	28	15	14	27	14	13	010	
946.71048	30	14	17	29	13	16	000	
946.84144	21	6	16	20	3	17	001	946.8386
946.87002	17	2	15	16	1	16	011	946.8648
947.07888	20	5	16	19	2	17	100	
947.13788	29	19	10	28	18	11	100	
947.31982	28	28	1	27	27	0	020	
947.35733	19	8	12	18	5	13	010	947.3549
947.46535	30	14	16	29	13	17	000	
947.55645	28	26	3	27	25	2	000	
947.79104	28	18	11	27	17	10	000	
947.93288	27	23	4	26	22	5	010	
948.62751	29	29	0	28	28	1	000	
948.90143	27	19	8	26	18	9	010	
948.93079	27	15	13	26	14	12	020	
949.09850	27	15	12	26	14	13	020	
949.41883	27	25	2	26	24	3	020	
949.53177	22	8	15	21	5	16	000	
949.91414	27	22	5	26	21	6	010	
949.93477	28	27	2	27	26	1	010	
950.03943	29	20	9	28	19	10	100	
950.15261	27	26	1	26	25	2	030	
950.44184	27	20	7	26	19	8	010	
950.75211	27	21	6	26	20	7	010	
951.07572	25	10	15	26	11	16	010-000	
951.37880	17	4	14	16	1	15	020	
951.51656	13	5	8	12	2	11	020	
951.75488	28	25	4	27	24	3	000	
951.96628	28	19	10	27	18	9	000	
952.00613	24	7	17	23	6	18	010	
952.04049	29	16	14	28	15	13	000	
952.16072	29	14	15	28	13	16	010	
952.19392	29	16	13	28	15	14	000	
952.60681	26	22	5	25	21	4	030	
953.15607	29	14	16	28	13	15	010	
953.19375	20	6	15	19	3	16	010	
953.39416	19	7	13	18	4	14	020	
953.70642	19	5	15	18	2	16	010	
953.85930	28	16	12	27	15	13	010	
953.99252	22	7	16	21	4	17	100	
954.23906	16	9	8	15	6	9	000	
954.62777	27	24	3	26	23	4	020	
954.64982	28	24	5	27	23	4	000	
954.69524	27	16	11	26	15	12	020	
954.82882	28	20	9	27	19	8	000	
954.84771	26	8	18	25	7	19	010	

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
954.90223	30	13	17	29	12	18	010	
954.96159	30	13	18	29	12	17	010	
955.14677	29	29	0	28	28	1	010	
955.26411	28	16	13	27	9	18	010-100	
955.76583	26	21	6	25	20	5	030	
955.83689	23	8	16	22	5	17	001	
955.89980	21	5	16	20	4	17	000	
956.25416	20	7	14	21	8	13	020-010	956.2517
956.39019	28	23	6	27	22	5	000	
956.45550	28	26	3	27	25	2	010	
956.48350	28	21	8	27	20	7	000	
956.83935	28	14	15	27	13	14	020	
956.98943	28	22	7	27	21	6	000	
957.20744	28	27	2	27	26	1	020	
957.62509	31	12	19	30	11	20	010	
957.74677	29	28	1	28	27	2	000	
958.04648	13	3	11	14	4	10	020-010	958.0415
958.30262	31	11	20	30	10	21	010	
958.41021	26	19	8	25	18	7	030	
958.56247	27	23	4	26	22	5	020	
958.60907	27	17	10	26	16	11	020	
958.62758	18	4	15	17	1	16	010	
958.89061	30	15	16	29	14	15	000	
959.13431	30	15	15	29	14	16	000	
959.18480	18	2	16	17	1	17	000	
959.22802	20	8	13	19	5	14	010	
959.25079	18	3	16	17	0	17	000	
959.61721	28	17	11	27	16	12	010	
959.63154	28	17	12	27	16	11	010	
959.68422	29	17	13	28	16	12	000	
959.73008	29	17	12	28	16	13	000	
960.48736	15	9	6	14	6	9	000	
960.65624	24	7	17	23	6	18	000	
960.76235	19	3	16	18	2	17	000	
960.98004	29	29	0	28	28	1	020	
961.01411	20	4	16	19	3	17	000	
961.09744	19	4	16	18	1	17	000	
961.21715	27	22	5	26	21	6	020	
961.26220	31	14	18	30	13	17	000	
961.43514	28	25	4	27	24	3	010	
961.44860	27	18	9	26	17	10	020	
961.85750	30	19	11	29	18	12	001	
962.60168	29	15	14	28	14	15	010	
962.91005	31	14	17	30	13	18	000	
962.97032	20	5	16	19	2	17	000	
963.27285	29	15	15	28	14	14	010	
963.40974	30	30	1	29	29	0	000	
963.54223	18	9	10	17	6	11	000	
963.84569	28	27	2	27	26	1	030	
963.89431	21	7	15	20	4	16	010	
963.93852	29	27	2	28	26	3	000	
964.21791	27	0	27	27	1	26	020-010	
964.29544	28	18	11	27	17	10	010	
964.42538	28	26	3	27	25	2	020	
964.72345	21	6	16	20	3	17	000	
964.94563	29	28	1	28	27	2	010	
965.03905	24	7	17	23	6	18	001	
965.07321	28	24	5	27	23	4	010	
965.13392	11	2	9	12	5	8	020-010	965.1337
965.18227	27	20	7	26	19	8	020	
965.42781	29	18	11	28	17	12	000	
967.09654	28	19	10	27	18	9	010	
967.15133	30	14	16	29	13	17	010	
967.42874	17	2	15	16	1	16	010	
967.45663	17	9	8	16	6	11	001	967.4523
967.62972	28	23	6	27	22	5	010	
967.66831	17	3	15	16	0	16	010	
967.74260	22	8	15	23	9	14	010-000	
968.11912	30	16	15	29	15	14	000	
968.56967	29	26	3	28	25	4	000	
968.65783	30	16	14	29	15	15	000	
968.81134	31	13	19	30	12	18	010	
968.91311	28	20	9	27	19	8	010	
969.05296	22	7	16	21	4	17	000	
969.11504	28	22	7	27	21	6	010	
969.35556	31	13	18	30	12	19	010	
969.55471	28	21	8	27	20	7	010	
969.85209	29	19	10	28	18	11	000	
970.04350	28	25	4	27	24	3	020	
970.55343	29	16	13	28	15	14	010	
970.69276	29	16	14	28	15	13	010	
971.65601	12	2	11	13	3	10	010-000	
971.75243	29	27	2	28	26	3	010	
971.78345	28	16	13	27	15	12	020	
971.86915	29	28	1	28	27	2	020	
971.89776	23	6	17	22	5	18	030	
971.96387	29	25	4	28	24	5	000	
972.26605	31	0	31	31	1	30	010-000	
972.61818	19	4	15	18	3	16	020	
972.70243	16	2	14	15	1	15	020	
972.73978	19	3	17	18	0	18	101	972.7381
972.95530	30	29	2	29	28	1	000	
972.97792	29	20	9	28	19	10	000	
973.25321	17	8	9	16	5	12	000	
973.49919	21	9	13	20	6	14	000	
973.91010	27	16	11	26	17	10	030	
973.96645	30	30	1	29	29	0	020	
974.01634	16	3	14	15	0	15	020	974.0150
974.16363	31	15	17	30	14	16	000	
974.20594	29	24	5	28	23	6	000	
974.26910	20	3	17	19	2	18	101	974.2642
974.43922	28	24	5	27	23	4	020	
974.45679	32	14	19	31	13	18	000	
974.67374	31	15	16	30	14	17	000	
974.91821	29	21	8	28	20	9	000	
975.52465	29	23	6	28	22	7	000	
975.59689	28	15	14	27	16	11	020	
975.65986							OH	
975.75032	29	22	7	28	21	8	000	
975.91914	21	8	13	22	9	14	020-010	975.9174
976.04084	8	0	8	9	3	7	030-020	976.0615
976.43510	30	17	14	29	16	13	000	
976.48074	29	17	12	28	16	13	010	
976.60618	30	17	13	29	16	14	000	
976.99597	29	26	3	28	25	4	010	
977.31238	23	6	17	22	5	18	100	
977.49346	31	31	0	30	30	1	000	
977.77297	28	23	6	27	22	5	020	
977.83960	11	2	10	12	3	9	020-010	977.8358
978.38345	20	7	14	19	4	15	020	
978.54868	17	9	8	18	10	9	030-020	978.5514
978.58751	30	15	15	29	14	16	010	

TABLE 1—*Continued*

$\nu_{sunspot}$	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	ν_{lab}
978.65856	29	27	2	28	26	3	020	
978.83241	21	5	16	20	4	17	010	
979.04865	30	15	16	29	14	15	010	
979.13257	19	10	9	20	11	10	100-010	
979.16460	30	29	2	29	28	1	010	
979.43428	30	28	3	29	27	2	000	
981.02652	28	21	8	27	20	7	020	
981.17448	29	25	4	28	24	5	010	
981.55492	29	15	14	28	14	15	020	
981.66850	29	18	11	28	17	12	010	
981.71118	31	14	17	30	13	18	010	
982.30492	31	31	0	30	30	1	010	
982.37175	30	18	13	29	17	12	000	
982.85042	23	8	16	22	5	17	000	
983.00561	15	8	7	14	5	10	010	
983.15745	22	9	14	21	6	15	000	
983.25663	16	10	6	17	11	7	110-020	983.2539
984.05368	20	9	12	21	10	11	020-010	
984.26072	29	24	5	28	23	6	010	
984.42750	30	27	4	29	26	3	000	
984.49973	29	26	3	28	25	4	020	
984.51548	29	19	10	28	18	11	010	
986.11271	30	28	3	29	27	2	010	
986.54635	29	20	9	28	19	10	010	
986.55825	30	16	15	29	15	14	010	
986.58906	29	23	6	28	22	7	010	
987.03964	30	19	12	29	18	11	000	
987.06327	29	22	7	28	21	8	010	
987.30024	20	7	14	21	8	13	010-000	
987.38366	31	30	1	30	29	2	000	
987.41387	29	21	8	28	20	9	010	
988.22096	30	26	5	29	25	4	000	
988.48874	32	15	18	31	14	17	000	
988.80719	17	7	10	16	4	13	000	
988.98631	21	5	16	20	4	17	010	
989.18490	20	6	15	19	3	16	020	
989.25958	29 -	25	4	28	24	5	020	
989.63800	23	10	13	24	11	14	010-000	
989.66087	32	15	17	31	14	18	000	
990.12676	12	1	12	11	8	3	000	
990.39639	30	20	11	29	19	10	000	
990.41385	25	7	18	24	6	19	020	
990.82440	19	3	17	18	0	18	001	990.8258
990.92071	23	6	17	22	5	18	000	
991.05122	32	32	1	31	31	0	000	
991.08576	30	25	6	29	24	5	000	
991.28823	20	3	17	19	2	18	001	
991.40277	16	5	12	17	6	11	020-010	991.3985
991.55904	29	17	12	28	16	13	020	
991.71592	23	7	17	22	4	18	001	
991.95101	30	27	4	29	26	3	010	
991.97597	30	28	3	29	27	2	020	
992.25540	21	5	17	20	2	18	001	
992.54424	31	17	15	30	16	14	000	
992.55894	30	17	14	29	16	13	010	
992.58647	30	21	10	29	20	9	000	
992.60362	31	30	1	30	29	2	010	
992.80564	24	12	13	25	13	12	010-000	
992.90092	30	24	7	29	23	6	000	
992.98131	10	1	9	11	4	8	020-010	992.9918
993.07067	29	24	5	28	23	6	020	
993.69305	30	22	9	29	21	8	000	
993.78560	30	23	8	29	22	7	000	
994.06564	31	29	2	30	28	3	000	
994.48335	31	15	16	30	14	17	010	
994.85211	22	9	14	23	10	13	010-000	
995.97669	9	0	9	10	3	8	020-010	995.9773
997.80078	21	8	14	22	9	13	010-000	
998.32780	22	8	15	21	5	16	010	
998.63763	31	18	14	30	17	13	000	
998.66923	31	18	13	30	17	14	000	
998.97206	21	6	16	20	3	17	010	
999.36050	31	28	3	30	27	4	000	
999.73695	30	25	6	29	24	5	010	
1000.31787	23	6	17	22	5	18	010	
1001.04811	32	31	2	31	30	1	000	
1001.09913	30	19	12	29	18	11	010	
1002.18118	30	24	7	29	23	6	010	
1002.76304	22	7	16	21	4	17	010	
1003.30446	30	20	11	29	19	10	010	
1003.42876	20	5	16	19	2	17	010	
1003.46770	18	6	13	19	7	12	010-000	
1003.54349	31	27	4	30	26	5	000	
1003.55466	31	19	12	30	18	13	000	
1003.94515	30	21	10	29	20	9	010	
1004.13003	14	4	11	15	5	10	020-010	1004.1276
1004.61573	33	33	0	32	32	1	000	
1005.36083	32	31	2	31	30	1	010	
1005.58715	31	28	3	30	27	4	010	
1005.62912	30	22	9	29	21	8	010	
1006.86426	31	26	5	30	25	6	000	
1007.10784	31	20	11	30	29	12	000	
1008.82103	20	7	13	21	8	14	020-010	1008.8206
1008.83413	22	10	13	23	11	12	010-000	
1009.15712	31	25	6	30	24	7	000	
1009.48711	21	4	17	20	3	18	000	
1010.42861	19	3	16	18	2	12	010	
1010.53651	9	1	9	10	2	8	020-010	1010.5324
1010.62056	31	24	7	30	23	8	000	

Sunspot frequencies are from (*11*) and have an estimated absolute accuracy of 0.002 cm^{-1}. Laboratory frequencies given to 5 decimal places are from (*12*) and have an estimated absolute accuracy of 0.001 cm^{-1}. Laboratory frequencies given to 4 decimal places are derived from experimental term values.

sorptions show 2–4% absorption, and there is a great deal of poorly resolved structure at the less than 2% absorption level. Comparison with our synthetic spectra suggest that going from the strong to medium echelons represents a drop in transition intensity by a factor of about 5. In this work we present assignments to all of the strong transitions, nearly all of the medium transitions, and some of the weak lines. We are confident that the extension of our calculations to higher vibrational states will lead to the assignment of the remaining weaker transitions.

A crucial step in our assignment procedure was the use of branches. For the purposes of this analysis, a branch was defined as a series of transitions with $K_a = J - n_a$, where n_a is constant for each branch. In the laboratory spectrum, which contains a significant number of transitions involving states of low K_a, we also followed branches defined by $K_c = J - n_c$ for a constant n_c.

Our variational calculations are not completely accurate, largely due to residual errors in the Born–Oppenheimer potential, but they give errors which vary slowly and systematically with J for a given branch. Typically, using our *ab initio* line list, the next member of a branch could be predicted with an accuracy of $\sim$0.02 cm^{-1}. It is thus possible to step along members of the branch starting from low J transitions, which are generally well characterized, to the previously unassigned higher J lines. For transitions observed both in the laboratory and in sunspots, a crude confirmation of each assignment was obtained by comparing the ratio of line intensities with that estimated from Boltzmann distributions at the appropriate temperature.

After assigning all strong and many medium lines in the sunspot spectrum by analyzing branches with high K_a, we were left with a set of approximately 50 unassigned medium-strength lines. These transitions were assigned to states with intermediate values of K_a and the assignments were checked by comparison with the line lists generated using spectroscopically determined potentials (*17–19*). We found the line list of Partridge and Schwenke (*19*), which became available after the bulk of the assignments reported here had been made, particularly useful for this purpose.

IV.2. Results

Table 1 presents the lines assigned in the sunspot spectrum. There are 1687 transitions, all of which, with the exception of the rotational difference transitions (*13*) discussed below, are pure rotational transitions which arise mainly from excited vibrational states. Transitions are assigned to the (000), (010), (020), (100), (001), (030), (110), (011), and (021) vibrational states.

Table 2 which can be obtained from the electronic archive, contains the 4700 lines observed in the laboratory spectrum of Polyansky *et al.* (*12*), for which we have been able to make some 3000 assignments. Nearly all of these are rotational transitions involving the (000), (010), (020), (100), (001), (030), (040), (110), (011), (021), (111), (120), and (101) vibrational states; there are also a few *P*-branch transitions from the (0,1,0) bending fundamental.

To illustrate both the success of our assignment procedure and some of the interesting features of the spectra, we have plotted two portions of both spectra labeled with assignments. Figure 1 shows the region 771.5–775.5 cm^{-1} in which transitions belonging to three distinct difference band transitions can be seen. Figure 2 shows the region 841.5–849.5 cm^{-1} in which two high K_a transitions which should appear as a single line are split by (presumably) Coriolis interactions with levels of a different vibrational state. It is not possible to plot the entire spectrum here. In paper I, we presented the region 870.0–875.4 cm^{-1}, in which many water transitions were observed in the laboratory, and the region 924.0–925.6 cm^{-1}, in which only one laboratory transition is observed.

With a definitive and complete set of assignments it is possible to build up stacks of observed energy levels for water. Such tabulations are particularly useful for making trivial assignments in other spectral regions (see Ref. *33*, for example). Table 3 presents the observed energy levels for the ground vibrational state. A full tabulation (Table 4) for the (000), (010), (020), (100), and (001) vibrational states has been placed in the electronic archive. These tabulations greatly extend the previous ones (*7, 12, 29, 32*), the results of which have been incorporated for completeness.

These tabulations are provided only for the convenience of the reader and it should be stressed that the fundamental data are the assigned transitions not these derived energy levels. In particular nearly all of our newly derived energy levels are based on a single transition, which means that one misassignment leads to a large number of erroneous energy levels. In addition, the propagation of experimental errors degrades the accuracy of the derived energy levels. Our data are not complete enough to build similar energy level ladders for the higher vibrational states. Table 3 shows that we have approximately doubled the energy range of the rotational levels and obtained a large increase in the range of observed K_a levels.

V. DISCUSSION

The newly assigned transitions show two phenomena which are not observed in low-temperature spectra. The first of these is a family of so-called rotational difference bands that we have discussed previously (*14, 15*). These transitions are caused by the mixing of rotational manifolds of neighboring vibrational states via Fermi interactions. The mixing results in intensity sharing between pure rotational transitions and what are nominally vibration–rotation transitions. The perturbations cause a doubling of the number of rotational transitions from 2 to 4 (see Fig. 3 in Ref. *15*). Differences between any three of these transitions give an exact prediction for the fourth transition, so that these quartets can be securely identified.

Isolated interactions between two individual rovibrational levels are to be expected. However, the interesting feature of the difference transitions is that they are not caused by such a single interaction but by a whole series of perturbations, which give rise to a series, or bands of transitions. Thus the (100)–(020) rotational difference band is strongest for rotational levels involving $K_a = 9$ but is also observable for $K_a = 8$, 10, and 11. In the course of the assignments reported here we also found rotational difference bands caused by

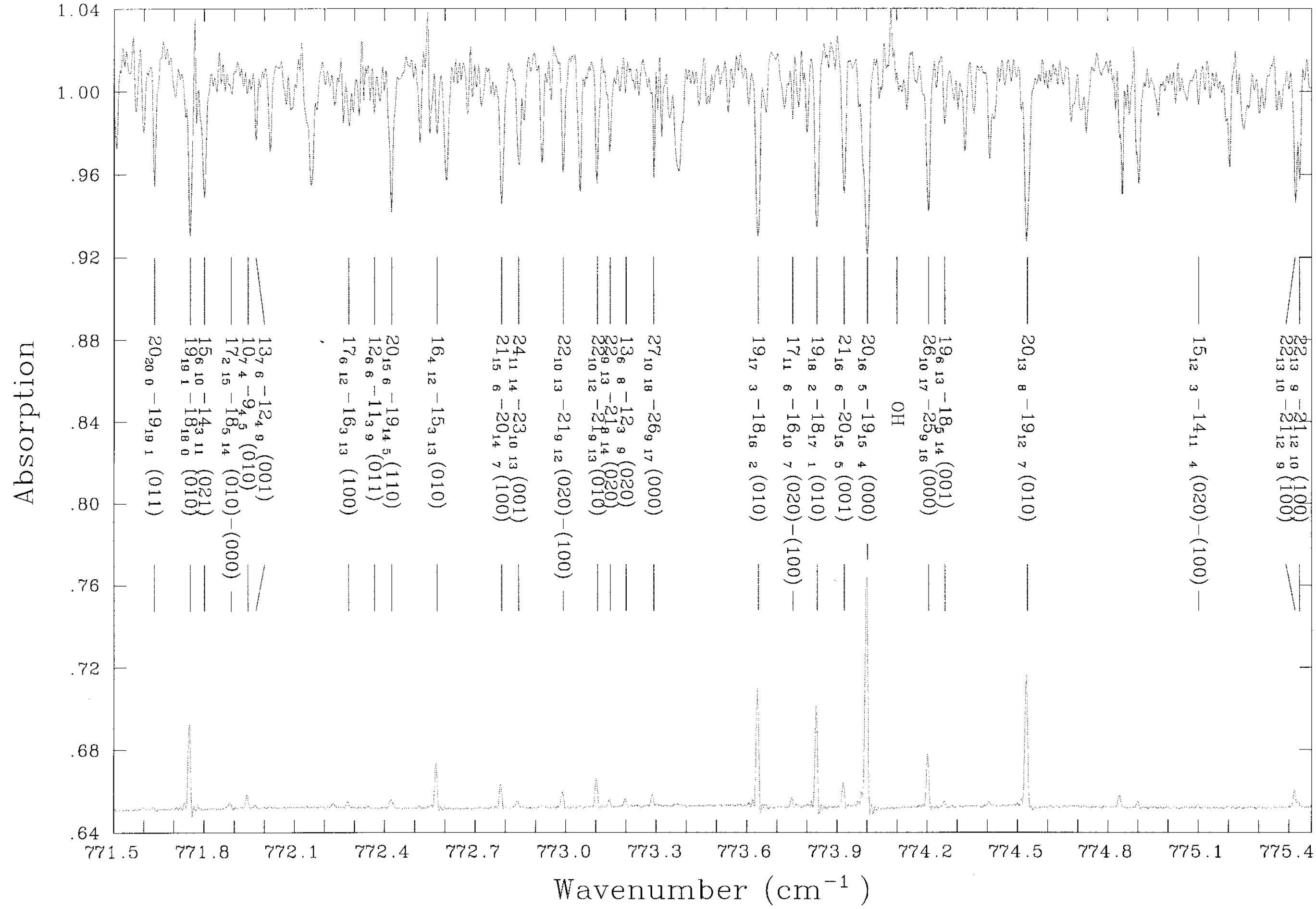

FIG. 1. Sunspot absorption spectrum (upper, Wallace *et al.* (*9, 11*) and laboratory emission spectrum (lower, Wallace *et al.* (*9*), Polyansky *et al.* (*12*)) in the wavenumber region 771.5–775.5 cm^{-1}. Newly assigned water transitions are labeled using standard notation $J_{K_aK_c}$ for rotational levels and $(\nu_1\nu_2\nu_3)$ for vibrational levels.

(110)–(030) and (120)–(040) interactions with the same values of K_a as found in the (100)–(020) case.

The second unusual feature we observe is the localized doubling of a number of pure rotational transitions with high K_a. It is a standard result of rotational spectroscopy that levels with $J_{K_aK_c}$ and $J_{K_a+1K_c}$ for high K_c and $J_{K_aK_c}$ and $J_{K_aK_c+1}$ for high K_a are degenerate. For water this leads to transitions for $J \sim 25$ which can be separated only at resolutions much higher than 0.001 cm^{-1}. In the course of this work we found many isolated examples where these transitions are split, presumably by Coriolis interactions with rotational levels belonging to other nearby vibrational states.

In the course of our variational calculations we have undertaken a number of comparisons with the line list and energy levels obtained by Partridge and Schwenke (PS) (*19*). PS optimized their *ab initio* potential using experimental line positions for low-lying rotational levels ($J \leq 5$) taken from the HITRAN data base (*34*). In the calculation of their full line list PS truncated the basis set used for the variational calculations for $J > 4$ at the level of their $J = 4$ calculations. Note that one would expect more uniform convergence if they had used a final basis whose size was proportional to $J + p$, where the rotational or Wang parity is given by $(-1)^{J+p}$.

For low J energy levels PS's calculations give superb results, reproducing experiment with a much higher accuracy than either the *ab initio* line list used here or Viti *et al.*'s (VTP1) previous line list, which was generated using an empirical potential derived from spectroscopic data (*35*). However, for higher rotational states, particularly those with $J > 20$, we find that a very high proportion of rotational states which one expects to be degenerate in fact show significant splittings in the PS line list. This phenomenon is not the same as the isolated splittings discussed above but seems to be a uniform property of the higher levels. Neither our analysis of the experimental levels, the present calculations, or the VTP1 line list shows any evidence for such splittings.

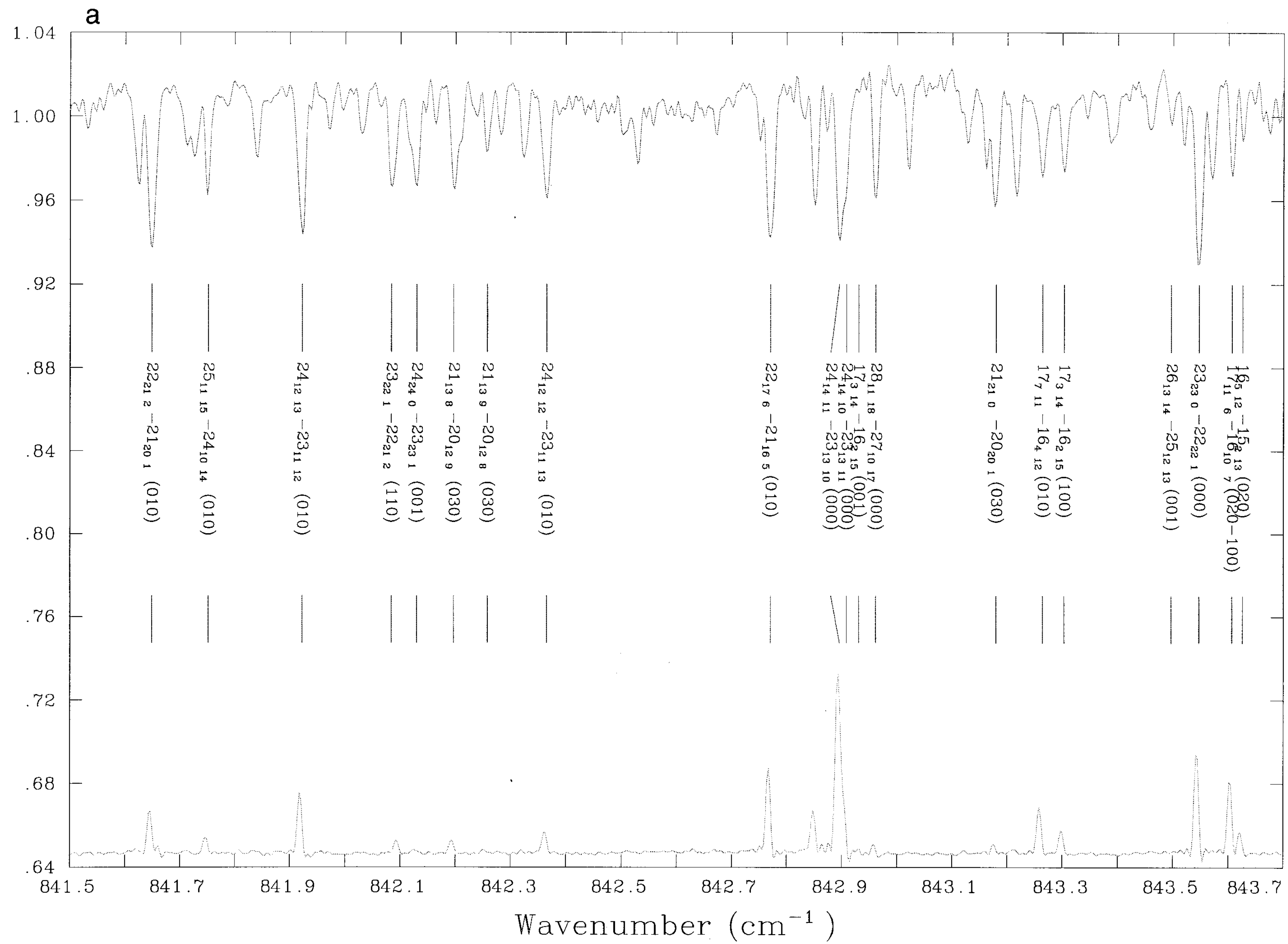

FIG. 2. Sunspot absorption spectrum (upper, Wallace *et al.* (*9, 11*)) and laboratory emission spectrum (lower, Wallace *et al.* (*9*), Polyansky *et al.* (*12*)) in the wavenumber region 841.5–849.5 cm^{-1}. Newly assigned water transitions are labeled using standard notation $J_{K_aK_c}$ for rotational levels and $(\nu_1\nu_2\nu_3)$ for vibrational levels. Note that some of the stronger sunspot absorption features are due to other molecules, particularly OH (*11*).

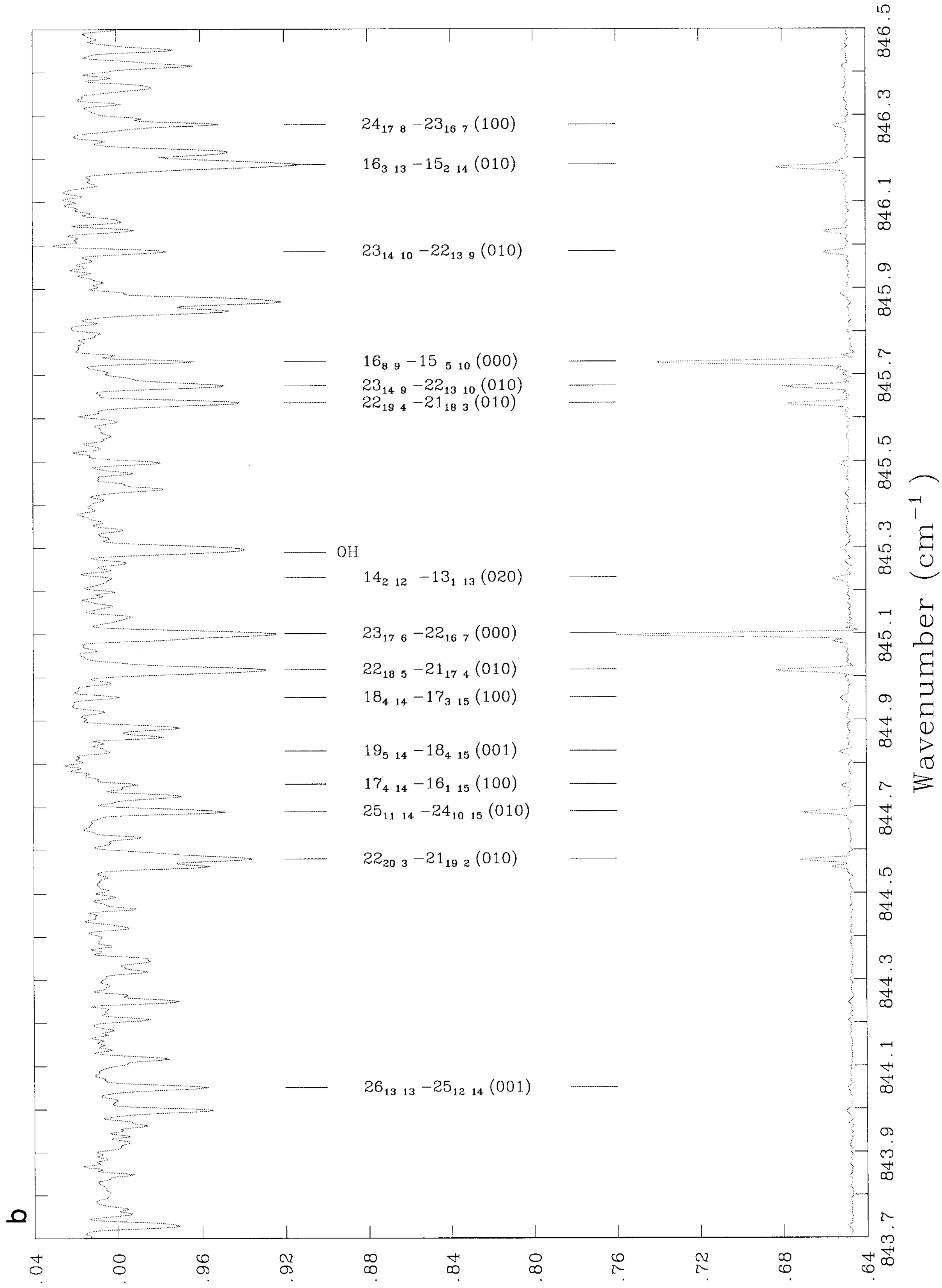

FIG. 2—*Continued*

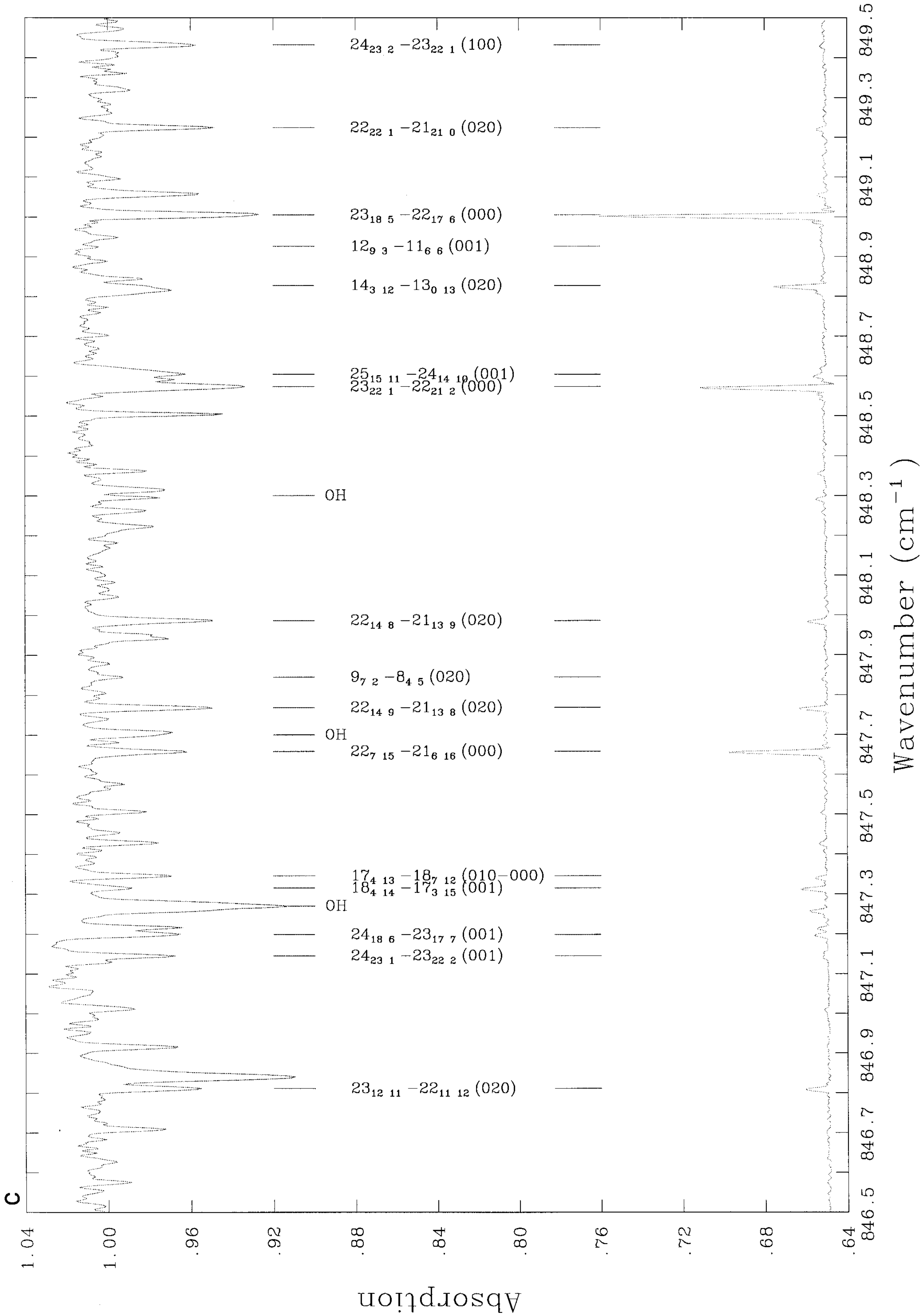

FIG. 2—*Continued*

To illustrate this point, Table 5 gives a comparison for the observed $J = 24$ rotational levels of the manifold of the (001) vibrational state.

It is clear from Table 5 that PS's line list systematically gives splittings which appear to be artificial. In particular, for the high K_a levels, the $p = 1$ parity rotational levels (those with K_c odd for this band) all lie below the $p = 0$ parity (K_c even) levels with which they should be quasi-degenerate. Since PS truncated their variational rotation–vibration calculations at 7500 energy-selected basis functions independent of the parity, p, this means that the $p = 1$ calculations will contain states of higher cutoff energy that the $p = 0$ calculation. Because of the variational principle, the $p = 1$ states will be better converged and hence lower in energy.

To test the hypothesis that the splitting found in PS's rotational levels is an artifact of a lack of variational convergence, we performed calculations using the spectroscopically optimized potential that PS used for their line lists. Our calculations were performed with the same basis set parameters that were used to construct our *ab initio* line list, as specified in Section III, and masses as specified by PS. For $J = 0$, our calculations agree to within 0.01 cm^{-1} with PS's up to ~25 000 cm^{-1}. However, for $J = 24$ our calculations gave energy levels which were systematically lower than those of PS (by up to 1 cm^{-1}). Furthermore none of the ''artificial'' splittings are present in these new levels (see Table 5).

This artificial splitting of lines has two possible consequences. The first is that it is more difficult to use the line list for assignments. The second consequence is perhaps more subtle. A major objective of PS was to construct a list of over 300 million water transitions in order to model the atmospheres of cool ($T \sim 2000$–4000 K) stars. An important consideration in these radiative transport models is how the line absorptions fill in the gaps in the spectrum. Two transitions which, to within their linewidth, are coincident will have a rather different effect than two well-separated transitions. In the latter case the overall stellar opacity will be overestimated. For $T \sim 2000$–4000 K, Boltzmann considerations suggest that transitions involving states with $J = 20$–30 are the dominant sources of opacity. Artificially doubling the number of lines for these J values could have serious consequences for the opacity prediction.

Although we have not discussed our assignment procedure in great detail, there are, in fact, two aspects to making correct line assignments. One step is associating a particular transition with a particular combination of upper and lower energy levels; the other step is assigning quantum number labels to these two energy levels. These labels take two forms: rigorously exact quantum numbers or symmetries and approximate labels. For water the only exact quantum numbers are the total rotational angular momentum, J, the rotational parity, p, and the vibrational parity or *ortho*/*para* designation which we normally denote q (*24*). The conventional vibrational quantum numbers (ν_1, ν_2, ν_3) and the rotational labels (K_a, K_c) are only approximate quantum numbers, although their values are constrained by J, p, and q.

Variational calculations are usually performed using the full symmetry of the system in question and therefore the calculated energy levels are automatically labeled with the exact quantum numbers. In this work, the other quantum numbers were determined as part of the procedure of following the branches in the spectrum. Although we have not implemented such an algorithm, it is attractive to have a method of automatically assigning approximate quantum numbers to the calculated energy levels. Indeed both PS and the recent HITEMP database (*18*) have implemented such procedures. A comparison with our manual assignments is interesting.

In both cases we find that the reliability of these automatic assignments shows a strong dependence on energy, particularly of the vibrational level involved. The approximate quantum numbers given by HITEMP become untrustworthy for states above about 10 000 cm^{-1}. PS's assignments are more reliable but they still give many wrong labels above about 15 000 cm^{-1}. In both cases, where a level is mislabeled, the labeling given usually appears to be very wild; that is, it belongs to a level which is distant in energy to the one being considered. Furthermore neither dataset gives a well-constructed set of energy labels in the sense that there are occasional energy levels with the same labels and certain sets of labels which are completely absent. This results in a number of distinct transitions with identical labels. It should be stressed that we found no evidence for chaotic behavior in the states of water we analyze here. As far as we can tell, our assignments have yet to reach parts of the water spectrum where the energy level labels become ambiguous, except possibly in the case of some of the accidental degeneracies discussed above. This is not the case for H_3^+ where the recorded high-resolution spectra already probe the region where such labeling becomes rather arbitrary (*20*).

Finally it should be noted that the sunspot spectrum is available at other wavelengths (*10*, *11*, *36*). We have recently undertaken a detailed analysis of transitions lying in the so-called K band (*33*) with a particular focus on the region 4860–4930 cm^{-1} where the water transitions are densest. This analysis commenced by using the energy levels determined here to make trivial assignments but resulted in assigning transitions between many states involving higher vibrational levels, not observed previously. These vibrational states are higher in energy than those probed here and a comparison with the energy levels of PS showed significant deviations between predictions and observations. Full results of this study will be presented elsewhere (*33*).

TABLE 3

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

J	K_a	K_c	level	J	K_a	K_c	level	J	K_a	K_c	level	J	K_a	K_c	level
23	0	23	5271.37411	24	4	20	7210.33599	25	7	18	8514.99803	26	9	17	9435.38546
23	1	23	5271.37411	24	5	20	7210.55657	25	8	18	8554.64488	26	10	17	9611.31636
23	1	22	5688.50232	24	5	19	7498.47251	25	8	17	8678.89917	26	10	16	9628.57372
23	2	22	5688.50232	24	6	19	7500.46238	25	9	17	8790.58702	26	11	16	9866.65071
23	2	21	6062.15310	24	6	18	7748.04653	25	9	16	8837.11141	26	11	15	9869.68222
23	3	21	6062.15310	24	7	18	7760.88997	25	10	16	9030.87628	26	12	15	10139.49024
23	3	20	6400.98369	24	7	17	7944.22951	25	10	15	9041.38213	26	12	14	10139.94033
23	4	20	6401.01619	24	8	17	7999.02552	25	11	15	9286.77776	26	13	14	10427.88892
23	4	19	6707.34300	24	8	16	8095.47464	25	11	14	9288.44113	26	13	13	10427.95222
23	5	19	6707.72403	24	9	16	8229.40248	25	12	14	9560.07912	26	14	13	10728.58265
23	5	18	6980.32723	24	9	15	8259.96511	25	12	13	9560.30266	26	14	12	10728.58809
23	6	18	6983.57445	24	10	15	8468.50880	25	13	13	9848.23810	26	15	12	11038.51162
23	6	17	7211.34923	24	10	14	8474.45827	25	13	12	9848.26472	26	15	11	11038.52429
23	7	17	7231.13773	24	11	14	8724.85220	25	14	12	10147.91442	26	16	11	11355.02857
23	7	16	7386.78497	24	11	13	8725.70330	25	14	11	10147.91209	26	16	10	11355.02857
23	8	16	7459.68364	24	12	13	8998.37215	25	15	11	10456.13516	26	17	10	11675.81753
23	8	15	7530.93378	24	12	12	8998.48265	25	15	10	10456.13516	26	17	9	11675.88171
23	9	15	7685.72328	24	13	12	9285.94754	25	16	10	10770.29950	26	18	9	11998.51570
23	9	14	7704.72241	24	13	11	9285.97092	25	16	9	10770.29950	26	18	8	11998.51570
23	10	14	7924.45036	24	14	11	9584.29400	25	17	9	11088.04695	26	19	8	12321.18454
23	10	13	7927.66396	24	14	10	9584.29675	25	17	8	11088.04695	26	19	7	12321.18454
23	11	13	8181.27384	24	15	10	9890.49983	25	18	8	11407.15261	26	20	7	12641.66618
23	11	12	8181.68512	24	15	9	9890.49983	25	18	7	11407.15261	26	20	6	12641.66618
23	12	12	8454.71303	24	16	9	10202.00363	25	19	7	11725.41494	26	21	6	12957.81322
23	12	11	8454.75352	24	16	8	10202.00363	25	19	6	11725.41494	26	21	5	12957.81322
23	13	11	8741.39041	24	17	8	10516.42851	25	20	6	12040.64744	26	22	5	13267.22952
23	13	10	8741.39712	24	17	7	10516.42851	25	20	5	12040.64744	26	22	4	13267.22952
23	14	10	9038.08784	24	18	7	10831.47701	25	21	5	12350.41846	26	23	4	13567.27828
23	14	9	9038.08784	24	18	6	10831.47701	25	21	4	12350.41846	26	23	3	13567.27828
23	15	9	9341.97633	24	19	6	11144.88246	25	22	4	12652.14433	26	24	3	13854.63043
23	15	8	9341.97633	24	19	5	11144.88246	25	22	3	12652.14433	26	24	2	13854.63043
23	16	8	9650.49864	24	20	5	11454.21803	25	23	3	12942.60679	26	25	2	14124.80131
23	16	7	9650.49864	24	20	4	11454.21803	25	23	2	12942.60679	26	25	1	14124.80131
23	17	7	9961.23237	24	21	4	11756.89295	25	24	2	13217.60348	26	26	1	14370.22004
23	17	6	9961.23237	24	21	3	11756.89295	25	24	1	13217.60348	26	26	0	14370.22004
23	18	6	10271.82893	24	22	3	12049.80148	25	25	1	13470.42252	27	0	27	7139.60644
23	18	5	10271.82893	24	22	2	12049.80148	25	25	0	13470.42252	27	1	27	7139.60644
23	19	5	10579.82069	24	23	2	12328.99890	26	0	26	6647.50624	27	1	26	7625.43808
23	19	4	10579.82069	24	23	1	12328.99890	26	1	26	6647.50624	27	2	26	7625.43808
23	20	4	10882.62994	24	24	1	12588.50126	26	1	25	7116.39258	27	2	25	8056.29214
23	20	3	10882.62994	24	24	0	12588.50126	26	2	25	7116.39258	27	3	25	8056.29214
23	21	3	11177.23557	25	0	25	6172.00890	26	2	24	7533.70885	27	3	24	8450.56357
23	21	2	11177.23557	25	1	25	6172.00890	26	3	24	7533.70885	27	4	24	8450.56782
23	22	2	11459.92108	25	1	24	6623.79422	26	3	23	7914.70255	27	4	23	8811.58958
23	22	1	11459.92108	25	2	24	6623.79422	26	4	23	7914.70871	27	5	23	8811.67586
23	23	1	11725.31531	25	2	23	7027.02838	26	4	22	8262.80968	27	5	22	9140.71359
23	23	0	11725.31531	25	3	23	7027.02838	26	5	22	8262.84844	27	6	22	9141.16883
24	0	24	5713.25385	25	3	22	7394.35709	26	5	21	8578.77074	27	6	21	9437.25411
24	1	24	5713.25385	25	4	22	7394.36814	26	6	21	8579.51288	27	7	21	9440.70518
24	1	23	6147.78510	25	4	21	7729.34367	26	6	20	8860.83290	27	7	20	9693.05987
24	2	23	6147.78510	25	5	21	7729.51054	26	7	20	8866.07375	27	8	20	9712.04325
24	2	22	6536.44916	25	5	20	8031.31748	26	7	19	9098.06796	27	8	19	9892.64235
24	3	22	6536.44916	25	6	20	8032.51572	26	8	19	9125.87080	27	9	19	9962.85935
24	3	21	6889.72294	25	6	19	8297.70595	26	8	18	9278.35895	27	9	18	10053.47385
24	4	21	6889.74164	25	7	19	8306.11612	26	9	18	9368.73030	27	10	18	10208.67782

TABLE 3—*Continued*

J	K_a	K_c	level	J	K_a	K_c	level	J	K_a	K_c	level	J	K_a	K_c	level
27	10	17	10236.30376	28	11	18	11079.15586	29	10	19	10512.38696	30	9	22	11835.22086
27	11	17	10463.94322	28	11	17	11087.99572	29	11	19		30	9	21	
27	11	16	10469.59745	28	12	17	11349.96849	29	11	18	11725.09120	30	10	21	
27	12	16	10736.15985	28	12	16	11351.58779	29	12	18	11980.28237	30	10	20	
27	12	15	10737.12630	28	13	16	11637.95003	29	12	17	11983.27426	30	11	20	12356.94950
27	13	15	11024.57467	28	13	15	11638.12136	29	13	17	12267.61042	30	11	19	
27	13	14	11024.70708	28	14	15	11939.70472	29	13	16	12268.15984	30	12	19	12628.62667
27	14	14	11325.96182	28	14	14	11939.76506	29	14	16	12569.37159	30	12	18	
27	14	13	11325.99313	28	15	14	12252.10840	29	14	15	12569.58352	30	13	18	12913.14222
27	15	13	11637.28107	28	15	13	12252.13330	29	15	15	12882.62089	30	13	17	12914.37592
27	15	12	11637.30223	28	16	13	12572.34044	29	15	14	12882.67997	30	14	17	13214.87032
27	16	12	11955.83445	28	16	12	12572.36625	29	16	14	13204.17378	30	14	16	13215.07577
27	16	11	11955.83457	28	17	12	12898.11394	29	16	13	13204.30232	30	15	16	13528.47413
27	17	11	12279.25046	28	17	11	12898.12931	29	17	13	13532.05047	30	15	15	13528.50590
27	17	10	12279.25046	28	18	11	13227.04150	29	17	12	13532.07052	30	16	15	13850.79909
27	18	10	12605.18627	28	18	10	13227.04150	29	18	12	13863.54175	30	16	14	13851.27872
27	18	9	12605.25045	28	19	10	13557.15255	29	18	11	13863.54175	30	17	14	14180.73742
27	19	9	12931.88282	28	19	9	13557.15255	29	19	11	14196.89359	30	17	13	14180.77997
27	19	8	12931.88282	28	20	9	13886.71164	29	19	10	14196.89359	30	18	13	14514.44227
27	20	8	13257.11494	28	20	8	13886.71164	29	20	10	14530.13047	30	18	12	14514.44227
27	20	7	13257.11494	28	21	8	14213.59844	29	20	9	14530.13047	30	19	12	14850.58139
27	21	7	13578.91493	28	21	7	14213.59844	29	21	9	14861.62985	30	19	11	14850.58139
27	21	6	13578.91493	28	22	7	14535.90436	29	21	8	14861.62985	30	20	11	15187.28998
27	22	6	13895.17847	28	22	6	14535.90436	29	22	8	15189.34876	30	20	10	15187.28998
27	22	5	13895.17847	28	23	6	14851.56866	29	22	7	15189.34876	30	21	10	15522.71694
27	23	5	14203.50888	28	23	5	14851.56866	29	23	7	15511.42901	30	21	9	15522.71694
27	23	4	14203.50888	28	24	5	15158.15870	29	23	6	15511.42901	30	22	9	15855.32290
27	24	4	14501.23478	28	24	4	15158.15870	29	24	6	15825.77460	30	22	8	15855.32290
27	24	3	14501.23478	28	25	4	15452.98966	29	24	5	15825.77460	30	23	8	16183.13436
27	25	3	14784.89230	28	25	3	15452.98966	29	25	5	16130.12257	30	23	7	16183.13436
27	25	2	14784.89230	28	26	3	15732.44875	29	25	4	16130.12257	30	24	7	16504.32993
27	26	2	15049.69715	28	26	2	15732.44875	29	26	4	16421.55933	30	24	6	16504.32993
27	26	1	15049.69715	28	27	2	15991.43408	29	26	3	16421.55933	30	25	6	16816.86036
27	27	0	15287.06939	28	27	1	15991.43408	29	27	3	16696.38727	30	25	5	16816.86036
27	27	0	15287.06939	28	28	1	16220.18434	29	27	2	16696.38727	30	26	5	17118.34353
28	0	28	7648.16725	28	28	0	16220.18434	29	28	2	16949.18085	30	26	4	17118.34353
28	1	28	7648.16725	29	0	29	8173.04103	29	28	1	16949.18085	30	27	4	17405.98683
28	1	27	8150.78359	29	1	29	8173.04103	29	29	1	17168.81185	30	27	3	17405.98683
28	2	27	8150.78359	29	1	28	8692.27824	29	29	0	17168.81185	30	28	3	17675.82155
28	2	26	8594.56629	29	2	28	8692.27824	30	0	30	8714.07594	30	28	2	17675.82155
28	3	26	8594.56629	29	2	27	9148.30135	30	1	30	8714.07594	30	29	2	17922.13615
28	3	25	9001.73829	29	3	27	9148.30135	30	1	29	9249.76628	30	29	1	17922.13615
28	4	25	9001.73829	29	3	26	9568.00949	30	2	29	9249.76628	30	30	1	18132.22159
28	4	24	9375.35418	29	4	26	9568.00949	30	2	28	9717.24697	30	30	0	18132.22159
28	5	24	9375.34330	29	4	25	9953.71754	30	3	28	9717.24697	31	0	31	9271.11563
28	5	23	9716.77751	29	5	25	9953.77404	30	3	27	10149.15935	31	1	31	9271.11563
28	6	23	9717.04337	29	5	24	10300.65479	30	4	27	10149.15935	31	1	30	9823.08723
28	6	22	10027.31750	29	6	24	10300.73832	30	4	26	10546.60704	31	2	30	9823.08723
28	7	22	10029.40140	29	6	23	10630.67501	30	5	26	10546.57785	31	2	29	10301.13144
28	7	21	10299.90494	29	7	23	10632.07155	30	5	25	10913.69668	31	3	29	10301.13144
28	8	21	10312.65220	29	7	22	10918.76389	30	6	25	10913.69737	31	3	28	10744.95953
28	8	20	10519.62692	29	8	22	10927.18777	30	6	24	11247.34447	31	4	28	10744.95953
28	9	20	10572.52789	29	8	21	11158.38390	30	7	24	11248.14329	31	4	27	11153.62441
28	9	19		29	9	21	11196.76072	30	7	23	11549.77222	31	5	27	11153.67148
28	10	19	10822.65589	29	9	20		30	8	23	11555.27029	31	5	26	11531.73609
28	10	18	10864.28244	29	10	20		30	8	22		31	6	26	

TABLE 3—*Continued*

J	K_a	K_c	level	J	K_a	K_c	level
31	6	25	11876.40817	31	24	8	17193.75492
31	7	25	11876.97593	31	24	7	17193.75492
31	7	24	12192.88249	31	25	7	17513.48705
31	8	24		31	25	6	17513.48705
31	8	23		31	26	6	17823.72462
31	9	23		31	26	5	17823.72462
31	9	22		31	27	5	18121.88702
31	10	22		31	27	4	18121.88702
31	10	21		31	28	4	18405.34733
31	11	21		31	28	3	18405.34733
31	11	20		31	29	3	18669.88719
31	12	20		31	29	2	18669.88719
31	12	19		31	30	2	18909.51981
31	13	19		31	30	1	18909.51981
31	13	18		31	31	1	19109.71505
31	14	18	13875.63810	31	31	0	19109.71505
31	14	17	13876.05227	32	0	32	9843.99974
31	15	17	14189.23940	32	1	32	9843.99974
31	15	16	14189.54406	32	1	31	10412.07770
31	16	16		32	2	31	10412.07770
31	16	15		32	2	30	10899.65821
31	17	15		32	3	30	10899.65821
31	17	14		32	3	29	11355.17582
31	18	14	15179.41760	32	4	29	11355.17582
31	18	13	15179.40665	32	4	28	11774.64111
31	19	13	15517.99693	32	5	28	11774.64111
31	19	12	15517.99693	32	15	17	14865.29899
31	20	12	15857.68923	32	15	18	14864.54101
31	20	11	15857.68923	32	30	3	
31	21	11		32	30	2	
31	21	10		32	31	2	19910.56792
31	22	10		32	31	1	19910.56792
31	22	9		32	32	1	20100.76627
31	23	9		32	32	0	20100.76627
31	23	8					

VI. CONCLUSIONS

In this work we present detailed assignments for hot water spectra obtained in a sunspot and in the laboratory. Although the work presented here concerns hot water, many of the characteristics of the spectrum will be common to the spectra of other light polyatomic molecules at high temperatures. It would seem, therefore, that a full quantum mechanical treatment based on variational calculations and high-quality potential energy surfaces, possibly with allowance for the failure of the Born–Oppenheimer approximation, will be necessary for spectral analysis and modeling of such systems. Indeed this is already the norm for much simpler diatomic systems, which display none of the spectral features described above, and for van der Waals complexes (*37*). This procedure has also been applied to the chemically bound H_3^+ molecule (*20*), which up until now has been something of a special case. This change will represent a major shift away from the traditional perturbation theory-based analysis of high-resolution spectra.

This new method of analysis is computationally much more expensive but is not without its benefits. Here, when confronted with a vast quantity of unanalyzed and seemingly unassignable data, we have based our calculations on *ab initio* potentials, occasionally reinforced by the use of calculations based on spectroscopically determined poten-

TABLE 5
Energy Levels for J = 24 Rotational Levels of the (001) State in cm^{-1}

J K_a K_c	Expt	PS	This work PS	This work *ab initio*
24 0 24	9379.493	9379.670	9379.656	9382.131
24 1 24	9379.493	9379.683	9379.656	9382.131
24 1 23	9803.442	9803.603	9803.590	9806.080
24 2 23	9803.442	9803.617	9803.590	9806.078
24 2 22	10183.350	10183.505	10183.486	10186.063
24 3 22	10183.350	10183.518	10183.486	10186.063
24 3 21	10529.434	10529.524	10529.505	10532.189
24 11 14	12297.529	12297.917	12296.525	12300.930
24 11 13	12299.281	12299.417	12299.346	12302.453
24 12 13	12554.999	12555.164	12555.078	12558.089
24 12 12	12555.210	12555.382	12555.276	12558.289
24 13 12	12826.246	12826.479	12826.360	12829.316
24 13 11	12826.324	12826.500	12826.390	12829.348
24 14 11	13108.367	13108.519	13108.393	13111.322
24 14 10	13108.364	13108.563	13108.406	13111.334
24 15 10	13398.573	13398.727	13398.552	13401.474
24 15 9	13398.573	13398.712	13398.553	13401.474
24 16 9	13693.277	13693.357	13693.171	13696.166
24 16 8	13693.277	13693.391	13693.171	13696.166
24 17 8	13991.433	13991.673	13991.437	13994.475
24 17 7	13991.433	13991.654	13991.437	13994.475
24 18 7	14290.330	14290.464	14290.220	14293.346
24 18 6	14290.330	14290.748	14290.220	14293.346
24 19 6	14587.427	14587.749	14587.336	14590.581
24 19 5	14587.427	14587.619	14587.336	14590.581
24 20 5	14880.626	14880.682	14880.407	14883.806
24 20 4	14880.626	14881.115	14880.407	14883.806
24 21 4	15167.074	15167.817	15166.816	15170.402
24 21 3	15167.074	15167.088	15166.816	15170.402
24 22 3	15443.810	15443.745	15443.505	15447.310
24 22 2	15443.810	15444.066	15443.505	15447.310
24 23 2	15707.030	15707.345	15706.651	15710.700
24 23 1	15707.023	15706.805	15706.651	15710.700
24 24 1	15951.702	15951.273	15951.150	15955.438
24 24 0	15951.702	15951.285	15951.150	15955.438

Note. Experimental levels with $K_a \leq 3$ are from Flaud *et al.* (*7*); levels with $K_a \geq 11$ are from this work. Calculated energy levels are from Partridge and Schwenke (*19*) (PS), from this work using PS's spectroscopically refined potential, and from this work, *ab initio.*

tials. However, spectroscopically determined potentials, derived from iterative variational calculations and fits to known spectroscopic data, are already widely used for molecules such as water (*18, 19, 35, 38*). The effective potentials derived from such calculations give a much more compact representation of the data than the traditional, vibrational-state by vibrational-state, perturbation theory-based approaches. They also have vastly superior extrapolation properties (*35*).

By the use of a full quantum mechanical treatment of the water nuclear motion problem we have managed to assign the seemingly unassignable high-temperature spectrum of water. Perturbation theory-based methods have proved to be excellent for interpreting the spectra of cool molecules. We suggest that a new spectroscopic paradigm is required for hot molecules based on variational calculations. This leaves superexcited molecules in the dissociation region as the final frontier for the theory of small-molecule rotation–vibration spectroscopy.

ACKNOWLEDGMENTS

We thank H. Partridge and D. W. Schwenke for supplying their potential energy surface prior to publication. The authors acknowledge NATO Grant 5-2-05/CRG951293 for making the experimental–theoretical collaboration possible. N.F.Z. thanks the Royal Society for funding his visit to the University College London. The work of O.L.P. was supported in part by the Russian Fund for Fundamental Studies. This work was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC). Acknowledgment is made to the Petroleum Research Fund for partial support of this work. Support was also provided by the NASA Laboratory Astrophysics Program, the UK Engineering and Science Research Council, and the UK Particle Physics and Astronomy Research Council.

REFERENCES

1. K. H. Hinkle and T. G. Barnes, *Astrophys. J.* **227,** 923–934 (1979).
2. F. Allard, P. H. Hauschildt, S. Miller, and J. Tennyson, *Astrophys. J.* **426,** L39–L41 (1994).
3. H. R. A. Jones, A. J. Longmore, F. Allard, P. H. Hauschildt, S. Miller, and J. Tennyson, *Mon. Not. R. Astron. Soc.* **277,** 767–776 (1995).
4. T. Tsuji and K. Ohnaka, *in* ''Elementary Processes in Dense Plasmas'' (S. Ichimaru and S. Ogata, Eds.), p. 193, Addison–Wesley, Reading, MA, 1995.
5. B. R. Oppenheimer, S. R. Kulkarni, K. Mathews, and T. Nakajima, *Science* **270,** 1478–1479 (1995).
6. H. Worden, R. Beer, and C. P. Rinsland, *J. Geophys. Res.* **102,** 1287–1299 (1997).
7. J.-M. Flaud, C. Camy-Peyret, and J.-P. Maillard, *Mol. Phys.* **32,** 499–521 (1976).
8. NATO AGARD (Advisory Group for Aerospace Research and Development), ''Termenology and Assessment Methods of Solid Propellant Rocket Exhaust Signatures,'' Advisory Report 287, Propulsion and Energetics Panel, Working Group 21, Feb. 1993.
9. L. Wallace, P. F. Bernath, W. Livingston, K. Hinkle, J. Busler, B. Guo, and K. Zhang, *Science* **268,** 1155–1158 (1995).
10. L. Wallace, W. Livingston, K. Hinkle, and P. F. Bernath, *Astrophys. J. Suppl. Ser.* **106,** 165–169 (1996).
11. L. Wallace, W. Livingston, and P. F. Bernath, ''An Atlas of the Sunspot Spectrum from 470 to 1233 cm^{-1} (8.1 to 21 μm) and the Photospheric Spectrum from 460 to 630 cm^{-1} (16 to 22 μm),'' NSO Technical Report 1994-01, Tucson, AZ, 1994.
12. O. L. Polyansky, J. R. Busler, B. Guo, K. Zhang, and P. Bernath, *J. Mol. Spectrosc.* **176,** 305–315 (1996).
13. O. L. Polyansky, N. F. Zobov, J. Tennyson, J. A. Lotoski, and P. F. Bernath, *J. Mol. Spectrosc.* **184,** 35–50 (1997).
14. O. L. Polyansky, J. Tennyson, and P. Bernath, *J. Mol. Spectrosc.*, in press.
15. O. L. Polyansky, N. F. Zobov, J. Tennyson, S. Viti, P. F. Bernath, and L. Wallace, *Science* **277,** 346–348 (1997).
16. P. F. Bernath, *Chem. Soc. Rev.* **25,** 111–115 (1996).
17. S. Viti, J. Tennyson, and O. L. Polyansky, *Mon. Not. R. Astron. Soc.* **287,** 79–86 (1997).
18. L. S. Rothman, R. Gamache, J. W. Schroeder, A. McCann, and R. B. Wattson, *SPIE Proc.* **2471,** 105 (1995); L. S. Rothman, private communication (1996).
19. H. Partridge and D. W. Schwenke, *J. Chem. Phys.* **106,** 4618–4639 (1997).
20. B. M. Dinelli, L. Neale, O. L. Polyansky, and J. Tennyson, *J. Mol. Spectrosc.* **181,** 142–150 (1997).
21. D. W. Schwenke, private communication (1996). [Preliminary fit to the *ab initio* data of Ref. (*19*)]
22. N. F. Zobov, O. L. Polyansky, C. R. Le Sueur, and J. Tennyson, *Chem. Phys. Lett.* **260,** 381–385 (1996).
23. W. Gabriel, E.-A. Reinsch, P. Rosmus, S. Carter, and N. C. Handy, *J. Chem. Phys.* **99,** 897–900 (1993).
24. J. Tennyson, J. R. Henderson, and N. G. Fulton, *Comput. Phys. Commun.* **86,** 175–198 (1995).
25. J. Tennyson and B. T. Sutcliffe, *Int. J. Quantum Chem.* **42,** 941–952 (1992).
26. N. G. Fulton, Ph.D. thesis, Chap. 4, University of London (1994).
27. J. Tennyson, S. Miller, and C. R. Le Sueur, *Comput. Phys. Commun.* **75,** 339–364 (1993).
28. J.-M. Flaud and C. Camy-Peyret, *J. Mol. Spectrosc.* **51,** 142–150 (1974).
29. C. Camy-Peyret, J.-M. Flaud, J. P. Maillard, and G. Guelachvili, *Mol. Phys.* **33,** 1641–1650 (1977).
30. J.-M. Flaud, C. Camy-Peyret, J.-P. Maillard, and G. Guelachvili, *J. Mol. Spectrosc.* **65,** 219–228 (1977).
31. C. Camy-Peyret, J.-M. Flaud, and J.-P. Maillard, *J. Phys. Lett.* **41,** L23–L26 (1980).
32. R. A. Toth, *J. Opt. Soc. Am. B* **10,** 1526–1544 (1993).
33. O. L. Polyansky, N. F. Zobov, J. Tennyson, S. Viti, P. F. Bernath, and L. Wallace, *Astrophys. J.* **489,** L205–L208 (1997).
34. L. S. Rothman, R. R. Gamache, R. H. Tipping, C. P. Rinsland, M. A. H. Smith, D. C. Benner, V. Malathy Devi, J.-M. Flaud, C. Camy-Peyret, A. Perrin, A. Goldman, S. T. Massie, L. R. Brown, and R. A. Toth, *J. Quant. Spectrosc. Radiat. Transfer* **48,** 55 (1992).
35. O. L. Polyansky, P. Jensen, and J. Tennyson, *J. Chem. Phys.* **101,** 7651–7657 (1994).
36. L. Wallace and W. Livingston, ''An Atlas of a Dark Sunspot Umbral Spectrum from 1970 to 8640 cm^{-1} (1.16 to 5.1 μm).'' NSO Technical Report, 1992-01, Tuscon, AZ, 1992.
37. J. M. Hutson, *Annu. Rev. Phys. Chem.* **41,** 123–154 (1990).
38. O. L. Polyansky, P. Jensen, and J. Tennyson, *J. Chem. Phys.* **105,** 6490–6497 (1996).