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Spectrum of Singly Charged Uranium (U II) : Theoretical Interpretation of Energy Levels, Partition Function and Classified Ultraviolet Lines

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Abstract: In an attempt to improve U II analysis, the lowest configurations of both parities have been interpreted by means of the Racah-Slater parametric method, using Cowan codes. In the odd parity, including the ground state, 253 levels of the interacting configurations $5f^37s^2 + 5f^36d7s + 5f^36d^2 + 5f^47p + 5f^5$ are interpreted by 24 free parameters and 64 constrained ones, with a root mean square (*rms*) deviation of 60 cm^{-1}. In the even parity, the four known configurations $5f^47s, 5f^46d, 5f^26d^27s, 5f^26d7s^2$ and the unknown $5f^26d^3$ form a basis for interpreting 125 levels with a *rms* deviation of 84 cm^{-1}. Due to perturbations, the theoretical description of the higher configurations $5f^37s7p + 5f^36d7p$ remains unsatisfactory. The known and predicted levels of U II are used for a determination of the partition function. The parametric study led us to a re-investigation of high resolution ultraviolet spectrum of uranium recorded at the Meudon Observatory in the late eighties, of which the analysis was unachieved. In the course of the present study, a number of 451 lines of U II has been classified in the region 2344 –2955 Å. One new level has been established as $5f^36d7p\ (^4I)^6K(J = 5.5)$ at 39113.98 ±0.1 cm^{-1}.

Keywords: uranium; actinide ions; emission spectrum; energy levels; energy parameters; partition function

1. Introduction

The spectroscopy of uranium is of interest in many respects. Being the element with the highest atomic number (Z = 92) naturally available, the nuclear decay of ^{238}U provides a tool for the evaluation of the age of the Universe [1]. In the astrophysical plasma models, the ionized uranium (U II) transition at 3859.572 Å ($5f^36d7s\ ^6L_{11/2} - 5f^36d7p\ ^6M_{13/2}$) is used for the diagnostics. Not only are specific radiative data for this transition needed, but so are partition functions that depend on energy levels relative to the ground level $5f^37s^2\ ^4I_{9/2}$. Therefore a comprehensive picture of the level scheme in ionized uranium is desired. For U II, as for other complex spectra of heavy elements, the interpretation of the observed emission lines does not allow a complete determination of the energy level scheme. Nevertheless, by application of the Racah-Slater parametric method, the energy parameters adjusted against known experimental energy values E_{exp} should lead to improved predictions of energies E_{th} for the levels left undetermined. The relevance of the methods that were used with success in lower-Z elements [2] was confirmed in the cases of several higher-Z elements, including thorium [3,4], despite the fact that the non-relativistic perturbative model was primarily unsatisfactory for these heavy systems. Due to the limited computer capacities in the early times, the previous calculations on U II [5,6] had to neglect configuration interaction (CI) effects or to use truncated bases of configurations. Therefore, the necessary limitation of core configurations $5f^3$ and $5f^4$ to their lowest LS terms impaired the calculated energies and wave functions for the $5f^3ll'$ and $5f^4l$ levels, consequence of the large spin-orbit interactions and the intermediate coupling conditions.

The critical compilation of energy levels and spectra of actinides published in 1992 by Blaise and Wyart [3] provided preliminary tables of energy levels of both parities in U II. The compilation of U II was based on emission data from Steinhaus et al. [7] and on new FTS measurements by Palmer et al. [8]. In particular, energy values of the lowest levels of configurations involving $5f, 6d, 7s, 7p$ electrons were reported, thus updating the previous estimates by Brewer [9]. The list of experimental energy levels in U II was further extended by Blaise et al. [6]. Although the earlier calculations [5,6] usefully supported the search for energy levels, it is worth taking advantage of the present possibilities of Cowan codes [10,11] implemented on modern computers for improving the interpretation of the level scheme in U II, and more generally in actinides. This is the main purpose of the present work.

On the experimental side, a set of uranium emission spectra in the ultraviolet range (1000–3000 Å) recorded in the late eighties at the Meudon Observatory was available at the beginning of the present work. The original aim of these recordings, involving one of the present authors (JFW), was to support the critical compilation of the U III spectrum in Blaise and Wyart [3] by supplementing the Fourier Transform measurements [12] in the range (2000 Å– 4 μ) with data in the shorter wavelength range. However the spectrograms had been only partly measured and had never been completely analyzed, leaving most of the experimental material unpublished. Only improvements for U III were reported in an EGAS conference [13] and in the compilation[3]. The analysis of the unknown spectrum of U IV was also planned but never initiated. With the recent publication of IR data on uranium [14], these unused ultraviolet data represent an opportunity for a new step in a comprehensive description of ionized uranium emission spectra.

2. Available Experimental Data

The available experimental spectra in the wavelength range 1000–3000 Å were emitted by a vacuum triggered spark source with uranium electrode and recorded on photographic plates using the high-resolution 10.7 m normal incidence vacuum ultraviolet spectrograph of the Meudon Observatory. The spectrograph is equipped with a 3600 lines/mm holographic concave grating, leading to a linear dispersion of 0.26 Å/mm on the plates. At the time of the experiment, only partial measurement of the plates was carried out on a semi-automatic comparator (microdensitometer). Wavelength calibration was insured by external reference lines in a superimposed spectrum from a iron Penning discharge source. In addition to U III lines, the spectrograms contain known lines from U V [15] and U VI [16], and a number of unidentified lines. Among the last ones, many likely belong to the unknown U IV spectrum. Although the discharge conditions were favorable for producing more than doubly charged ions, many sharp lines were present at the long wavelength end, which we presumed to belong to U II. In the present work, more complete measurements have been resumed for the wavelength range 2250–2955 Å, by digitizing the spectral plates using a flatbed scanner. The plates were scanned simultaneously with a precision ruler with markings every 1 mm, allowing interpolation between markings for correction of possible distortions, as described in [17]. Then the positions of lines were determined by superimposing two symmetrical profiles of the line displayed by a "homemade" software that mimics the rotating prism set-up of the comparator [18]. For wavelength calibration, internal standards were preferred. These were chosen among the U III wavelengths from Fourier Transform Spectrometry (FTS) [12] and the U II Ritz wavelengths calculated from level energies determined by FTS [6]. For the wavelength range shorter than 2350 Å, some U V wavelengths [15] were used. The uncertainty of the wavelength measurements varies between ±0.001 and ±0.003 Å.

Figure 1 shows a section of the triggered spark spectrum between 2863–2875Å. The shape of the lines, from relatively sharp (for U II) to hazy (for U IV) may be attributed to Doppler broadening as higher charged ions are produced in hotter part of the sparks. Identified U II lines are numbered. The numbers and corresponding wavelengths can be found in Table 9.

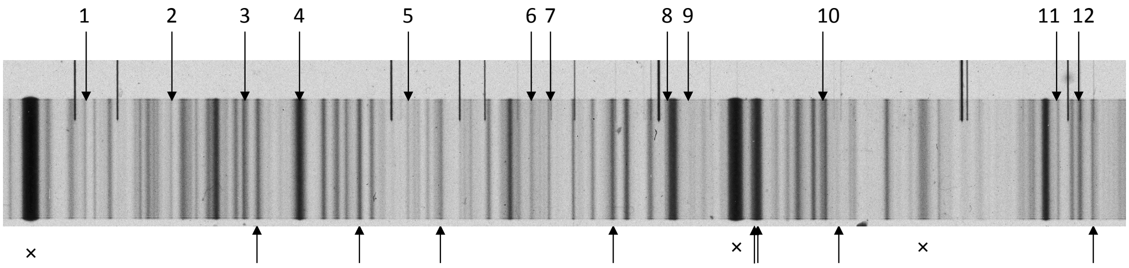

Figure 1. Section of a vacuum triggered spark spectrum (2863–2875 Å). Downward arrows: the U II lines identified in the present work, their numbers and corresponding wavelengths can be found in Table 9; Upward arrows: U III lines from [12]; x: Unidentified lines, likely from U IV. The superimposed iron spectrum is visible above the uranium spectrum but not used in the present work.

3. Theoretical Interpretation of the Energy Levels

Figure 2 shows a diagram of U II configurations of both parities included in the present study. The energy levels spread as predicted by ab initio calculations in the Relativistic Hartree-Fock mode (Cf text below).

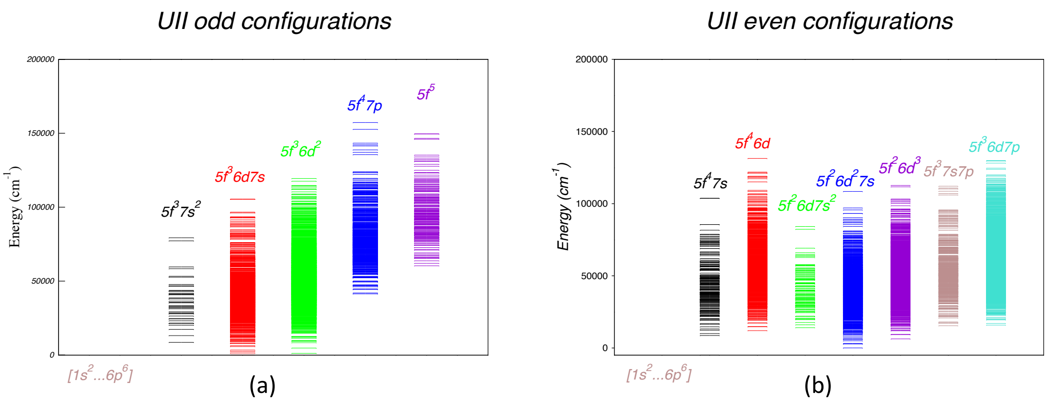

Figure 2. Energy levels of U II belonging to the configurations included in the present study as predicted by ab initio HFR calculations. (**a**) Odd parity configurations. (**b**) Even parity configurations.

We started our work from the energy values tabulated in the final publication on U II [6]. Table 1 recalls the account of various observables available in [6] used for checking the validity of theoretical calculations. The lowest levels of configurations with $5f, 6d, 7s$ and $7p$ electrons, as determined in [6], may be supplemented by predictions for unknown configurations given in [3] according to Brewer's work [9]. This guided our choice of the bases of interacting electronic configurations.

Table 1. Summary of experimental data available for the parametric interpretation of U II levels. N_{tot}: total number of levels; N_{ZE}: number of levels with Landé factor measured by Zeeman effect, N_{IS}: number of levels with measured isotope shift; N_{ident}: number of levels with empirical identification. The number of classified lines per level was not given in [6].

	Odd Parity Levels	Even Parity Levels
N_{tot}	354	809
N_{ZE}	137	355
N_{IS}	114	401
N_{ident}	109	113

3.1. Odd Parity Levels

The present work benefited from the similarities between lanthanides and actinides elements. In the periodic table of elements, neodymium occupies the same position in the lanthanide row as does uranium in the actinide row. Similarities between the two spectra do exist, although configurations built on the $5f^3$ core are much lower relative to the core $5f^4$ in U II than are those built on $4f^3$ relative to $4f^4$ in Nd II.

In Nd II, the basis set of overlapping odd configurations $4f^35d6s + 4f^35d^2 + 4f^36s^2 + 4f^46p + 4f^5$ was adopted for the parametric interpretation of 596 energy levels of these configurations [19,20] by means of the Cowan's codes [10,11]. It had been proven to be adequate by a *root mean square* (*rms*) deviation as small as 53 cm^{-1}. Since in U II the corresponding configurations (with principal quantum numbers increased by one) are also the lowest ones in the parity, we used the same basis set for resuming the calculation of odd parity levels, including the lowest odd parity levels listed in [6]. However, in the case of U II, the $5f^5$ configuration is unknown but is involved by electrostatic interaction with the $5f^36d^2$ configuration. The next higher unknown configuration $5f^26d7s7p$ was not included in the basis. Since its lowest level is expected at 38000 $\pm$ 5000 cm^{-1} above the ground state, according to Brewer's estimates [9], it should not overlap the other odd levels included in the calculation, although CI repulsion effects could be present.

In the first step of the calculation, the *RCN* and *RCN*2 codes were used in the Relativistic Hartree-Fock (*HFR*) mode. The electrostatic and spin-orbit radial integrals were then scaled with factors obtained as averages from earlier actinide calculations [4] and helped for generating the set of parameters for the first diagonalization by the *RCG* code. Appropriate corrections on the average energy E_{av} parameters were made for establishing a fair correspondence between calculated and experimental energies and Landé factors [6] for the low levels of f^3ds, f^3d^2 and f^3s^2. Then the iterative Least Squares Fit (LSF) of the energy parameters was performed by means of the *RCE* code, minimizing the *rms* deviation $\Delta E = \sqrt{\sum_i (E_i^{exp} - E_i^{th})^2/(N_i - N_p)}$, where N_i and N_p are respectively the number of experimental energies and the number of free parameters, with a few dozens of experimental energies to start. Constraints on the parameters were applied for preventing uncontrolled divergence problems. Step by step, the number of levels in the fit was increased up to 253 with a final *rms* deviation of 60 cm^{-1}. Final values for 22 free parameters and 64 constrained ones are reported in Table 2. The electrostatic and spin-orbit integrals are listed with their fitted values and their *HFR* values from which the scaling factors $SF(P)$=P_{fit}/P_{HFR} are derived. In addition to the explicit CI effects, second order CI effects of distant configurations have been taken into account by using effective parameters. These are α, β and γ for the $5f^n$ core configurations and *Slater forbidden* parameters for $5f^nnl$ (enabled by a specific option of the *RCG* code). Their initial values were chosen semi-empirically by comparison with earlier works [4].

The comparison of experimental and calculated levels is given in Table 3, which is ordered by increasing theoretical energies E_{th}. One may notice that leading *LS* components of eigenfunctions often represent a small part of the total wave functions. As an example, the eigenfunction of the level at E_{exp} = 8379.697 cm^{-1} has three leading components representing respectively only 14, 11 and

10 percent of the total wavefunction. However, the calculation seems correct, as shown by the small deviations for both energies and Landé factors: E_{exp}–E_{th} = 22 cm^{-1} and g_{exp}– g_{th} = 0.002. At higher energies, in the bulk of calculated levels, it occurs that leading *LS* components become as small as 3% only. Considering that the configuration sharing is more meaningful than tiny term components, we have summed the squared amplitudes in the wave functions separately for the 5 configurations. The dominant configuration and its percentage are respectively reported in the last two columns of the table.

Below 20,000 cm^{-1}, it was possible to establish a reliable correspondence between experimental and theoretical energies for the LSF procedure, which was generally supported by agreement between g_{th} and g_{exp} Landé factors, when availabie [6]. However, a few exceptions have been observed. As an example, the two J = 7.5 levels at 8394.362 and 8521.922 cm^{-1} were previously [6] assigned respectively as $f^3d^2\ {}^6M_{15/2}$ and $f^3ds\ {}^6K_{15/2}$, based on the empirical identification of Landé factors and isotope shifts. In the present work, the initial HFR step predicted these two levels in an inverted order of energies at respectively 8536 and 8438 cm^{-1}, with strongly mixed eigenfunctions. Furthermore, the LSF following this inverted order led to smaller deviations, although physically unsatisfactory. Therefore this order has been adopted in Table 3. Above 20,000 cm^{-1} Landé factors are missing for a majority of levels and the quantum number J is reported as ambiguous for some of them. Since the correspondence between calculated and experimental energies becomes uncertain as energy increases, identifications above 25,726 cm^{-1} are not reported here.

At an intermediate step of the parametric fitting, the previously assigned J value, $J = 11/2$, of the level E_{exp} = 13,695.737 cm^{-1} raised questions. It was found that on one hand, no other level with $J = 11/2$ was predicted between the two experimental levels at 13,270.612 and 13,961.850 cm^{-1}, and on the other hand, one $J = 9/2$ level was missing between E_{exp} = 13,450.490 and 14,265.976 cm^{-1}. The possibility for correcting the J-value for E_{exp} = 13,695.737 was thus examined. Indeed, while a $J = 11/2$ attribution can be justified by only one unique transition with a $J = 13/2$ even level, a $J = 9/2$ value is supported by 16 lines of [7] and by two unidentified lines from the infrared line list of [14] that fit transitions with $J = 7/2$ even levels. Table 4 collects the transitions supporting the present assignation of a $J = 9/2$ for this level. Similar ambiguity for some other levels led us to be cautious and to avoid inclusion of too many E_{exp} values in the LSF fitting process with no other reason but a small ΔE value.

Table 2. Fitted parameters (in cm^{-1}) for odd parity configurations of U II compared with HFR radial integrals. The scaling factors $SF(P) = P_{fit}/P_{HFR}$ (dimensionless) are replaced by $\Delta E = E_{fit} - E_{HFR}$ for E_{av} average energies (in cm^{-1}). Constraints on some parameters are in the second column under 'Cstr.' (denoted 'f' for fixed parameters or 'rn' , which link parameters of the same 'rn' to vary in a constant ratio). The HFR values of E_{av} parameters are relative to the ground state configuration $5f^3 7s^2$ taken as zero value.

		$5f^3 7s^2$				$5f^3 6d7s$				$5f^3 6d^2$			
Param. *P*	**Cstr.**	P_{fit}	**Unc.**	P_{HFR}	$\Delta E/SF$	P_{fit}	**Unc.**	P_{HFR}	$\Delta E/SF$	P_{fit}	**Unc.**	P_{HFR}	$\Delta E/SF$
E_{av}		22711	54	0	22711	30141	35	4716	25425	41875	29	15459	26916
$F^2(ff)$	r1	47923	244	70159	0.683	47163	241	69047	0.683	46426	237	67969	0.683
$F^4(ff)$	r2	31974	437	45448	0.704	31411	429	44648	0.704	30868	422	43877	0.704
$F^6(ff)$	r3	21971	563	33210	0.662	21568	552	32601	0.662	21180	542	32015	0.662
α	r4	36.3	1			36.3	1			36.3	1		
β	f	−600				−600				−600			
γ	f	1500				1500				1500			
$F^2(dd)$										23885	401	33922	0.704
$F^4(dd)$										12305	782	22307	0.551
$\alpha_d{}^2$	f									10			
ζ_f	r5	1732.4	4	1868.5	0.927	1705.7	4	1839.8	0.927	1681.2	4	1813.4	0.927
ζ_d	r6					1531.8	14	1793.1	0.854	1410.4	13	1650.9	0.854
$F^1(fd)$	r7					880	202			880	202		
$F^2(fd)$	r8					19605	205	28026	0.700	18724	196	26766	0.700
$F^4(fd)$	r9					13940	363	15151	0.920	13251	345	14404	0.920
$G^1(fd)$	r10					11304	81	18156	0.623	10995	78	17660	0.623
$G^2(fd)$	r11					833	295			833	295		
$G^3(fd)$	r12					11699	227	13054	0.896	11236	218	12535	0.896
$G^4(fd)$	r13					2858	355			2858	355		
$G^5(fd)$	r14					8054	353	9682	0.832	7696	337	9250	0.832
$G^3(fs)$						2583	88	4198	0.615				
$G^2(ds)$						13609	247	21081	0.646				

Table 2. *Cont.*

	$5f^47p$					$5f^5$				
Param. P	**Cstr.**	P_{fit}	**Unc.**	P_{HFR}	$\Delta E/SF$	**Cstr.**	P_{fit}	**Unc.**	P_{HFR}	$\Delta E/SF$
E_{av}		60158	196	42943	17215	f	61000		58456	2544
$F^2(ff)$	r1	43973	224	64376	0.683	f	38003		55478	0.686
$F^4(ff)$	r2	29072	397	41323	0.704	f	24513		35118	0.691
$F^6(ff)$	r3	19894	509	30071	0.662	f	17151		25410	0.675
α	r4	37.7	1				36.5	1		
β	f	−600					−600			
γ	f	1500					1500			
ζ_f	r5	1550.4	4	1672.2	0.927		1333.5	3	1437.9	0.927
ζ_p	f	3325.8	209	3293.7	1.01					
$F^1(fp)$	f	100								
$F^2(fp)$	f	7215		8016	0.900					
$G^2(fp)$	f	2058		2058	1.000					
$G^4(fp)$	f	1800		1800	1.000					

Table 2. *Cont.*

Param. P	**Cstr.**	P_{fit}	**Unc.**	P_{HFR}	$\Delta E/SF$
Configuration Interaction					
$5f^37s^2 - 5f^36d7s$					
$R^2(fs,fd)$	r15	−6614	71	−10104	0.65
$R^3(fs,df)$	r15	−1442	15	−2204	0.65
$5f^3s^2 - 5f^3d^2$					
$R^2(ss,dd)$	r15	14670	157	22412	0.65
$5f^37s^2 - 5f^5$					
$R^3(ss,ff)$	r15	4516	48	6900	0.65
$5f^36d7s - 5f^36d^2$					
$R^2(fs,fd)$	r15	−6605	71	−9955	0.65
$R^3(fs,df)$	r15	−1500	16	−2284	0.65
$R^2(ds,dd)$	r15	−16091	172	−24584	0.65
$5f^36d7s - 5f^47p$					
$R^1(ds,fp)$	r15	−9384	101	−14337	0.65
$R^3(ds,pf)$	r15	−2805	30	−4286	0.65
$5f^36d7s - 5f^5$					
$R^3(ds,ff)$	r15	−3507	38	−5357	0.65
$5f^36d^2 - 5f^47p$					
$R^1(dd,fp)$	r15	5580	60	8526	0.66
$R^3(dd,fp)$	r15	2490	27	3805	0.66
$5f^36d^2 - 5f^5$					
$R^1(dd,ff)$	r15	15269	164	23326	0.66
$R^3(dd,ff)$	r15	10171	109	15537	0.66
$R^5(dd,ff)$	r15	7325	78	11191	0.66
$5f^47p - 5f^5$					
$R^2(fp,ff)$	r15	−2887	31	−4410	0.66
$R^4(fp,ff)$	r15	−2501	27	−3821	0.66

Table 3. Energy levels of U II, odd parity. Comparison of experimental energies and Landé factors with values calculated from the parameter set of Table 2. $\Delta E = E^{exp} - E^{th}$. The percentage of the leading term (notations from Cowan codes) and its configuration are specified by columns 7–9. The dominant configuration and its percentage are reported in the last two columns.

J	E^{exp} (cm^{-1})	E^{th} (cm^{-1})	ΔE (cm^{-1})	g_L^{th}	g_L^{exp}	% 1^{st} comp	Conf	Term	Main conf	%
4.5	0.000	−56.8	56	0.756	0.765	77	f3s2	(4I)4I	f3s2	91.7
5.5	289.041	224.4	64	0.656	0.655	77	f3ds	(4I)6L	f3ds	99.9
4.5	914.765	930.2	−15	0.604	0.605	71	f3ds	(4I)6K	f3ds	96.2
6.5	1749.123	1715.5	33	0.864	0.865	45	f3ds	(4I)6L	f3ds	93.8
5.5	2294.696	2320.7	−26	0.868	0.865	47	f3ds	(4I)6K	f3ds	97.5
5.5	4420.871	4406.4	14	0.971	0.97	89	f3s2	(4I)4I	f3s2	93.6
6.5	4585.434	4577.9	7	0.793	0.785	28	f3d2	(4I)6M	f3d2	51.8
2.5	4706.273	4674.8	31	0.477	0.480	33	f3ds	(4I)6H	f3ds	96.8
7.5	5259.653	5247.0	12	1.007	1.015	68	f3ds	(4I)6L	f3ds	97.6
3.5	5401.503	5352.6	48	0.767	0.690	26	f3ds	(4I)6I	f3ds	98.0
6.5	5526.750	5549.1	−22	1.019	1.020	70	f3ds	(4I)6K	f3ds	98.3
3.5	5667.331	5695.5	−28	0.657	0.735	51	f3ds	(4I)6I	f3ds	96.9
5.5	5790.641	5827.3	−36	0.851	0.860	39	f3ds	(4I)6K	f3ds	95.5
6.5	6283.431	6392.9	−109	0.785	0.790	39	f3d2	(4I)6M	f3ds	54.5
4.5	6445.035	6471.2	−26	0.835	0.840	43	f3ds	(4I)6I	f3ds	97.6
0.5		6999.4		2.398		20	f3ds	(4F)4Pa	f3ds	97.8
1.5	7017.172	7096.0	−78	0.612	0.620	58	f3s2	(4F)4F	f3s2	90.8
4.5	7166.632	7259.7	−93	0.945	0.940	20	f3ds	(4I)6H	f3ds	94.9
5.5	7598.353	7626.3	−27	0.971	0.980	18	f3ds	(4I)4Ia	f3ds	98.0
3.5	7547.374	7629.2	−81	0.802	0.790	21	f3ds	(4I)4Ha	f3ds	84.8
6.5	8276.733	8248.0	28	1.093	1.090	84	f3s2	(4I)4I	f3s2	89.9
4.5	8379.697	8357.5	22	0.841	0.840	14	f3ds	(4I)6I	f3ds	76.1
1.5	8400.125	8426.1	−25	0.086	0.150	68	f3ds	(4I)6G	f3ds	97.7
2.5	8430.185	8432.6	−2	0.719	0.720	38	f3ds	(4I)6G	f3ds	94.3
7.5	8394.362	8437.9	−43	1.052	0.960	55	f3ds	(4I)6K	f3ds	74.2
5.5	8510.866	8446.9	63	0.854	0.860	11	f3ds	(4I)4Kb	f3ds	78.7
7.5	8521.922	8535.6	−13	0.968	1.060	41	f3d2	(4I)6M	f3d2	57.1
6.5	8755.640	8767.9	−12	1.042	1.040	14	f3ds	(4I)4Lb	f3ds	92.2
8.5	8853.748	8815.5	38	1.105	1.105	83	f3ds	(4I)6L	f3ds	98.6
3.5	9075.732	9020.5	55	0.873	0.870	15	f3ds	(4I)6H	f3ds	68.6
2.5	9344.625	9250.9	93	0.751	0.79	25	f3s2	(4G)4G	f3s2	47.1
4.5	9241.971	9254.9	−12	1.023	1.015	12	f3ds	(4I)6H	f3ds	77.6
5.5	9553.187	9584.8	−31	1.053	1.060	56	f3ds	(4I)6I	f3ds	96.4
6.5	9626.113	9637.3	−11	0.946	0.950	39	f3ds	(4I)4Kb	f3ds	83.9
4.5	9690.665	9707.7	−17	0.991	0.995	10	f3s2	(2H)2H2	f3ds	60.9
1.5	9881.618	9911.4	−29	0.272		51	f3ds	(4F)6G	f3ds	98.3
3.5	9933.226	9916.5	16	0.823	0.82	27	f3ds	(4I)4Hb	f3ds	88.1
4.5	9882.726	9967.6	−84	0.878	0.875	16	f3s2	(4I)4Ib	f3ds	43.9
2.5	10285.072	10178.1	106	0.454	0.42	35	f3ds	(4F)6H	f3ds	93.1
7.5	10198.312	10250.6	−52	0.968	0.960	44	f3ds	(4I)4Lb	f3ds	79.5
2.5	10366.253	10437.7	−71	0.922		58	f3s2	(4F)4F	f3s2	68.1
3.5	10444.432	10437.7	6	0.878	0.865	12	f3ds	(4F)4Hb	f3ds	74.7
1.5	-	10643.1		1.731		30	f3ds	(4F)6D	f3ds	97.8
5.5	10740.958	10688.6	52	0.690	0.685	68	f3d2	(4I)6L	f3d2	84.1
2.5	10732.087	10867.1	−135	0.953		29	f3ds	(4F)6G	f3ds	92.0
2.5	11350.714	11227.9	122	1.254		17	f3ds	(4F)6D	f3ds	95.3
1.5	-	11230.7		1.617		58	f3s2	(4S)4S	f3s2	91.6
3.5	11363.537	11289.2	74	1.033		13	f3d2	(4I)6Ia	f3ds	69.2
8.5	11382.321	11330.6	51	1.179	1.185	75	f3ds	(4I)6K	f3ds	96.4
4.5	11544.672	11426.0	118	0.673	0.690	45	f3d2	(4I)6Ka	f3d2	61.1
3.5	-	11571.9		0.994		23	f3s2	(4F)4F	f3s2	52.5
7.5	11708.483	11664.6	43	1.175	1.175	77	f3s2	(4I)4I	f3s2	92.2

Table 3. *Cont.*

J	E^{exp} (cm^{-1})	E^{th} (cm^{-1})	ΔE (cm^{-1})	g_L^{th}	g_L^{exp}	% 1^{st} comp	Conf	Term	Main conf	%
3.5	11707.835	11743.7	−35	0.781	0.705	37	f3ds	(4G)6I	f3ds	60.0
5.5	11784.953	11809.2	−24	1.097		36	f3ds	(4I)6H	f3ds	97.0
6.5	11813.450	11833.5	−20	1.008	1.09	26	f3ds	(4I)6I	f3ds	81.0
6.5	11787.315	11841.2	−53	1.030	0.940	37	f3ds	(4I)6I	f3ds	83.9
4.5	11797.343	11854.3	−56	1.005		16	f3ds	(4I)6G	f3ds	96.3
0.5	-	11902.1		1.361		22	f3ds	(4F)2P	f3ds	95.6
2.5	12112.402	12095.7	16	0.957		10	f3ds	(4F)6G	f3ds	94.6
4.5	12055.788	12117.5	−61	0.976		18	f3ds	(4G)6I	f3ds	93.8
8.5	12033.378	12121.2	−87	1.014	1.005	78	f3d2	(4I)6M	f3d2	90.9
3.5	12092.319	12161.5	−69	0.823		22	f3ds	(4F)6H	f3ds	86.6
9.5	12350.555	12255.1	95	1.176	1.200	89	f3ds	(4I)6L	f3ds	99.0
1.5	-	12392.5		0.562		19	f3ds	(4G)4Fa	f3ds	90.4
5.5	12530.613	12519.6	10	0.987	1.000	12	f3d2	(4I)6Ka	f3ds	74.9
6.5	12629.355	12578.1	51	1.044	1.095	23	f3d2	(4I)6L	f3ds	65.8
3.5	12627.826	12582.6	45	0.965		24	f3s2	(4G)4G	f3ds	49.3
7.5	12660.559	12591.2	69	1.072	1.015	8	f3ds	(4I)4Lb	f3ds	88.1
5.5	12638.060	12690.0	−51	0.997		14	f3ds	(4I)4Ib	f3ds	78.1
2.5	-	12691.9		0.713		33	f3s2	(4G)4G	f3ds	47.4
4.5	12687.308	12718.0	−30	0.916		13	f3d2	(4I)6Ia	f3d2	49.9
1.5	-	12891.3		0.905		8	f3ds	(4F)4Db	f3ds	78.5
7.5	13015.838	12958.6	57	1.070	1.125	30	f3ds	(4I)4Kb	f3ds	96.0
3.5	13183.793	13117.1	66	0.982		22	f3ds	(4F)6G	f3ds	70.5
2.5	-	13125.8		0.997		20	f3ds	(4F)6G	f3ds	83.5
5.5	13089.590	13133.0	−43	0.941	0.940	34	f3d2	(4I)6Ka	f3d2	53.3
4.5	13275.365	13247.5	27	0.956		15	f3ds	(4I)6H	f3ds	78.9
5.5	13270.612	13272.1	−1	1.134		20	f3ds	(4I)6G	f3ds	92.7
6.5	13344.198	13275.1	69	0.905	0.910	35	f3d2	(4I)6L	f3d2	60.6
3.5	13450.362	13423.3	27	0.979		19	f3ds	(4I)6G	f3ds	80.0
4.5	13450.490	13449.0	1	1.014		15	f3ds	(4G)6I	f3ds	69.0
7.5	13503.319	13524.3	−20	1.101	1.13	19	f3ds	(4I)6I	f3ds	87.2
4.5	13695.737	13683.4	12	1.058		21	f3ds	(4F)6H	f3ds	85.3
3.5	13733.500	13730.8	2	0.934		22	f3ds	(4F)6G	f3ds	64.9
2.5	-	13751.0		0.638		17	f3d2	(4I)6Ha	f3ds	61.8
0.5	-	13817.0		0.009		51	f3ds	(4F)6F	f3ds	94.3
6.5	13975.278	13932.4	42	1.021		19	f3ds	(4I)2K	f3ds	81.3
2.5	13967.812	13944.8	23	0.734		18	f3ds	(4I)4Ga	f3ds	87.9
5.5	13961.850	13980.2	−18	0.972		14	f3ds	(4I)4Ib	f3ds	63.9
3.5	14107.329	14042.4	64	0.829		16	f3ds	(4F)4Hb	f3ds	84.4
9.5	-	14049.9		1.232		72	f3ds	(4I)6K	f3ds	97.9
1.5	-	14142.4		1.176		34	f3ds	(4F)6F	f3ds	88.8
8.5	14177.723	14148.0	29	1.072	1.085	60	f3ds	(4I)4Lb	f3ds	86.1
4.5	14265.976	14230.0	35	1.110		17	f3ds	(4I)4Hb	f3ds	81.3
4.5	14366.889	14399.2	−32	1.078		8	f3ds	(4I)6H	f3ds	90.1
1.5	-	14477.7		1.043		14	f3ds	(4S)6D	f3ds	65.8
6.5	-	14496.9		1.142		16	f3ds	(4I)4Ia	f3ds	96.8
6.5	14599.600	14557.6	42	0.934		17	f3d2	(4I)6L	f3d2	61.8
4.5	14654.181	14628.3	25	1.057		12	f3ds	(4F)6G	f3ds	75.8
2.5	-	14660.8		0.777		17	f3ds	(4F)4Gb	f3ds	71.4
7.5	14724.776	14738.1	−13	1.170	1.170	34	f3ds	(4I)6I	f3ds	96.5
5.5	14709.266	14771.1	−61	0.925	0.920	10	f3ds	(4I)4Ka	f3ds	49.4
3.5	14900.134	14873.4	26	1.010		7	f3ds	(4G)6G	f3ds	84.7
0.5	-	14905.3		1.636		32	f3ds	(4S)6D	f3ds	92.3
4.5	-	14981.0		1.177		44	f3s2	(4F)4F	f3s2	71.3
6.5	14991.377	14993.8	−2	1.180		17	f3ds	(4F)6H	f3ds	88.6
2.5	-	15013.4		1.198		13	f3ds	(4F)6P	f3ds	89.2

Table 3. *Cont.*

J	E^{exp} ($\mathbf{cm^{-1}}$)	E^{th} ($\mathbf{cm^{-1}}$)	ΔE ($\mathbf{cm^{-1}}$)	g_L^{th}	g_L^{exp}	% 1^{st}*comp*	*Conf*	*Term*	*Main conf*	%
3.5	15147.878	15080.0	67	0.989		9	f3ds	(4F)4Gb	f3ds	79.0
1.5	-	15205.3		1.007		10	f3ds	(4G)6G	f3ds	66.4
5.5	15234.383	15205.3	29	1.058		7	f3ds	(4F)6H	f3ds	78.7
2.5	-	15280.5		1.147		33	f3ds	(4F)6F	f3ds	71.8
1.5	-	15308.6		1.985		55	f3ds	(4F)6P	f3ds	93.4
5.5	15330.434	15334.3	−3	1.123		14	f3ds	(4I)6G	f3ds	82.6
4.5	15413.346	15397.6	15	0.984		14	f3ds	(4G)6I	f3ds	52.3
0.5	-	15411.9		0.611		25	f3ds	(4S)4Db	f3ds	81.9
3.5	15587.280	15423.3	164	1.031		9	f3ds	(4I)4Ga	f3ds	63.2
5.5	15430.900	15483.0	−52	1.073		16	f3s2	(2H)2H2	f3ds	54.4
9.5	15534.868	15604.8	−69	1.093	1.095	89	f3d2	(4I)6M	f3ds	97.5
7.5	15692.655	15633.9	58	1.005		62	f3d2	(4I)6L	f3d2	92.4
10.5	-	15655.2		1.230		91	f3ds	(4I)6L	f3ds	99.7
8.5	15767.762	15683.0	84	1.200		36	f3ds	(4I)6I	f3ds	96.2
3.5	-	15689.4		1.136		11	f3ds	(4F)6P	f3ds	82.3
6.5	15717.452	15736.5	−19	1.026	1.04	35	f3d2	(4I)6Ka	f3d2	69.0
5.5	15863.755	15811.3	52	1.027		14	f3d2	(4I)6Ia	f3d2	51.9
4.5	15916.166	15879.5	36	0.971		28	f3d2	(4I)6Kb	f3ds	55.2
2.5	-	15883.4		0.628		10	f3d2	(4I)6Ha	f3d2	49.2
6.5	15884.560	15900.5	−15	1.072	1.150	12	f3ds	(4I)4Ka	f3ds	72.3
7.5	16156.487	16066.8	89	1.150		19	f3ds	(4I)6H	f3ds	82.9
2.5	16213.945	16073.4	140	1.010		7	f3ds	(4G)2F	f3ds	84.5
0.5	-	16099.2	0	2.345		32	f3ds	(4F)6D	f3ds	93.9
4.5	16063.244	16101.2	−37	0.889		21	f3d2	(4I)6Kb	f3ds	44.9
5.5	16003.163	16120.1	−116	1.091		20	f3ds	(4G)6I	f3ds	75.8
3.5	-	16140.4		1.052		15	f3ds	(4G)6H	f3ds	75.0
1.5	-	16176.8		1.130		9	f3ds	(4F)4Pa	f3ds	85.5
2.5	16336.514	16281.8	54	1.161		7	f3ds	(4F)6P	f3ds	74.4
3.5	16239.757	16285.9	−46	1.230		14	f3ds	(4F)6P	f3ds	83.5
4.5	16338.719	16290.5	48	1.040		6	f3ds	(4I)4Ia	f3ds	87.9
8.5	-	16419.3		1.098		22	f3ds	(4I)4La	f3ds	78.7
3.5	16376.820	16443.1	−66	1.048		9	f3ds	(4I)4Gb	f3ds	63.7
6.5	16532.589	16466.5	66	1.043		14	f3ds	(4I)2I	f3ds	77.6
1.5	-	16471.3		1.008		12	f3ds	(4F)2D	f3ds	86.2
2.5	16473.747	16481.7	−7	0.952		13	f3ds	(4F)6F	f3ds	65.1
5.5	16397.828	16490.5	−92	1.045		13	f3s2	(2H)2H2	f3ds	51.3
1.5	-	16528.6		0.844		10	f3s2	(4D)4D	f3ds	49.5
4.5	16514.265	16528.9	−14	0.986		16	f3s2	(4G)4G	f3ds	51.5
6.5	16618.369	16650.2	−31	0.987		60	f3s2	(2K)2K	f3s2	68.2
2.5	-	16660.2		1.339		22	f3ds	(4F)6P	f3ds	80.3
3.5	16672.399	16723.4	−51	1.019		7	f3ds	(4G)6G	f3ds	69.2
7.5	16690.212	16731.2	−40	0.986		14	f3ds	(2K)4M	f3ds	51.9
4.5	16819.694	16758.4	61	1.033		11	f3ds	(4F)6G	f3ds	68.2
5.5	16699.409	16782.6	−83	1.114		16	f3ds	(4I)6H	f3ds	78.5
2.5	16838.258	16808.1	30	0.982		10	f3ds	(4G)6H	f3ds	83.1
0.5	-	16830.2		0.230		14	f3d2	(4I)6F	f3d2	71.1
2.5	-	16867.1		1.060		8	f3ds	(4G)6H	f3ds	58.8
3.5	16857.015	16868.5	−11	0.838		10	f3d2	(4F)6I	f3ds	54.8
5.5	16758.024	16899.5	−141	1.026		12	f3ds	(4I)4Ka	f3ds	65.5
8.5	16982.510	16958.9	23	1.143		22	f3ds	(4I)4Kb	f3ds	91.3
4.5	-	16964.3		1.026		11	f3ds	(4F)4Hb	f3ds	64.7
6.5	16990.271	17005.7	−15	1.118		12	f3ds	(4I)4Ib	f3ds	59.7
1.5	-	17006.8		0.859		9	f3d2	(4I)6F	f3ds	55.0
2.5	17008.229	17102.2	−94	1.154		10	f3ds	(4F)6D	f3ds	84.7
3.5	-	17117.2		0.920		8	f3ds	(4G)4Hb	f3ds	60.7

Table 3. *Cont.*

J	E^{exp} ($\mathbf{cm^{-1}}$)	E^{th} ($\mathbf{cm^{-1}}$)	ΔE ($\mathbf{cm^{-1}}$)	g_L^{th}	g_L^{exp}	% 1^{st} *comp*	*Conf*	*Term*	*Main conf*	%
5.5	17205.372	17170.4	34	1.120		28	f3ds	(4F)6G	f3ds	76.8
1.5	-	17192.9		0.957		17	f3ds	(4F)2P	f3ds	82.7
0.5	-	17217.5		0.499		30	f3s2	(2P)2P	f3s2	53.9
4.5	17200.903	17280.6	−79	0.979	0.970	10	f3ds	(4G)4Ib	f3d2	50.5
7.5	17259.216	17301.3	−42	1.118		12	f3ds	(4I)4Ib	f3ds	79.9
2.5	-	17320.0		0.619		18	f3ds	(4G)6H	f3ds	48.2
3.5	17381.930	17363.1	18	1.184		17	f3ds	(4F)6D	f3ds	84.2
1.5	-	17364.5		0.679		7	f3ds	(4F)4Fa	f3ds	77.1
4.5	17388.631	17392.7	−4	1.010		13	f3ds	(4I)4Hb	f3ds	65.2
6.5	17461.883	17423.5	38	1.155		18	f3ds	(4I)6G	f3ds	84.6
3.5	-	17481.4		1.163		15	f3ds	(4S)6D	f3ds	67.6
7.5	17556.776	17523.7	33	1.055		11	f3d2	(4I)6L	f3ds	68.6
1.5	-	17579.4		0.960		15	f3d2	(4I)6F	f3ds	57.4
2.5	17621.175	17607.3	13	0.941		5	f3d2	(4I)6Hb	f3ds	57.1
3.5	17560.922	17619.6	−58	0.991		10	f3ds	(4G)4Gb	f3ds	72.9
5.5	17755.028	17785.9	−30	1.050		11	f3ds	(2H)4K2	f3ds	84.0
6.5	17775.960	17808.2	−32	1.046		15	f3d2	(4I)6Ka	f3d2	57.7
0.5	-	17812.2		0.076		13	f3d2	(4I)6F	f3ds	51.0
3.5	17823.434	17820.9	2	0.950		12	f3d2	(4F)6I	f3d2	51.4
2.5	-	17857.4		0.987		5	f3s2	(4D)4D	f3d2	44.1
5.5	17922.769	17934.8	−12	0.973		11	f3d2	(4I)4Ka	f3d2	65.0
6.5	17888.312	17935.3	−47	1.157		21	f3ds	(4F)6H	f3ds	90.7
3.5	-	17959.5		0.963		12	f3d2	(4I)6Ha	f3ds	48.7
4.5	18009.838	17965.3	44	1.119		12	f3ds	(4F)6F	f3ds	71.6
9.5	-	17995.9		1.146		68	f3ds	(4I)4Lb	f3ds	81.7
8.5	18032.564	18015.8	16	1.044		25	f3d2	(4I)6L	f3d2	92.4
3.5	18041.437	18095.3	−53	0.913		9	f3d2	(4F)6I	f3ds	51.0
2.5	18178.854	18128.3	50	1.074		5	f3s2	(4D)4D	f3ds	54.7
5.5	18102.958	18150.0	−47	1.117		7	f3ds	(4F)6F	f3ds	79.1
4.5	-	18182.7		1.081		8	f3d2	(4I)6Ha	f3ds	70.3
3.5	-	18232.9		0.974		7	f3d2	(4I)6Ha	f3d2	40.4
3.5	18291.412	18326.3	−34	0.893		19	f3d2	(4I)6Ib	f3d2	63.0
1.5	-	18385.9		0.921		8	f3ds	(4F)6F	f3ds	59.8
4.5	-	18424.3		1.061		8	f3ds	(4F)4Hb	f3ds	68.1
0.5	-	18436.4		0.102		30	f3ds	(4G)6F	f3ds	59.7
1.5	-	18451.3		0.966		10	f3ds	(4S)6D	f3ds	54.7
2.5	18594.848	18459.0	135	0.995		4	f3d2	(4I)6Ha	f3d2	49.9
7.5	-	18486.3		1.112		7	f3ds	(4I)4Ia	f3ds	50.0
4.5	18526.283	18503.5	22	0.990		10	f3d2	(4I)6Ia	f3d2	54.0
3.5	-	18505.9		0.955		6	f3d2	(4I)6Ia	f3ds	50.6
7.5	18539.154	18523.8	15	1.098		10	f3ds	(4I)4Ia	f3ds	50.6
6.5	18451.979	18576.6	−124	1.116		40	f3ds	(4G)6I	f3ds	89.1
0.5	-	18623.1		1.461		35	f3ds	(4F)4Pb	f3ds	79.0
1.5	-	18664.9		1.001		11	f3ds	(4F)4Pb	f3ds	57.2
2.5	18852.922	18728.5	124	1.145		5	f3ds	(4S)6D	f3ds	72.2
5.5	18754.949	18740.0	14	1.013		12	f3d2	(4I)6Kb	f3d2	60.4
6.5	18788.827	18792.5	−3	1.042		14	f3d2	(4I)4La	f3d2	67.4
8.5	-	18796.5		1.153		29	f3ds	(2H)4K2	f3ds	90.2
3.5	18796.998	18857.5	−60	0.841		15	f3d2	(4I)6Hb	f3d2	61.4
5.5	18892.289	18858.6	33	0.969		24	f3d2	(4I)6Kb	f3d2	61.0
2.5	-	18913.1		1.008		5	f3d2	(4F)6Ga	f3ds	60.9
7.5	19017.870	18939.8	78	1.161		16	f3ds	(4I)4Ka	f3ds	81.9
10.5	-	18945.7		1.157		92	f3d2	(4I)6M	f3d2	100.
0.5	-	18964.1		0.717		10	f3ds	(4F)4Db	f3ds	72.7
4.5	19004.689	18967.7	36	1.024		5	f3ds	(4F)4Gb	f3ds	65.0
2.5	-	19032.8		0.700		14	f3d2	(4I)6Hb	f3ds	52.2

Table 3. *Cont.*

J	E^{exp} $(\mathbf{cm^{-1}})$	E^{th} $(\mathbf{cm^{-1}})$	ΔE $(\mathbf{cm^{-1}})$	g_L^{th}	g_L^{exp}	% 1^{st}comp	Conf	Term	Main conf	%
1.5	-	19059.2		1.033		16	f3ds	(4G)6F	f3ds	59.4
1.5	-	19112.9		1.073		13	f3ds	(4F)4Fb	f3ds	76.4
4.5	19147.489	19141.1	6	1.179		16	f3ds	(4F)6F	f3ds	70.5
5.5	19129.394	19157.3	−27	1.019		11	f3ds	(4I)4Gb	f3ds	62.9
8.5	19242.364	19215.9	26	1.042		48	f3d2	(4I)6L	f3d2	89.0
4.5	19237.394	19219.6	17	1.174		12	f3s2	(4G)4G	f3ds	66.2
6.5	19276.989	19249.2	27	1.166		8	f3ds	(4I)6G	f3ds	67.6
0.5	-	19274.8		0.018		13	f3ds	(4F)4Da	f3ds	62.7
4.5	19375.292	19300.7	74	1.031		11	f3d2	(4G)6K	f3ds	58.0
3.5	19316.823	19365.5	−48	1.211		16	f3ds	(4F)6P	f3ds	78.0
1.5	-	19372.2		0.983		12	f3d2	(4I)6G	f3ds	49.7
5.5	19473.367	19473.3		0.982		13	f3d2	(4I)6Kb	f3d2	64.7
3.5	-	19490.5		1.086		11	f3ds	(4F)4Fb	f3d2	50.5
7.5	19510.817	19551.1	−40	1.045		8	f3ds	(2K)4K	f3ds	71.7
7.5	-	19592.9		1.049		23	f3s2	(2K)2K	f3s2	47.0
4.5	19627.056	19598.3	28	1.093		9	f3d2	(4G)6K	f3ds	64.9
3.5	19570.868	19600.8	−29	1.017		5	f3ds	(4S)4Db	f3d2	56.0
2.5	19469.535	19630.2	−160	1.085		9	f3ds	(4G)6F	f3ds	68.6
1.5	-	19743.7		0.654		26	f3d2	(4I)6G	f3d2	48.0
7.5	19748.316	19758.5	−10	1.078		20	f3d2	(4I)6Ka	f3d2	46.6
2.5	-	19760.1		1.182		9	f3s2	(2D)2D1	f3ds	59.1
6.5	19694.329	19779.6	−85	1.023		9	f3ds	(2K)4K	f3ds	61.3
5.5	19733.338	19797.2	−63	1.079		13	f3ds	(4G)6H	f3ds	68.9
4.5	19869.609	19841.7	27	1.053		7	f3d2	(4I)6Hb	f3d2	52.8
3.5	-	19846.5		0.967		7	f3ds	(4S)4Db	f3ds	68.2
9.5	-	19865.8		1.141		23	f3ds	(4I)4La	f3ds	81.4
6.5	-	19922.7		1.035		15	f3d2	(4I)6Kb	f3d2	56.3
4.5	20018.685	19953.9	64	0.910		28	f3d2	(4G)6K	f3d2	52.5
5.5	-	19960.6		1.063		16	f3ds	(2K)4K	f3ds	79.3
2.5	-	20001.7		0.970		10	f3d2	(4I)6G	f3d2	51.3
1.5	-	20038.3		0.807		8	f3d2	(4I)6G	f3ds	50.0
3.5	20084.775	20039.4	45	0.978		6	f3ds	(4F)4Gb	f3d2	45.1
0.5	-	20067.8		1.423		16	f3ds	(4G)6D	f3ds	58.5
6.5	20055.098	20097.5	−42	1.129		19	f3ds	(4F)6G	f3ds	66.5
5.5	-	20103.3		1.080		11	f3ds	(4G)6G	f3ds	73.9
3.5	20263.434	20107.4	156	1.038		11	f3d2	(4F)6H	f3d2	54.8
7.5	20148.474	20124.4	24	0.985		18	f3d2	(4I)4Ma	f3d2	51.4
8.5	-	20130.9		1.093		26	f3d2	(4I)6Ka	f3d2	83.3
4.5	20033.114	20149.0	−115	1.128		13	f3d2	(4I)6Ha	f3ds	47.2
2.5	-	20196.5		1.138		8	f3ds	(4G)6F	f3ds	49.0
1.5	-	20202.8		1.050		10	f3ds	(4D)6F	f3ds	67.7
6.5	-	20217.0		1.067		9	f3d2	(4I)4Lb	f3ds	66.3
5.5	-	20249.0		1.138		16	f3s2	(2H)2H1	f3ds	47.4
0.5	-	20290.5		0.067		17	f3ds	(4G)6F	f3ds	58.5
4.5	20340.780	20306.0	34	1.083		13	f3d2	(4F)6I	f3d2	51.7
2.5	-	20356.6		1.013		16	f3s2	(2D)2D1	f3ds	59.5
4.5	-	20458.9		0.949		7	f3ds	(2H)4I2	f3ds	52.5
6.5	-	20499.6		1.108		23	f3ds	(4I)4Hb	f3ds	86.7
3.5	20514.235	20526.7	−12	1.030		9	f3ds	(4G)6H	f3ds	68.5
4.5	20500.810	20528.4	−27	1.006		8	f3d2	(4F)6I	f3ds	61.3
2.5	-	20537.7		1.034		6	f3ds	(2G)4G1	f3ds	54.5
5.5	-	20541.7		1.078		9	f3ds	(4G)4Ib	f3ds	51.7
3.5	-	20595.8		1.055		7	f3ds	(4F)6F	f3ds	58.1
1.5	-	20632.0		1.171		7	f3ds	(4G)6F	f3ds	64.4
5.5	-	20634.6		1.069		8	f3ds	(2H)4I2	f3ds	67.9
4.5	-	20658.4		1.023		11	f3d2	(4I)6Hb	f3ds	49.6

Table 3. *Cont.*

J	E^{exp} $(\mathbf{cm^{-1}})$	E^{th} $(\mathbf{cm^{-1}})$	ΔE $(\mathbf{cm^{-1}})$	g_L^{th}	g_L^{exp}	% 1st comp	Conf	Term	Main conf	%
7.5	-	20663.4		1.098		21	f3ds	(4G)6I	f3ds	71.6
8.5	-	20670.8		1.068		14	f3ds	(2K)4M	f3d2	50.5
2.5	-	20704.1		1.122		19	f3ds	(4G)6F	f3ds	65.7
7.5	-	20771.0		1.031		11	f3d2	(4I)4Ma	f3ds	52.3
6.5	-	20779.4		1.008		10	f3ds	(2K)4L	f3ds	61.0
3.5	-	20780.2		1.054		7	f3d2	(4F)6H	f3d2	52.7
0.5	-	20796.7		1.267		16	f3ds	(4G)6D	f3ds	65.5
4.5	20899.429	20808.9	90	1.065		8	f3ds	(4G)6G	f3ds	61.3
2.5	-	20851.8		0.970		26	f3s2	(2D)2D1	f3s2	33.0
5.5	-	20951.3		1.110		15	f3d2	(4I)6Ib	f3d2	55.1
1.5	-	20961.9		0.786		8	f3ds	(2P)4F	f3ds	58.5
3.5	20890.426	20965.3	−74	1.130		9	f3ds	(4F)4Fb	f3ds	50.1
5.5	-	21022.3		1.084		7	f3ds	(2H> 2I2	f3ds	59.9
7.5	20946.239	21023.1	−76	1.008		23	f3d2	(4I)4Mb	f3d2	79.4
4.5	21103.432	21118.7	−15	1.078		7	f3d2	(4F)6H	f3ds	50.6
1.5	-	21159.6		0.906		11	f3ds	(4G)6F	f3ds	54.0
3.5	21107.881	21165.2	−57	0.870		14	f3d2	(4G)6I	f3d2	49.3
7.5	-	21215.3		1.111		13	f3ds	(4F)6H	f3ds	84.4
4.5	-	21232.1		1.062		14	f3ds	(4G)4Hb	f3ds	55.3
6.5	-	21247.7		1.005		6	f3ds	(2H)2K2	f3d2	52.8
2.5	-	21256.4		1.004		6	f3d2	(4I)6G	f3d2	51.8
1.5	-	21288.7		1.046		5	f3ds	(4S)6D	f3ds	71.5
4.5	21387.040	21309.6	77	0.940		9	f3d2	(4G)6I	f3d2	74.1
5.5	-	21309.5		1.129		13	f3ds	(4F)6F	f3ds	62.0
2.5	-	21350.9		1.045		10	f3ds	(4G)6F	f3ds	57.4
0.5	-	21372.9		1.981		13	f3ds	(4D)6D	f3ds	64.7
3.5	-	21415.6		1.018		9	f3ds	(4F)2G	f3ds	70.7
5.5	-	21494.8		1.104		4	f3ds	(4F)6G	f3ds	66.0
1.5	-	21502.1		0.977		6	f3ds	(4G)4Fb	f3ds	64.9
8.5	-	21531.9		1.072		12	f3ds	(2K)4M	f3d2	58.7
2.5	-	21553.7		1.045		7	f3ds	(4D)6F	f3ds	65.9
8.5	-	21582.8		1.058		24	f3ds	(4I)4Kb	f3ds	78.3
6.5	21645.939	21597.3	48	1.152		12	f3d2	(4I)6Ha	f3ds	51.0
0.5	-	21604.6		0.518		11	f3s2	(2P)2P	f3ds	44.8
9.5	-	21618.8		1.159		73	f3d2	(4I)6L	f3d2	99.9
3.5	-	21651.4		1.144		11	f3ds	(4G)4Gb	f3ds	67.0
4.5	-	21656.8		1.177		21	f3ds	(2H)4F2	f3ds	82.7
5.5	-	21662.8		1.075		6	f3d2	(4I)6Hb	f3d2	65.7
2.5	-	21718.6		1.114		7	f3d2	(4F)6Ga	f3ds	51.7
0.5	-	21721.7		0.048		14	f3d2	(4S)6F	f3d2	58.4
4.5	21793.334	21750.4	42	1.067		10	f3d2	(4F)6Ga	f3d2	65.1
7.5	-	21768.7		1.100		9	f3ds	(2H)2K2	f3ds	92.0
6.5	-	21803.0		1.117		7	f3ds	(4I)4Ha	f3ds	75.2
5.5	-	21819.9		1.081		7	f3d2	(4I)6Ha	f3ds	51.0
4.5	-	21821.1		1.070		7	f3d2	(4G)6I	f3ds	52.6
3.5	-	21855.1		1.096		6	f3ds	(2H> 2F2	f3ds	63.9
6.5	21858.433	21863.2	−4	1.015		31	f3d2	(4I)6Kb	f3d2	80.9
2.5	-	21873.3		1.090		7	f3ds	(4F)4Pb	f3ds	70.7
5.5	-	21886.1		1.088		7	f3ds	(4F)4Gb	f3ds	53.7
2.5	-	21942.1		1.178		8	f3d2	(4F)6P	f3d2	70.4
1.5	-	21944.2		0.872		8	f3d2	(4S)6F	f3ds	44.7
4.5	-	21981.2		1.074		8	f3d2	(4F)6H	f3ds	65.1
3.5	-	22046.5		1.089		6	f3d2	(4F)6Ga	f3ds	61.1
1.5	-	22059.7		1.278		11	f3ds	(4G)6D	f3ds	58.5
2.5	-	22070.4		0.903		6	f3ds	(4G)4Gb	f3ds	60.4
5.5	-	22089.4		1.062		24	f3s2	(2I)2I	f3d2	33.5

Table 3. *Cont.*

J	E^{exp} $(\mathbf{cm^{-1}})$	E^{th} $(\mathbf{cm^{-1}})$	ΔE $(\mathbf{cm^{-1}})$	g_L^{th}	g_L^{exp}	*% 1st comp*	*Conf*	*Term*	*Main conf*	*%*
5.5	-	22123.0		1.023		14	f3d2	(4G)6K	f3d2	62.3
1.5	-	22127.9		1.207		88	f3d2	(4I)6M	f3d2	100.
8.5	-	22150.9		1.120		16	f3ds	(4I)6I	f3ds	84.2
3.5	-	22152.9		1.206		18	f3ds	(4G)6F	f3ds	74.8
3.5	-	22197.0		1.101		8	f3d2	(4I)6F	f3d2	59.6
4.5	22230.453	22197.0	33	1.114		7	f3s2	(2G)2G1	f3d2	41.3
6.5	-	22225.0		1.093		4	f3ds	(4G)6G	f3d2	51.3
2.5	-	22226.7		1.125		8	f3ds	(2H)4F2	f3ds	70.4
4.5	-	22262.3		0.943		8	f3d2	(4G)6I	f3ds	49.9
1.5	-	22269.6		1.121		6	f3ds	(4D)6D	f3d2	50.6
6.5	-	22273.6		1.086		10	f3ds	(4F)4Hb	f3ds	64.9
4.5	22305.305	22289.0	16	1.090		15	f3ds	(4I)2G	f3ds	55.5
7.5	-	22300.7		1.062		15	f3ds	(4I)4Ib	f3ds	58.6
3.5	-	22350.7		0.985		9	f3d2	(4I)4Hc	f3d2	61.8
4.5	-	22398.8		1.054		8	f3s2	(2G)2G1	f3ds	42.7
1.5	-	22425.5		1.053		9	f3ds	(4F)4Fb	f3ds	62.9
3.5	-	22449.8		1.049		7	f3ds	(4G)6G	f3d2	50.1
5.5	-	22470.4		1.019		17	f3d2	(4G)6K	f3d2	78.5
5.5	22567.167	22555.9	11	1.080		11	f3d2	(4G)6K	f3d2	50.3
7.5	-	22582.5		1.220		23	f3ds	(4G)6H	f3ds	68.3
2.5	-	22589.1		0.927		6	f3d2	(4I)4Gb	f3d2	58.8
4.5	-	22604.6		1.115		5	f3ds	(4I)4Ga	f3ds	49.4
0.5	-	22620.1		0.894		11	f3ds	(4D)6D	f3ds	60.9
3.5	-	22645.0		1.020		5	f3ds	(4I)4Ga	f3ds	51.8
6.5	-	22692.1		1.223		23	f3ds	(4G)6G	f3ds	80.8
2.5	-	22693.8		1.021		6	f3ds	(2D)4F2	f3ds	61.9
5.5	-	22708.2		1.185		6	f3ds	(4G)6G	f3ds	53.5
3.5	-	22729.6		1.131		7	f3ds	(4D)6D	f3ds	58.6
5.5	22813.792	22788.4	25	1.049		6	f3ds	(2K)4I	f3ds	52.7
3.5	-	22793.4		1.215		8	f3s2	(4D)4D	f3ds	68.0
7.5	-	22819.3		1.048		12	f3d2	(4I)6Kb	f3d2	64.3
6.5	-	22820.8		1.050		7	f3ds	(4G)4Ib	f3ds	55.7
0.5	-	22833.5		1.834		20	f3ds	(2D)2S1	f3ds	80.9
1.5	-	22833.8		1.287		9	f3d2	(4F)6P	f3d2	59.8
5.5	-	22851.9		1.043		7	f3d2	(4F)6I	f3d2	61.3
3.5	-	22857.0		1.182		7	f3s2	(4D)4D	f3ds	58.4
8.5	-	22888.2		1.135		34	f3d2	(4I)6Ka	f3d2	82.6
1.5	-	22942.6		1.091		7	f3ds	(4G)6D	f3ds	72.5
3.5	-	22963.0		1.051		8	f3ds	(2H> 2F2	f3ds	64.5
2.5	-	22972.1		1.012		5	f3ds	(4G)4Fb	f3ds	62.2
1.5	-	22991.6		0.806		8	f3d2	(4F)6Ga	f3ds	51.1
4.5	-	23006.5		1.047		3	f3d2	(4I)6Ib	f3d2	46.1
2.5	-	23031.6		1.181		4	f3ds	(2H> 2F2	f3ds	53.7
2.5	-	23062.2		1.204		14	f3ds	(4G)6D	f3ds	66.3
4.5	23106.350	23094.0	12	1.023		7	f3d2	(4G)6I	f3d2	63.8
6.5	23013.222	23100.7	−87	1.066		9	f3ds	(4G)6H	f3d2	53.5
8.5	-	23125.4		1.173		34	f3ds	(4G)6I	f3ds	84.5
5.5	23043.896	23135.7	−91	1.111		11	f3s2	(4G)4G	f3ds	49.8
0.5	-	23170.1		0.636		11	f3d2	(4F)6Fa	f3d2	53.0
5.5	-	23170.0		1.131		9	f3ds	(2H)4G2	f3ds	76.9
1.5	-	23225.8		1.043		5	f3ds	(2D)4P1	f3ds	54.4
3.5	-	23259.0		1.082		6	f3d2	(4F)6Fb	f3d2	51.4
7.5	23371.611	23282.8	88	1.047		26	f3d2	(4I)6Kb	f3d2	82.3
2.5	-	23293.3		0.964		5	f3d2	(4F)6Fa	f3ds	48.9
9.5	-	23318.7		1.196		47	f3d2	(4I)6Ka	f3d2	99.9

Table 3. *Cont.*

J	E^{exp} $(\mathbf{cm^{-1}})$	E^{th} $(\mathbf{cm^{-1}})$	ΔE $(\mathbf{cm^{-1}})$	g_L^{th}	g_L^{exp}	% 1^{st} comp	Conf	Term	Main conf	%
6.5	-	23329.5		1.092		7	f3d2	(4F)6H	f3d2	69.3
2.5	-	23330.0		1.174		6	f3ds	(2D)4P1	f3ds	73.2
1.5	-	23364.1		1.369		14	f3d2	(4F)6P	f3d2	49.4
0.5	-	23375.3		1.338		23	f3ds	(2D)2S1	f3ds	78.6
4.5	-	23397.0		1.097		11	f3ds	(4F)4Fb	f3ds	60.5
3.5	-	23461.6		1.152		6	f3d2	(4F)6P	f3d2	54.8
4.5	-	23474.8		1.020		13	f3d2	(4I)6G	f3d2	69.7
8.5	-	23507.1		1.032		28	f3d2	(4I)4Ma	f3d2	79.9
6.5	-	23534.5		1.060		5	f3ds	(2K)4L	f3ds	53.0
2.5	-	23557.4		1.091		6	f3d2	(4I)6F	f3d2	45.6
5.5	23528.305	23572.0	−43	1.079		6	f3d2	(4F)6H	f3d2	59.3
3.5	-	23585.2		1.047		4	f3ds	(2H)4G2	f3ds	54.3
5.5	-	23594.8		1.146		9	f3ds	(2H)4H2	f3ds	56.3
3.5	-	23601.2		1.214		9	f3ds	(4G)6D	f3ds	51.7
1.5	-	23648.2		0.829		9	f3ds	(2D)4F1	f3ds	62.1
7.5	-	23651.9		1.084		15	f3ds	(2H)4K2	f3ds	75.8
5.5	-	23671.9		1.137		6	f3d2	(4F)6Ga	f3d2	58.2
0.5	-	23688.3		0.487		15	f3d2	(4F)6Fa	f3ds	49.3
4.5	-	23706.2		1.100		8	f3d2	(4I)6G	f3d2	58.8
3.5	-	23726.6		1.131		3	f3ds	(4D)6F	f3ds	56.0
9.5	-	23730.0		1.088		41	f3ds	(2K)4M	f3ds	99.9
6.5	-	23735.2		1.093		8	f3d2	(4F)6I	f3ds	62.3
4.5	-	23760.6		1.112		10	f3d2	(4I)6F	f3d2	51.8
0.5	-	23774.7		0.513		14	f3s2	(4D)4D	f3ds	46.4
2.5	-	23811.4		0.973		9	f3d2	(4S)6F	f3d2	64.0
1.5	-	23813.8		0.906		15	f3d2	(4F)6Fa	f3d2	47.4
5.5	-	23814.8		1.095		5	f3s2	(4G)4G	f3d2	65.2
6.5	-	23819.7		1.094		5	f3ds	(4G)4Ib	f3d2	51.7
7.5	-	23823.9		1.037		21	f3d2	(4I)4Mb	f3d2	89.3
2.5	-	23844.1		1.166		5	f3ds	(2D)4P1	f3ds	62.3
6.5	-	23916.1		1.130		11	f3d2	(4I)6Ib	f3d2	65.2
2.5	-	23926.4		1.092		6	f3ds	(4F)4Ga	f3ds	75.7
1.5	-	23940.0		0.948		6	f3ds	(4D)6G	f3ds	65.3
3.5	-	23945.5		1.031		4	f3d2	(4G)6I	f3d2	52.2
4.5	23924.333	23956.4	−32	1.100		5	f3ds	(2K)4I	f3ds	70.9
0.5	-	23978.6		1.410		10	f3d2	(4S)6F	f3d2	66.6
8.5	-	23985.8		0.995		13	f3d2	(4I)4N	f3d2	54.4
5.5	-	24014.6		1.150		11	f3d2	(4F)6H	f3ds	49.7
5.5	-	24061.4		1.115		8	f3ds	(4G)6F	f3ds	70.7
7.5	-	24091.8		1.123		10	f3d2	(4I)6Ha	f3d2	64.6
4.5	-	24098.6		1.129		7	f3d2	(4I)6G	f3ds	50.5
1.5	-	24104.3		0.872		10	f3d2	(4F)6Gb	f3ds	43.9
5.5	-	24163.8		1.111		8	f3ds	(4G)4Gb	f3ds	54.0
3.5	-	24199.1		0.952		6	f3d2	(4I)4Hc	f3d2	62.1
0.5	-	24202.1		0.767		9	f3ds	(2D)4P1	f3ds	61.4
2.5	-	24214.8		1.139		5	f3ds	(4F)4Db	f3ds	62.7
3.5	-	24215.6		1.249		8	f3ds	(4G)6F	f3ds	48.6
4.5	-	24232.9		1.084		11	f3d2	(4F)6Ga	f3d2	58.8
6.5	-	24278.4		1.060		7	f3d2	(4G)6K	f3d2	64.9
9.5	-	24314.3		1.013		50	f3d2	(4I)4N	f3d2	99.9
2.5	-	24319.2		0.969		8	f3d2	(4G)6Ha	f3d2	57.6
2.5	-	24359.1		1.202		6	f3d2	(4F)6P	f3ds	48.6
1.5	-	24369.2		1.084		6	f3ds	(2D)4P1	f3ds	53.5
4.5	-	24377.2		1.100		4	f3ds	(4F)2H	f3d2	63.1
5.5	-	24383.2		1.098		7	f3ds	(2K)4I	f3ds	65.1
6.5	-	24388.0		1.063		10	f3ds	(2K)4K	f3ds	57.9

Table 3. *Cont.*

J	E^{exp} (cm^{-1})	E^{th} (cm^{-1})	ΔE (cm^{-1})	g_L^{th}	g_L^{exp}	% 1stcomp	Conf	Term	Main conf	%
3.5	-	24403.0		1.168		8	f3ds	(4D)6G	f3ds	51.2
10.5	-	24433.6		1.209		71	f3d2	(4I)6L	f3d2	99.9
7.5	-	24441.5		1.077		12	f3ds	(2K)4K	f3ds	53.7
1.5	-	24488.1		0.673		20	f3d2	(4F)6Gb	f3d2	57.1
1.5	-	24505.5		1.121		5	f3ds	(2D)4P1	f3ds	65.9
4.5	24446.491	24505.8	−59	1.070		4	f3d2	(4I)2Ha	f3d2	47.6
3.5	-	24548.7		1.089		5	f3ds	(4D)4Gb	f3ds	53.8
2.5	-	24570.0		1.060		6	f3d2	(4I)4Ga	f3d2	59.3
1.5	-	24602.0		1.162		9	f3ds	(4D)6D	f3ds	63.0
8.5	-	24605.5		1.069		19	f3d2	(4I)4Mb	f3d2	58.0
4.5	-	24707.3		0.959		4	f3d2	(4I)4Ib	f3ds	46.1
5.5	24771.463	24720.3	51	1.096		7	f3d2	(4G)6I	f3ds	58.6
6.5	-	24735.1		1.056		36	f3d2	(4G)6K	f3d2	91.9
2.5	-	24740.2		1.161		11	f3ds	(4G)4Db	f3d2	49.4
7.5	-	24754.0		1.125		8	f3d2	(4I)6Ha	f3d2	52.1
3.5	-	24790.7		1.124		4	f3ds	(4D)6D	f3d2	55.0
6.5	-	24812.7		1.058		7	f3ds	(4G)4Hb	f3d2	53.6
0.5	-	24840.6		0.546		9	f3d2	(4I)6F	f3d2	55.9
7.5	-	24851.5		1.093		10	f3ds	(2K)4L	f3ds	53.1
3.5	-	24861.8		1.247		9	f3ds	(4G)6D	f3ds	60.8
2.5	-	24877.5		1.259		6	f3ds	(4D)6D	f3ds	53.9
1.5	-	24889.3		0.985		3	f3d2	(4F)6Fa	f3d2	54.6
5.5	-	24920.7		1.094		5	f3ds	(4G)6F	f3d2	58.8
4.5	24888.132	24945.0	−56	1.161		9	f3ds	(4G)6F	f3ds	50.8
2.5	-	24964.3		1.135		5	f3ds	(2P)4F	f3ds	52.9
6.5	-	24986.3		1.073		5	f3d2	(4G)6K	f3ds	50.2
4.5	24984.711	25008.7	−23	1.023		3	f3ds	(2H)4I1	f3ds	57.1
8.5	-	25008.2		1.077		14	f3d2	(4I)6Ia	f3d2	52.8
7.5	-	25019.1		1.182		11	f3d2	(4F)6H	f3d2	78.6
3.5	-	25045.7		1.077		4	f3ds	(2P)2Fa	f3d2	54.7
5.5	25111.924	25063.7	48	1.170		6	f3ds	(4F)4Gb	f3ds	56.2
3.5	-	25082.7		1.126		5	f3ds	(4G)6G	f3d2	49.5
1.5	-	25084.7		1.215		11	f3d2	(4F)6Da	f3d2	56.5
6.5	-	25130.0		1.110		10	f3ds	(4G)6H	f3ds	50.0
4.5	-	25154.2		1.173		7	f3ds	(2H> 2G2	f3ds	51.7
2.5	-	25158.7		1.017		8	f3ds	(2H)2F2	f3d2	49.9
2.5	-	25179.5		1.213		5	f3d2	(4F)6Fa	f3d2	51.9
1.5	-	25219.2		0.913		7	f3d2	(4I)4Fb	f3ds	51.9
4.5	-	25236.5		1.036		9	f3s2	(2H)2H1	f3ds	48.1
5.5	25245.183	25237.4	7	1.021		25	f3d2	(4G)6I	f3d2	71.9
8.5	-	25302.6		1.037		23	f3d2	(4I)4Mb	f3d2	54.4
2.5	-	25320.0		1.094		8	f3d2	(4S)6F	f3d2	49.8
4.5	-	25325.8		1.152		6	f3ds	(4F)4Fb	f3ds	58.6
6.5	-	25376.5		1.091		8	f3s2	(2I)2I	f3d2	68.6
0.5	-	25379.7		1.245		11	f3ds	(4D)6D	f3ds	67.7
3.5	-	25396.3		1.018		5	f3ds	(4F)2G	f3d2	47.5
6.5	-	25411.7		1.092		9	f3s2	(2I)2I	f3d2	50.4
3.5	-	25453.7		1.070		4	f3d2	(4I)2G	f3d2	47.5
4.5	25439.103	25463.6	−24	1.076		5	f3d2	(4S)6F	f3d2	58.6
5.5	25423.490	25476.5	−53	0.977		7	f3ds	(2I)4K	f3d2	54.5
1.5	-	25482.2		1.014		8	f3ds	(2D)4S1	f3ds	53.0
3.5	-	25516.3		1.045		4	f3d2	(4G)6I	f3d2	56.6
0.5	-	25521.6		0.983		6	f3ds	(2D> 2P1	f3ds	53.1
5.5	25514.656	25537.8	−23	1.082		10	f3ds	(4G)2I	f3ds	49.4
4.5	-	25545.5		1.169		12	f3d2	(4S)6F	f3d2	58.7
6.5	-	25558.5		1.096		7	f3ds	(4G)4Ia	f3ds	63.1

Table 3. *Cont.*

J	E^{exp} (cm^{-1})	E^{th} (cm^{-1})	ΔE (cm^{-1})	g_L^{th}	g_L^{exp}	% 1^{st}comp	*Conf*	*Term*	*Main conf*	%
2.5	-	25582.3		1.134		9	f3d2	(4F)6Fa	f3ds	53.6
2.5	-	25603.8		0.986		6	f3ds	(4D)4Fb	f3d2	48.7
6.5	-	25647.8		1.088		42	f3s2	(2I)2I	f2s2	44.7
4.5	-	25665.7		1.137		4	f3ds	(4G)6F	f3d2	57.5
1.5	-	25666.4		1.063		7	f3ds	(4D)6G	f3d2	49.1
7.5	-	25671.0		1.079		7	f3ds	(2L)4M	f3ds	67.3
5.5	25726.260	25729.7	−3	1.101		4	f3d2	(4I)6G	f3ds	60.1
1.5	-	25754.9		1.030		6	f3d2	(4F)6Gb	f3d2	64.2

Table 4. Transitions of the U II odd parity level at 13695.737 cm^{-1} with $J = 4.5$ to even levels of $J = 3.5$.

wl_{Ritz} in Air (Å)	wn_{Ritz} (cm^{-1})	wn_{exp} (cm^{-1})	E_{even} (cm^{-1})	J	E_{odd} (cm^{-1})	J	Int	*Ref*
14539.464	6875.953	6875.950	20571.690	3.5	13695.737	4.5	18.15	[14]
13112.082	7624.469	7624.468	21320.206	3.5	13695.737	4.5	9.22	[14]
4566.3396	21893.243	21893.239	35588.980	3.5	13695.737	4.5	142	[7]
4452.1493	22454.758	22454.757	36150.495	3.5	13695.737	4.5	112	[7]
4354.3144	22959.274	22959.276	36655.011	3.5	13695.737	4.5	135	[7]
4343.3456	23017.256	23017.274	36712.993	3.5	13695.737	4.5	139	[7]
4299.6016	23251.430	23251.429	36947.167	3.5	13695.737	4.5	131	[7]
4103.8897	24360.253	24360.293	38055.990	3.5	13695.737	4.5	236	[7]
4058.3724	24633.463	24633.459	38329.200	3.5	13695.737	4.5	269	[7]
4036.9830	24763.977	24763.973	38459.714	3.5	13695.737	4.5	138	[7]
4026.7550	24826.878	24826.899	38522.615	3.5	13695.737	4.5	151	[7]
3990.6927	25051.223	25051.233	38746.960	3.5	13695.737	4.5	126	[7]
3965.9476	25207.524	25207.546	38903.261	3.5	13695.737	4.5	133	[7]
3891.9441	25686.821	25686.815	39382.558	3.5	13695.737	4.5	171	[7]
3765.4517	26549.697	26549.706	40245.434	3.5	13695.737	4.5	166	[7]
3734.8311	26767.359	26767.361	40463.096	3.5	13695.737	4.5	157	[7]
3728.6081	26812.033	26812.083	40507.770	3.5	13695.737	4.5	141	[7]
3697.7707	27035.628	27035.603	40731.365	3.5	13695.737	4.5	217	[7]

3.2. Even Parity Levels

Similarly to the odd parity study, the *RCN* and *RCN*2 codes were used in the Relativistic Hartree-Fock (*HFR*) mode. Considering the large CI interaction integrals within the group $5f^2(6d+7s)^3$, the previously undetermined configuration $5f^26d^3$ was added to the four lowest configurations $5f^47s, 5f^46d, 5f^26d^27s, 5f^26d7s^2$. Appropriate scaling of Slater and spin-orbit integrals and corrections on the average energy parameters were applied for preparing the initial input data of the *RCG* code and of the LSF in the *RCE* code. In the final cycle of optimization, 125 levels and 22 free parameters led to a *rms* deviation of 84 cm^{-1}, i.e., which is less satisfactory than in the odd parity. One of these levels, given at E_{exp} = 22917.453 cm^{-1} without any label in [6] has been identified as the lowest level of the $5f^26d^3$ configuration, slightly above the error bars of Brewer's predictions [9]. It is seen that the scaling factors of fitted parameters reported in Table 5 are not very different from those obtained in the opposite parity (Table 2). With regard to the unachieved status of the parametric interpretation in the even parity, only the dominant configuration and the first component of the eigenfunctions are given in Table 6, together with the energies and Landé factors calculated in the final LSF.

Attempts to interpret $5f^37s7p + 5f^36d7p$ with the same method of parametric fitting could not go beyond the optimization of the average energy E_{av} and spin-orbit ζ_{5f} parameters. In Table 7 energy parameters adopted for $5f^37s7p + 5f^36d7p$ are reported and they lead to the calculated energies in Table 8. The empirical attribution of E_{exp} levels to configurations derived from isotope shifts and transition intensities in [6] are not fully supported by the present calculations. There were more

$5f^37s7p$ labels in Table 2 of [6] than predicted from the present work (Cf Table 8). The quantitative evaluation of the CI effects within the whole group $5f^4(7s+6d)+5f^2(6d+7s)^3 + 5f^37s7p + 5f^36d7p$ has been attempted but has failed.

Table 5. Fitted parameters (in cm^{-1}) for even parity configurations of U II with $5f^2$ and $5f^4$ cores compared with HFR radial integrals. The scaling factors are $SF(P) = P_{fit}/P_{HFR}$ (dimensionless). They are replaced by $\Delta E = E_{fit} - E_{HFR}$ for E_{av} average energies (in cm^{-1}). Constraints on some parameters are in the 'Cstr' columns (denoted 'f' for fixed parameters or 'rn' , which link parameters of the same 'rn' to vary in a constant ratio). The HFR values of E_{av} parameters are relative to the lowest odd configuration $5f^37s^2$ taken as zero value.

	$5f^47s$					**$5f^46d$**				
Param. P	P_{fit}	Cstr.	Unc.	P_{HFR}	$\Delta E/SF$	P_{fit}	Cstr.	Unc.	P_{HFR}	$\Delta E/SF$
E_{av}	32165		112	15872	16293	46815		153	29044	17771
$F^2(ff)$	42100	r1	471	63821	0.660	41167	r1	461	62408	0.660
$F^4(ff)$	25599	r2	810	40934	0.625	24977	r2	790	39939	0.625
$F^6(ff)$	18480	r3	814	29779	0.621	18016	r3	794	29030	0.621
α	19.5	r4	2			19.5	r4	2		
β	−600	f				−600	f			
γ	1600	f				1600	f			
ζ_f	1557	r5	9	1661	0.938	1529	r5	9	1631	0.938
ζ_d						1145	r6	19	1369	0.836
$F^1(fd)$						509	f			
$F^2(fd)$						20390	r8	520	24906	0.819
$F^4(fd)$						14468	r9	776	13477	1.074
$G^1(fd)$						11163	r10	248	18109	0.616
$G^2(fd)$						1524	f	197		
$G^3(fd)$						13293	r11	511	12342	1.077
$G^4(fd)$						2691	f			
$G^5(fd)$						7527	r12	923	8963	0.840
$G^3(fs)$	2132		113	4561	0.467					
	$5f^26d7s^2$					**$5f^26d^27s$**				
Param. P	P_{fit}	Cstr.	Unc.	P_{HFR}	$\Delta E/SF$	P_{fit}	Cstr.	Unc.	P_{HFR}	$\Delta E/SF$
E_{av}	39115		305	11841	27274	43050		208	12973	30077
$F^2(ff)$	49005	r1	548	74289	0.660	48413	r1	542	73381	0.660
$F^4(ff)$	30284	r2	958	48424	0.625	29870	r2	945	47763	0.625
$F^6(ff)$	22025	r3	971	35490	0.621	21710	r3	957	34984	0.621
α	19.5	r4	2			19.5	r4	2		
β	−600	f				−600	f			
γ	1600	f				1600	f			
$F^2(dd)$						23302	r13	1546	37756	0.617
$F^4(dd)$						14997	r16	3057	25080	0.598
$\alpha(dd)$						10	f			
ζ_f	1908	r5	11	2036	0.937	1884	r5	11	2010	0.937
ζ_d	1889	r6	32	2259	0.931	1760	r6		2104	0.837
$F^1(fd)$	509	f				509	f			
$F^2(fd)$	25399	r8	647	31025	0.819	24437	r8	623	29850	0.819
$F^4(fd)$	18040	r9	968	16803	1.074	17283	r9	927	16099	1.074
$G^1(fd)$	11285	r10	250	18306	0.616	11030	r10	245	17892	0.616
$G^2(fd)$	1524	f				1524	f			
$G^3(fd)$	14821	r11	570	13760	1.077	14324	r11	551	13299	1.077
$G^4(fd)$	2691	f				2691	f			
$G^5(fd)$	8727	r12	1071	10389	0.840	8394	r12	1030	9996	0.840
$G^3(fs)$	1578	f		2450	0.644	1885	r6	100	4033	0.467
$G^2(ds)$						12984		597	20874	0.622

Table 5. *Cont.*

			$5f^26d^3$		
Param. P	P_{fit}	Cstr.	Unc.	P_{HFR}	$\Delta E/SF$
E_{av}	52093	401	20882	31211	
$F^2(ff)$	47830	r1	535	74289	0.660
$F^4(ff)$	29460	r2	932	44131	0.625
$F^6(ff)$	21410	r3	943	34500	0.621
α	19.5	r4	2		
β	−600	f			
γ	1600	f			
$F^2(dd)$	22416	r13	1488	36319	0.617
$F^4(dd)$	14359	r16	2926	24013	0.598
$\alpha(dd)$	10	f			
ζ_f	1860	r5	11	1986	0.937
ζ_d	1635	r6	27	1956	0.836
$F^1(fd)$	509	f			
$F^2(fd)$	25399	r8	647	31025	0.819
$F^4(fd)$	18040	r9	968	16803	1.074
$G^1(fd)$	11285	r10	250	18306	0.616
$G^2(fd)$	1524	f			
$G^3(fd)$	13799	r11	570	12811	1.077
$G^4(fd)$	2691	f			
$G^5(fd)$	8050	r12	988	9587	0.840
Configuration Interaction					
$5f^47s-5f^46d$					
$R^2(fs,fd)$	−6216	r14	357	−10574	0.588
$R^3(fs,df)$	−1875	r14	108	−3189	0.588
$5f^47s-5f^26d7s^2$					
$R^3(ff,ds)$	−2310	r14	133	−3930	0.588
$5f^47s-5f^26d^27s$					
$R^1(ff,dd)$	10962	r15	214	23117	0.474
$R^3(ff,dd)$	7708	r15	150	16225	0.474
$R^5(ff,dd)$	5672	r15	111	11961	0.474
$5f^46d-5f^26d7s^2$					
$R^3(ff,ss)$	3556	r14	204	6050	0.588
$5f^46d-5f^26d^27s$					
$R^3(ff,ds)$	−2385	r14	137	−4056	0.588
$5f^46d-5f^26d^3$					
$R^1(ff,dd)$	10762	r15	210	22694	0.474
$R^3(ff,dd)$	7466	r15	146	15745	0.474
$R^5(ff,dd)$	5465	r15	107	11525	0.474
$5f^26d7s^2-5f^26d^27s$					
$R^2(fs,fd)$	−5657	r14	324	−9621	0.588
$R^3(fs,df)$	−908	r14	52	−1545	0.588
$R^2(ds,dd)$	−14874	r14	853	−25302	0.588
$5f^26d7s^2-5f^26d^3$					
$R^2(ss,dd)$	13119	r14	752	22316	0.588
$5f^26d^27s-5f^26d^3$					
$R^2(fs,fd)$	−5558	r14	319	−9454	0.588
$R^4(fs,df)$	−938	r14	54	−1596	0.588
$R^2(ds,dd)$	−14638	r14	840	−24900	0.588

Table 6. Energy levels of U II, even parity with $5f^2$ and $5f^4$ parent configurations. Comparison of experimental energies and Landé factors with values calculated from the parameter set of Table 5. ΔE = $E^{exp} - E^{th}$. The percentage, the configuration and the *LS* name of the leading component in the corresponding configuration are given in the last three columns.

J	E^{exp} (cm^{-1})	E^{th} (cm^{-1})	ΔE (cm^{-1})	g_L^{th}	g_L^{exp}	% 1^{st} *comp*	*Conf*	*Term*
3.5	4663.803	4647	16	0.500	0.490	71	f4s	(5I)6I
4.5	5716.449	5564	152	0.830	0.830	40	f4s	(5I)6I
5.5	8347.690	8327	19	1.030	1.040	62	f4s	(5I)6I
4.5	8423.418	8423		0.797	0.790	41	f4s	(5I)4I
6.5	10740.265	10772	−31	1.142	1.145	72	f4s	(5I)6I
1.5	10987.204	10954	32	0.690	0.645	24	f4s	(5F)6F
2.5	11252.337	11138	114	1.175		22	f4s	(5F)6F
5.5	11389.469	11419	−30	0.961	0.970	59	f4s	(5I)4I
0.5		12254		−0.516		70	f4s	(5F)6F
5.5	12513.881	12493	19	0.676	0.680	61	f4s	(5I)6L
3.5	12804.950	12821	−16	0.922		12	f4s	(3G)4G2
7.5	12862.155	12880	−17	1.206	1.22	69	f4s	(5I)6I
4.5	13023.114	12905	118	1.134		11	f4s	(3G)4G2
1.5	13006.990	13044	−37	0.701		34	f4s	(5F)6F
5.5	13783.030	13733	49	0.695	0.685	56	f2d2s	(3H)6L
2.5	13758.142	13807	−49	0.931		30	f4s	(5G)6G
6.5	13865.969	13875	−9	1.068	1.10	61	f4s	(5I)4I
3.5	14018.821	13979	39	1.260		46	f4s	(5F)6F
1.5		14204		0.370		34	f4s	(5F)4F
2.5	14239.503	14439	−199	1.517		34	f4s	(5S)6S
8.5	14796.725	14742	54	1.245		61	f4s	(5I)6I
3.5	14767.466	14759	8	1.044		30	f4s	(5G)6G
2.5	14848.575	14955	−107	1.004		26	f4s	(5F)4F
2.5	15087.785	15088		0.951		23	f4s	(5G)4G
6.5	15392.416	15353	38	0.871	0.880	72	f4d	(5I)6L
3.5	15679.555	15734	−55	0.589	0.615	20	f2d2s	(3H)6Ia
3.5	15812.498	15857	−44	0.588	0.590	17	f2d2s	(5I)6I
1.5	15888.905	15870	18	1.529		42	f4s	(5S)4S
7.5	15992.765	15937	55	1.129	1.20	53	f4s	(5I)4I
6.5	15962.320	15959	3	0.903	0.900	46	f2d2s	(3H)6L
4.5	16211.704	16356	−145	0.663	0.615	53	f4d	(5I)6K
5.5	16379.878	16364	14	1.283		24	f4s	(5F)6F
4.5	16804.920	16546	259	0.759	0.845	19	f2d2s	(3H)6K
4.5	16656.412	16711	−55	1.318		52	f4s	(5F)6F
5.5	16706.303	16913	−207	0.788	0.790	36	f4s	(3K)4K2
4.5	17225.885	17216	9	0.991		14	f4s	(3H)6K
5.5	17434.363	17438	−4	0.795	0.800	20	f2ds2	(3K)4K2
6.5	17380.868	17463	−82	0.973		31	f4s	(3K)4K2
4.5	17392.211	17604	−212	0.860	0.785	16	f2d2s	(3H)6K
3.5		17683		1.115		49	f4s	(5F)4F
2.5		18060		0.680		17	f4d	(5I)4G
7.5	18136.366	18062	73	1.004	1.005	76	f4d	(5I)6L
4.5	18084.435	18154	−69	0.971		19	f4d	(5G)6G
4.5	18200.092	18334	−134	0.836	0.780	27	f2ds2	(3H)4I
3.5		18599		0.980		25	f4s	(5G)4G
4.5	18536.705	18600	−63	0.967		26	f4d	(5I)6I
2.5		18675		0.575		10	f4d	(5I)6H
5.5	18827.008	18694	133	0.908	0.945	36	f2d2s	(3H)6K
7.5	18656.355	18699	−42	1.053		21	f4s	(3L)4L
0.5		18737		2.635		39	f4s	(5D)6D
6.5	18617.807	18791	−173	0.908		42	f4s	(3L)4L
5.5	18654.316	18850	−196	0.874	0.880	70	f4d	(5I)6K
2.5		19047		0.751		12	f4s	(3G)4G2

Table 6. *Cont.*

J	E^{exp} $(\mathbf{cm^{-1}})$	E^{th} $(\mathbf{cm^{-1}})$	ΔE $(\mathbf{cm^{-1}})$	g_L^{th}	g_L^{exp}	% 1^{st} *comp*	*Conf*	*Term*
5.5	19097.594	19096	1	1.330		42	f4s	(5F)6F
2.5		19134		0.933		10	f4s	(5F)6F
1.5		19159		0.448		17	f2d2s	(3F)6Ga
3.5		19246		1.001		13	f4s	(3G)4G2
2.5	19395.168	19330	64	0.779		7	f2d2s	(3H)6Ha
2.5		19354		1.001		10	f4s	(3H)6Ha
1.5		19412		0.996		17	f4s	(5F)6F
3.5	19517.729	19546	−28	0.821	0.815	15	f4d	(5I)6I
7.5	19743.511	19756	−12	1.017	1.000	67	f2d2s	(3H)6L
1.5		19796		0.191		48	f4d	(5I)6G
2.5		19863		0.909		12	f2d2s	(3H)6Ha
5.5	19840.514	19899	−58	0.947		8	f4d	(5I)6K
6.5	19977.100	19935	41	0.969	0.960	32	f2d2s	(3H)6L
3.5	19971.328	19977	−5	0.857	0.860	11	f4d	(5I)4H
8.5	20230.479	20127	102	1.099		20	f4s	(5I)6I
5.5	20353.992	20310	43	1.029	1.015	29	f2d2s	(3H)6Ia
4.5		20365		1.208		50	f4s	(5F)4F
7.5	20425.567	20445	−20	0.975		32	f4s	(3M)4M
3.5	20571.690	20474	97	0.947	0.935	8	f4d	(3H)6Ha
0.5		20496		1.065		26	f4s	(3P)4P2
1.5		20530		1.274		20	f4s	(5D)6D
8.5	20739.844	20612	127	1.095	1.11	74	f4d	(5I)6L
2.5	20678.779	20672	6	1.066		8	f4s	(1D)2D3
4.5	20635.272	20721	−86	0.914	0.945	13	f2d2s	(3H)6Ia
6.5	20702.037	20789	−87	1.034	0.990	40	f4d	(5I)6K
1.5		20828		1.079		12	f4s	(3P)4P2
6.5	20934.186	20858	76	1.265		45	f4s	(5G)6G
3.5	20961.720	20901	60	0.877	0.855	11	f4d	(5I)6H
2.5		20917		0.750		14	f4d	(5I)6H
5.5	20742.878	20940	−197	1.012		29	f4d	(5I)6I
5.5	20932.139	21050	−118	1.173		25	f4s	(5G)6G
1.5		21053		1.534		31	f4s	(5D)6D
4.5	21154.557	21066	88	1.061	1.010	13	f4d	(5I)4H
4.5	21053.528	21089	−35	1.215		21	f4s	(3F)4F4
3.5	21207.738	21190	17	1.303	1.150	19	f4s	(5D)6D
3.5	21320.206	21514	−194	0.822	0.835	14	f4d	(3H)6Ia
5.5	21691.517	21532	159	0.961	0.975	15	f2d2s	(3H)4I
4.5	21555.275	21619	−63	0.915	1.025	9	f2d2s	(3H)4Ic
6.5	21710.768	21641	68	0.917	0.915	31	f2d2s	(3H)4Lb
3.5		21650		1.062		9	f4s	(3F)2F4
2.5		21719		0.862		15	f4d	(5F)6G
4.5		21720		1.001		26	f4s	(5G)4G
1.5		21728		0.478		12	f4s	(3F)4F3
0.5		21778		0.852		34	f4s	(5D)4D
0.5		21942		1.493		33	f4s	(3P)4P2
2.5		21953		1.186		15	f4s	(3D)2D1
3.5	21860.051	21954	−94	0.718	0.67	16	f2d2s	(3H)6Ia
3.5	22158.070	22053	104	0.910		11	f4d	(5I)6H
5.5	22157.162	22058	98	1.171		39	f4s	(5G)4G
6.5	21975.590	22058	−82	1.030	1.03	29	f4d	(5I)6K
2.5		22142		1.003		8	f4s	(3F)4F3
1.5		22153		0.300		25	f4d	(5F)6G
4.5	22165.179	22197	−32	1.007	0.895	12	f4d	(5F)6H
3.5	22250.398	22216	34	0.863	0.885	12	f2d2s	(3F)6I
4.5	22429.865	22303	126	0.874	0.935	13	f4s	(3I)4I1
5.5	22389.574	22326	62	0.992	1.040	6	f2d2s	(3H)6K

Table 6. *Cont.*

J	E^{exp} (cm^{-1})	E^{th} (cm^{-1})	ΔE (cm^{-1})	g_L^{th}	g_L^{exp}	% 1^{st} *comp*	*Conf*	*Term*
6.5	22615.319	22534	80	0.986	0.995	28	f2d2s	(3H)4K
0.5		22613		1.207		14	f2ds2	(3F)2P
5.5	22764.904	22625	139	1.030	0.980	17	f4s	(1H)2H1
4.5	22642.478	22634	8	0.936	0.875	8	f2d2s	(3I)4I1
2.5		22696		1.168		14	f2d2s	(5D)6D
3.5	22815.123	22740	74	0.786		26	f2ds2	(3F)4H
7.5		22776		1.032		40	f4d	(5I)6K
3.5	22960.667	22891	69	0.997	0.945	9	f2d2s	(3H)6Ha
4.5	22868.033	22902	−34	0.943	0.980	9	f2d2s	(5I)6H
5.5	22917.453	22942	−25	0.759	0.860	38	f2d3	(3H)6L
6.5	23107.566	22945	161	1.120	1.060	29	f2d2s	(3H)6Ia
2.5	23029.458	23039	−9	0.988		17	f4d	(5I)6G
9.5		23076		1.160		71	f4d	(5I)6L
1.5		23104		1.446		15	f2d2s	(3H)6D
5.5	23241.365	23121	119	0.968	0.96	17	ds2	(3H)4I *
2.5		23148		1.070		13	f2d2s	(5D)6D
4.5	23241.033	23168	72	0.959	1.050	6	f2d2s	(5I)6I
3.5	23257.613	23205	52	0.597		21	f4d	(5G)6I
6.5	23234.820	23223	11	1.024	1.090	29	f4d	(5I)6I
2.5	23353.601	23264	89	0.779		20	f2d2s	(3H)6Ha
7.5	23262.359	23350	−87	1.102	1.070	24	f2d2s	(3H)6K
3.5		23412		0.960		13	f4d	(5I)6G
0.5		23428		2.116		14	f2d2s	(3H)6D
8.5		23441		1.107		73	f2d2s	(3H)6L
6.5		23492		1.202		24	f4s	(3H)4H3
4.5		23501		1.073		12	f4s	(3G)4G2
5.5		23628		1.033		11	f4d	(5I)4H
3.5		23644		0.849		11	f2d2s	(3H)6Ib
1.5	23673.649	23648	25	1.276		25	f4d	(5D)4D
6.5	23635.919	23712	−77	0.986	0.920	18	f2d2s	(3H)4Lb
2.5	23700.946	23739	−38	0.868		17	f2d2s	(3F)6H
5.5		23792		0.923		22	f2ds2	(3H)4I
4.5	23817.508	23802	15	0.958	0.870	11	f2d2s	(3H)6K
0.5		23827		1.989		9	f4d	(5S)6D
2.5	23905.877	23828	77	1.085		9	f4d	(3F)6H
3.5	23803.252	23831	−27	0.991		7	f4d	(3F)4G
7.5	24071.418	23927	143	1.023		41	f4s	(3L)4L
1.5		23943		0.969		7	f2d2s	(3H)6Ga
4.5		23962		0.947		8	f2d2s	(3H)6K
3.5	23895.471	24064	−169	0.969	0.735	10	f4s	(3G)2G2
6.5	24159.696	24072	86	0.922	0.965	31	f4s	(3L)4L
8.5		24074		1.069		42	f4s	(3L)4L
5.5	24010.467	24077	−66	0.934	0.975	18	f4d	(5I)4K
7.5	24247.529	24122	124	1.113		22	f4d	(5I)6I
4.5	24220.675	24158	62	1.094		7	f4d	(5F)6G
5.5		24168		0.989		7	f2d2s	(3H)2H3
2.5		24213		1.052		11	f4d	(5F)6F
3.5	24209.303	24243	−34	1.086		12	f2d2s	(3F)6Ga
1.5		24292		0.768		17	f2d2s	(5F)6F
2.5		24299		1.004		17	f4d	(5F)6G
6.5		24375		1.024		9	f4d	(5I)4K
7.5	24423.656	24381	42	0.995		38	f4d	(3L)2L
5.5		24432		1.037		12	f4s	(5G)4G
4.5		24440		1.016		12	f2d2s	(3F)6I
3.5		24491		1.262		17	f4s	(5D)6D
1.5		24501		0.628		15	f2d2s	(3H)6Ga
4.5		24593		1.023		13	f4d	(3H)6K

Table 6. *Cont.*

J	E^{exp} (cm^{-1})	E^{th} (cm^{-1})	ΔE (cm^{-1})	g_L^{th}	g_L^{exp}	% 1st comp	Conf	Term
0.5		24650		0.273		29	f2d2s	(3F)6Fa
7.5		24675		0.974		17	f4d	(3K)4M2
8.5		24686		1.084		30	f4d	(5I)6K
0.5		24712		−0.082		43	f4d	(5F)6F
3.5	24709.449	24720	−10	0.943		16	f2d2s	(3H)6Ib
5.5		24722		1.007		11	f4d	(5I)6H
1.5		24746		1.386		15	f4d	(5F)6D
4.5	24684.135	24802	−117	0.981	0.935	7	f2d2s	(3H)6K
2.5		24840		0.805		12	f2d2s	(3F)4G
9.5		24845		1.114		46	f4s	(3L)4L
5.5	24857.570	24893	−35	1.068		7	f2d2s	(3H)4Ga
4.5		24928		0.975		11	f2d2s	(3H)6K
3.5	24862.698	24946	−83	0.993		10	f2d2s	(3H)6Ib
6.5		24977		1.111		18	f4s	(3I)4I1
4.5		24981		1.159		16	f4s	(3F)4F2
2.5		24984		0.830		8	f2d2s	(3H)4Gc
8.5	25053.005	25075	−22	1.063		43	f4s	(3M)4M
3.5		25132		1.140		9	f4d	(3F)4F3
2.5		25247		0.917		7	f4s	(3F)2F3
6.5		25248		1.000		14	f2d2s	(3H)6L
3.5		25294		1.056		8	f4d	(5I)6G
5.5	25356.972	25334	22	0.997	1.020	9	f4d	(3H)4Kb
4.5		25343		1.003		9	f2d2s	(3H)4H
3.5		25346		1.020		10	f4d	(3H)6Ha
4.5		25424		0.904		23	f2d2s	(3H)6Ib
1.5		25434		0.868		7	f4d	(5F)6F
8.5		25458		1.157		22	f4d	(5I)6I
0.5		25477		1.513		12	f4d	(5G)4D
7.5	25399.465	25518	−119	0.986		32	f4s	(3M)4M
3.5		25532		0.989		9	f4s	(3F)2F2
4.5		25537		0.950		7	f2d2s	(3H)4I
1.5	25582.631	25561	21	1.305		14	f4d	(5S)6D
2.5		25564		0.793		9	f4d	(5G)6H
8.5		25575		1.040		44	f4s	(3M)2M
2.5		25628		0.942		7	f2d2s	(3H)6Ga
5.5	25626.941	25635	−8	1.038		8	f4s	(5I)6H
3.5		25637		1.038		8	f2d2s	(5F)6F
10.5		25657		1.215		72	f4d	(5I)6L
1.5		25669		0.638		15	f2d2s	(3H)4F
6.5		25714		1.088		14	f4d	(3H)6L
7.5	25667.906	25733	−65	1.164	1.100	29	f4s	(3I)4I1
5.5		25746		0.978		20	f2d2s	(3H)4Kb
2.5		25748		1.061		6	f2d2s	(3F)6Ga
3.5		25784		1.051		13	f2d2s	(3H)6Ga
7.5		25784		1.078		15	f2d2s	(3H)6L
2.5		25875		1.115		9	f4d	(5F)6F
6.5		25892		0.998		20	f2d2s	(3H)6L
5.5		25894		1.083		22	f2d2s	(3H)6Ha
1.5		25981		0.913		21	f2d2s	(3F)6Fa
0.5		26012		1.555		14	f4d	(5S)6D
4.5		26038		1.116		7	f2d2s	(5F)6G
6.5		26058		1.176		12	f4d	(5I)6G
2.5		26094		1.261		16	f4s	(3P)4P2
0.5		26143		0.461		29	f4s	(3D)4D1
5.5	26158.897	26164	−5	1.010		18	f2d2s	(3F)6I
1.5		26166		1.167		18	f4s	(3P)4P2
3.5		26246		0.996		7	f2d2s	(3H)4Hb

Table 6. *Cont.*

J	E^{exp} (cm^{-1})	E^{th} (cm^{-1})	ΔE (cm^{-1})	g_L^{th}	g_L^{exp}	% 1^{st} *comp*	*Conf*	*Term*
5.5		26321		1.134		8	f4d	(3G)4G2
4.5		26343		1.008		9	f2d2s	(3H)6Ib
2.5		26364		1.209		16	f4s	(5D)4D
6.5		26375		1.035		18	f4s	(3I)2I1
8.5		26386		1.162		13	f2d2s	(3H)4Ka
1.5		26397		1.140		12	f4s	(3P)2P2
3.5		26446		1.063		4	f4d	(3H)4H2
4.5		26457		1.042		7	f4d	(5F)6G
2.5		26470		0.912		5	f4s	(3H)6D
7.5	26527.106	26493	33	1.095	1.075	17	f4d	(3H)4Lb
1.5		26521		1.308		10	f4d	(5F)6P
5.5		26544		1.093		9	f2d2s	(3H)4Kb
4.5		26569		1.066		7	f4d	(5D)6D
3.5		26623		1.160		6	f4d	(5S)6D
5.5	26628.496	26633	−5	1.065	1.155	19	f4d	(3H)6K
9.5		26641		1.176		41	f4d	(5I)6K
0.5		26642		0.493		8	f2d2s	(5G)6F
8.5		26703		1.050		30	f4d	(5I)6K
4.5		26717		1.094		7	f4s	(1G)2G4
0.5		26793		0.457		14	f4d	(5F)4D
2.5		26801		1.049		18	f2d2s	(3F)6Fa
3.5		26811		0.980		7	f2.d	(3H)4Hh
6.5		26842		1.015		12	f4d	(3H)4I
4.5		26856		1.076		6	f2d2s	(3G)2G2
5.5	26989.437	26863	125	1.103	1.095	13	f4d	(3H)6K
7.5		26868		1.061		34	f4s	(3H)6K
5.5		26903		1.059		12	f4d	(3H)6K
1.5		26918		0.766		6	f2d2s	(5F)6G
3.5		26919		1.111		14	f4s	(3F)4F4
7.5	26931.699	26961	−29	1.058		18	f4d	(5I)4L
2.5		26966		1.098		4	f2d2s	(3H)6D
3.5		26974		1.143		5	f4d	(5D)4D
4.5		26984		1.056		9	f4d	(5F)6F
5.5		27019		1.135		9	f4d	(5I)6G
6.5		27037		0.995		14	f2d2s	(3H)4Ka
1.5		27069		0.490		17	f2d2s	(3F)6Gb
2.5		27161		1.031		5	f4d	(5F)6G
6.5		27170		1.006		6	f4d	(3H)4Ka
4.5		27177		1.117		9	f4d	(5S)6D
3.5		27192		0.990		5	f4d	(5D)4D
4.5		27287		1.014		13	f2d2s	(3F)6H
5.5		27295		1.094		6	f4d	(5I)6G
3.5		27356		1.029		5	f2d2s	(3H)4H2
1.5		27358		1.067		9	f2d2s	(3H)6F
3.5		27382		1.005		4	f2d2s	(3F)6H
2.5		27385		0.982		7	f4d	(5S)6D
4.5		27390		1.060		5	f2d2s	(3G)2G2
2.5		27434		0.998		9	f4d	(3F)2F4
6.5		27439		1.033		17	f2d2s	(3H)4I
4.5		27484		1.089		9	f2d2s	(3F)4H

Table 6. *Cont.*

J	E^{exp} (cm^{-1})	E^{th} (cm^{-1})	ΔE (cm^{-1})	g_L^{th}	g_L^{exp}	% 1st comp	Conf	Term
6.5		27508		1.098		9	f2d2s	(3H)6Ia
1.5		27520		0.933		6	f4d	(3F)6P
9.5		27553		1.178		89	f2d2s	(3H)6L
0.5		27574		1.729		17	f2d2s	(3F)4P
7.5		27597		1.181		15	f4d	(5I)6H
5.5		27618		1.033		9	f2d2s	(3H)6Ib
3.5		27629		1.046		6	f4d	(5F)6D
4.5		27659		0.944		9	f2d2s	(3H)6Ib
2.5		27661		0.922		7	f2d2s	(3H)6Hb
3.5		27737		0.930		9	f2d2s	(3H)4Hb
7.5	27695.597	27788	−92	1.073	1.090	9	f4d	(3H)4Lb

*: The level at 23241.365 cm^{-1} has a leading component belonging to the $5f^26d7s^2$ configuration but the dominant configuration is $5f^26d^27s$.

Table 7. Adopted parameters (in cm^{-1}) for even parity configurations $5f^37s7p$ and $5f^36d7p$ of U II compared with HFR radial integrals. The scaling factors are $SF(P) = P_{fit}/P_{HFR}$. Constraints on some parameters (denoted 'rn' in the 'Unc' columns of standard errors) link parameters of the same 'rn' to vary in a constant ratio. The HFR values of E_{av} parameters are relative to the lowest even configuration $5f^47s$ taken as zero value.

	$5f^37s7p$					$5f^36d7p$				
Param. P	P_{fit}	**Cstr.**	**Unc.**	P_{HFR}	$\Delta E/SF$	P_{fit}	**Cstr.**	**Unc.**	P_{HFR}	$\Delta E/SF$
E_{av}	54614		598	10338	44276	61291		312	17718	43573
$F^2(ff)$	48327	f		70448	0.686	47577	f		69355	0.686
$F^4(ff)$	45655	f		45655	0.691	31003	f		44867	0.691
$F^6(ff)$	22523	f		33367	0.675	22117	f		32766	0.675
α	36.5	f				36.5	f			
β	−600	f				−600	f			
γ	1500	f				1500	f			
ζ_f	1809	r1	102	1875	0.965	1781	r1	100	1846	0.965
ζ_d						1624	f		1902	0.854
ζ_p	5118	f		4490	1.14	4232	f		3713	1.14
$F^2(fp)$	7201	f		9001	0.80	6461	f		8077	0.80
$F^2(fd)$						20160	f		29007	0.695
$F^4(fd)$						15386	f		15765	0.976
$F^2(dp)$						13971	f		17464	0.80
$G^1(fd)$						11676	f		18742	0.623
$G^3(fd)$						12558	f		13562	0.926
$G^5(fd)$						8692	f		10084	0.862
$G^2(fp)$	2205	f		2205		1552	f		1939	0.8
$G^4(fp)$	1978	f		1978		1382	f		1727	0.8
$G^3(fs)$	2618	f		4328	0.605					
$G^1(dp)$						6543	f		10904	0.6
$G^3(dp)$						4812	f		8019	0.6
$G^1(sp)$	23515	f		26415	0.89					
Configuration Interaction										
$5f^37s7p - 5f^36d7p$										
$R^2(fs,fd)$	−6710	f	−10167	0.66						
$R^3(fs,df)$	−1442	f	−2185	0.66						
$R^2(sp,dp)$	−11708	f	−17742	0.66						
$R^1(sp,pd)$	−10971	f	−16622	0.66						

Table 8. Energy levels for even parity configurations $5f^37s7p$ and $5f^36d7p$ of U II. $\Delta E = E^{exp} - E^{th}$. The percentage, the configuration and the *LS* name of the leading component in the corresponding configuration are given in the last three columns.

J	E^{exp} (cm^{-1})	E^{th} (cm^{-1})	ΔE (cm^{-1})	g_L^{th}	g_L^{exp}	% 1^{st} *comp*	*Conf*	*Term*
4.5	23315.092	22981	333	0.649	0.875	56	$5f^37s7p$	(4I)6I
5.5	24608.168	24608		0.874	0.910	30	$5f^37s7p$	(4I)6I
3.5	24342.199	24688	−345	0.577	0.760	53	$5f^37s7p$	(4I)6I
4.5	25437.162	25193	243	0.887	0.930	15	$5f^37s7p$	(4I)6I
6.5	26191.312	25937	253	0.753	0.890	49	$5f^36d7p$	(4I)6M
5.5		26810		0.733		33	$5f^36d7p$	(4I)6La
5.5		27873		0.834		25	$5f^37s7p$	(4I)6K
4.5		28301		0.729		30	$5f^36d7p$	(4I)4If
5.5	28154.447	28532	−378	0.862	0.890	18	$5f^37s7p$	(4I)6Lb
6.5		28989		1.033		48	$5f^37s7p$	(4I)6K
5.5		29614		0.970		18	$5f^37s7p$	(4I)6K
4.5		29689		0.865		42	$5f^37s7p$	(4I)6I
2.5		30187		0.362		65	$5f^37s7p$	(4I)6H
3.5		30321		0.723		31	$5f^37s7p$	(4I)6H
1.5		30387		0.375		46	$5f^37s7p$	(4F)6G
7.5	30341.673	30527	−185	0.910	1.010	59	$5f^36d7p$	(4I)6M
4.5		30725		0.874		19	$5f^37s7p$	(4I)6H
2.5		31004		0.787		8	$5f^36d7p$	(4I)4Ga
6.5		31106		0.919		36	$5f^36d7p$	(4I)6La
5.5		31210		0.965		15	$5f^37s7p$	(4I)4Ka
3.5		31231		0.705		14	$5f^36d7p$	(4I)6Ia
6.5		31719		1.005		21	$5f^37s7p$	(4I)6I
0.5		31781		0.118		28	$5f^37s7p$	(4F)6F
1.5		32017		1.030		12	$5f^37s7p$	(4F)6F
2.5		32113		0.862		34	$5f^37s7p$	(4F)6G
6.5	32535.021	32250	283	0.940	0.990	29	$5f^36d7p$	(4I)6Lb
5.5		32326		0.930		35	$5f^36d7p$	(4I)6Kb
6.5		32464		1.093		21	$5f^37s7p$	(4I)6H
4.5		32642		0.693		40	$5f^36d7p$	(4I)6Ka
6.5		32856		0.840		27	$5f^36d7p$	(4I)4Ld
7.5		32894		1.139		47	$5f^37s7p$	(4I)6K
3.5		33045		0.673		31	$5f^36d7p$	(4I)4Hf
5.5		33215		0.799		25	$5f^36d7p$	(4I)6Lb
4.5		33289		0.888		11	$5f^37s7p$	(2H)4I2
0.5		33509		0.499		12	$5f^36d7p$	(4F)6F
4.5		33651		0.809		21	$5f^36d7p$	(4I)6Kb
6.5		33806		1.036		21	$5f^37s7p$	(4I)4Ka
2.5		33859		1.057		10	$5f^37s7p$	(4F)6G
5.5		33985		1.026		22	$5f^37s7p$	(4I)4Ia
5.5	34207.000	34347		0.837		15	$5f^36d7p$	(4I)6La
3.5		34351		0.951		22	$5f^37s7p$	(4F)6G
6.5		34409		0.936		11	$5f^36d7p$	(4I)4Lc
5.5		34427		1.048		12	$5f^37s7p$	(4I)6I
2.5		34433		0.540		26	$5f^37s7p$	(4G)6H
1.5		34435		0.866		14	$5f^37s7p$	(4G)6G
3.5		34466		0.698		25	$5f^36d7p$	(4I)6I
4.5		34496		0.920		11	$5f^36d7p$	(4I)6Ia
7.5		34524		0.959		17	$5f^36d7p$	(4I)4Mb
4.5		34560		0.990		14	$5f^37s7p$	(4I)6H
3.5		34761		0.935		17	$5f^37s7p$	(4F)6G
1.5		34812		1.605		42	$5f^37s7p$	(4S)6P
8.5	34632.367	34911	−279	1.024	1.085	60	$5f^36d7p$	(4I)6M

Table 8. *Cont.*

J	E^{exp} (cm^{-1})	E^{th} (cm^{-1})	ΔE (cm^{-1})	g_L^{th}	g_L^{exp}	% 1st comp	Conf	Term
2.5		35093		0.837		17	$5f^37s7p$	(4F)4Ga
3.5		35149		0.908		9	$5f^37s7p$	(4I)6H
7.5		35301		1.085		17	$5f^36d7p$	(4I)6I
4.5		35338		0.895		10	$5f^36d7p$	(4I)6K
2.5		35498		1.074		17	$5f^37s7p$	(4F)6F
6.5		35514		0.990		31	$5f^36d7p$	(4I)6Kb
7.5		35529		1.051		27	$5f^36d7p$	(4I)6La
3.5		35552		0.873		12	$5f^36d7p$	(4I)6H
3.5		35666		0.834		6	$5f^36d7p$	(4I)6H
4.5		35696		0.811		13	$5f^36d7p$	(4I)6H
5.5		35744		0.966		19	$5f^37s7p$	(4I)2I
4.5		35780		0.867		11	$5f^36d7p$	(4I)4Ia
5.5		35804		0.901		14	$5f^36d7p$	(4I)4Ke
6.5		35809		1.064		30	$5f^37s7p$	(4I)2K
7.5		35892		1.196		34	$5f^37s7p$	(4I)6H
3.5		35906		1.009		9	$5f^36d7p$	(4F)6G
5.5		35985		0.961		13	$5f^36d7p$	(4I)6Ka
1.5		36046		0.867		14	$5f^37s7p$	(4F)6F
3.5		36064		1.089		10	$5f^37s7p$	(4F)6D
4.5		36137		0.865		10	$5f^36d7p$	(4I)6Ib
2.5		36149		1.444		33	$5f^37s7p$	(4S)6P
8.5		36364		1.210		31	$5f^37s7p$	(4I)6I
7.5		36389		1.059		29	$5f^36d7p$	(4I)6Lb
6.5		36410		1.019		14	$5f^36d7p$	(4I)6I
2.5		36417		0.607		17	$5f^36d7p$	(4F)6Ha
1.5		36462		1.200		14	$5f^37s7p$	(4S)2P
5.5		36516		0.934		39	$5f^36d7p$	(4I)6Ka
0.5		36680		1.812		15	$5f^36d7p$	(4S)4Pa
3.5		36721		0.935		9	$5f^37s7p$	(4F)6I
4.5		36849		0.904		18	$5f^36d7p$	(4I)4Hf
2.5		36946		1.020		5	$5f^36d7p$	(4F)4Fa
4.5		37004		1.163		34	$5f^37s7p$	(4F)6G
3.5		37008		0.949		10	$5f^36d7p$	(4I)6Ia
1.5		37053		0.995		12	$5f^36d7p$	(4I)6Ga
0.5		37112		2.063		27	$5f^37s7p$	(4F)6D
2.5		37313		0.864		6	$5f^36d7p$	(4I)6Ga
3.5		37369		0.935		16	$5f^37s7p$	(4G)6H
2.5		37477		0.897		13	$5f^36d7p$	(4G)6H
1.5		37537		0.695		14	$5f^36d7p$	(4F)4Ff
7.5		37620		1.065		13	$5f^37s7p$	(4I)4Ka
6.5		37789		1.127		26	$5f^37s7p$	(4I)4Ha
3.5		37822		0.986		8	$5f^37s7p$	(4F)4Ga
1.5		37855		1.172		15	$5f^36d7p$	(4F)6F
5.5		37879		0.929		11	$5f^36d7p$	(4I)6Kb
7.5		37917		0.996		18	$5f^36d7p$	(4I)4Mb
2.5		37960		0.861		9	$5f^36d7p$	(4G)6H
8.5	37308.326	37991	−683	1.062	1.070	18	$5f^36d7p$	(4I)6M
4.5		38040		0.895		18	$5f^36d7p$	(4I)6I
3.5		38063		0.821		10	$5f^36d7p$	(4F)6I
1.5		38080		0.578		23	$5f^36d7p$	(4G)6G
6.5		38156		0.931		15	$5f^36d7p$	(4I)4Ld
5.5		38183		0.896		13	$5f^36d7p$	(4I)6K
4.5		38205		0.863		12	$5f^36d7p$	(4I)6I
2.5		38217		0.816		9	$5f^36d7p$	(4I)6Hb
0.5		38228		2.117		26	$5f^37s7p$	(4F)6D

Table 8. *Cont.*

J	E^{exp} (cm^{-1})	E^{th} (cm^{-1})	ΔE (cm^{-1})	g_L^{th}	g_L^{exp}	% 1^{st} *comp*	*Conf*	*Term*
3.5		38436		0.941		9	$5f^36d7p$	(4F)4Hd
2.5		38452		0.879		17	$5f^37s7p$	(4G)2F
7.5		38497		1.029		25	$5f^36d7p$	(4I)4Lc
2.5		38554		0.760		11	$5f^36d7p$	(4I)6Gb
4.5		38630		1.028		10	$5f^36d7p$	(4G)6H
6.5		38721		0.974		15	$5f^36d7p$	(4I)6Kb
1.5		38794		1.134		8	$5f^36d7p$	(4F)6D
5.5		38809		0.916		22	$5f^36d7p$	(4I)6K
8.5		38835		1.187		29	$5f^37s7p$	(4I)6K
2.5		38916		1.074		12	$5f^36d7p$	(4F)6F
4.5		38931		1.064		7	$5f^36d7p$	(4I)6I
4.5		38975		0.830		20	$5f^36d7p$	(4G)6K
3.5		38993		0.936		8	$5f^37s7p$	(4I)4Ha
2.5		39000		0.891		14	$5f^37s7p$	(4G)6G
1.5		39006		0.407		30	$5f^36d7p$	(4I)6Gb
9.5	39809.365	39050	758	1.111	1.105	48	$5f^36d7p$	(4I)6M
5.5		39065		1.092		5	$5f^36d7p$	(4I)6Kb
6.5		39122		1.038		14	$5f^36d7p$	(4I)6Ka
4.5		39161		1.136		14	$5f^36d7p$	(4F)6D

3.3. Partition Function

To get an idea of how semi-empirical parametric calculations could influence the value of the partition function $Q(T) = \sum_i (2J_i + 1)exp(-E_i/k_BT)$ (k_B : Boltzmann constant), we made an estimation of the partition function of U II for a typical stellar temperature. The temperature chosen is 4825 K ($k_BT = 3353.54$ cm^{-1}), which is the temperature quoted by Cayrel et al. [1] for a metal-poor star showing the U II line at 3859.57 Å in its spectrum.

Since experimental levels are incompletely determined, a partition function calculated with only known experimental energies would be underestimated. Therefore we calculated the partition function with all the available experimental energies supplemented by the final least squares fitted energies when experimental ones are missing. In the expression of the partition function we included all the levels below 46 000 cm^{-1} of both parities. The result is : $Q_{exp/LSF}(T)$ = 122.99, which is the best value possible in the present case. When the partition function is calculated with the same number of levels, but with all the fitted energies, the result is: Q_{LSF}(T) = 120.99, which agrees with $Q_{exp/LSF}(T)$ within 2%. When *ab initio* HFR energy values are used, we have Q_{HFR}(T) = 89.19, which is 26% smaller. Consequently, in absence of complete experimental level energies, the energies calculated from fitted parameters provide a realistic estimation of the partition function.

3.4. Transition Probabilities

The parametric calculations provide gA values for transition probabilities (g: upper level statistical weight; A: Einstein coefficient of spontaneous emission) between calculated levels. Extensive comparison with experimental transition probabilities is not possible because of the scarcity of measurements. Furthermore, because of the strongly mixed wave functions, weak transitions are sensitive to small changes of energy parameters and may not be reliable for comparison. Nevertheless, it is interesting to consider the line at 3859.6 Å, which is strong and used as cosmochronometer [1]. Chen and Borzileri [21] measured the gA value for this line and found 2.8×10^8 s^{-1}, to be compared with previous measurement 1.1×10^8 s^{-1} by Corliss [22]. Nilsson et al. [23] derived branching ratios from relative intensities measured in FTS spectra and combined with radiative lifetime of the upper level at 26191 cm^{-1} to find a g_lf value of 0.856 for the oscillator strength weighted by the lower level degeneracy. The corresponding gA value (Equation (1) of [23]) is 3.8×10^8 s^{-1} in agreement with the value of 3.5 × 10^8 s^{-1} calculated by Kurucz [24]. Our calculations lead to gA = 1.53 × 10^9 s^{-1}, four times larger, but they confirm the order of magnitude. However, the parametric study for the high even levels of $5f^37s7p + 5f^36d7p$ is still unachieved, since treated without all the interacting even configurations. Its results should be taken with caution.

4. Classified Lines of U II in the Ultraviolet

On our spectrograms described in Section 2, some lines were relatively sharp and were likely emitted by singly charged uranium ions. For identification of U II lines, we searched experimental wave numbers matching the Ritz wave numbers calculated from the energy differences of known U II energy levels reported in [6], even when the level was not assigned with quantum numbers. The maximum uncertainty of the wavelength measurements is estimated to be ±0.003 Å . Thus the corresponding uncertainty on wave numbers should be less than ±0.05 cm^{-1}. To take into account any possible perturbations in the spark spectrum, we chose a tolerance of ±0.1 cm^{-1} for a criterion of identification. Indeed, according to [14], the level energies in [6], therefore the Ritz wave numbers, have negligible uncertainties of about ±0.01 cm^{-1}. Table 9 lists the 451 lines between 2344 and 2955 Å identified as U II transitions, with calculated Ritz wavelengths, experimental wavelengths, deviations exp-Ritz and line intensities, together with the corresponding upper and lower levels. One line has triple identification and 24 lines have double identification. These concern mostly lines with two deviations of opposite signs. Otherwise, the line with the smallest deviation is retained. No gA values were available here for confirmation of identifications since the even levels involved in these transitions have only experimental energy values but no quantum numbers assigned except the J values.

Search of new levels of $5f^36d7p$ close to the predicted energies of Table 8 was attempted using the possible U II lines left unidentified. Unfortunately, only one chain of transitions supported by calculated transition probabilities could be found leading to a level $5f^36d7p$ $(^4I)^6K$ with $J = 5.5$ at 39113.98 ± 0.1 cm^{-1}. Table 10 lists the six transitions that establish this level.

Table 9. Ultraviolet transitions of U II emitted from a vacuum spark source. wl_{Ritz} : Ritz wavelength calculated with experimental energies from [6]; wl_{exp}: experimental wavelength ; $\Delta wl = wl_{exp} - wl_{Ritz}$; wn_{exp}: experimental wavenumbers; $\Delta wn = wn_{exp} - (E_{even} - E_{odd})$.

wl_{Ritz} in Air (Å)	wl_{exp} in Air (Å)	*Int*	*Note*	wn_{exp} (cm^{-1})	Δwl (Å)	Δwn (cm^{-1})	E_{odd} (cm^{-1})	J_{odd}	E_{even} (cm^{-1})	J_{even}
2343.5696	2343.5707	49		42656.867	0.0012	−0.021	0.000	4.5	42656.888	5.5
2348.8952	2348.8968	73		42560.149	0.0016	−0.029	289.041	5.5	42849.219	5.5
2390.9748	2390.9742	10		41811.216	−0.0006	0.011	0.000	4.5	41811.205	5.5
2401.1302	2401.1330	125		41634.329	0.0029	−0.050	289.041	5.5	41923.420	6.5
2423.7052	2423.7102	52		41246.529	0.0051	−0.086	0.000	4.5	41246.615	4.5
2427.0021	2427.0022	43		41190.593	0.0001	−0.001	914.765	4.5	42105.359	5.5
2448.0954	2448.0942	97		40835.731	−0.0012	0.020	289.041	5.5	41124.752	6.5
2448.9324	2448.9265	7		40821.854	−0.0059	0.099	0.000	4.5	40821.755	4.5
2471.0901	2471.0868	55		40455.794	−0.0033	0.054	2294.696	5.5	42750.436	6.5
2477.1835	2477.1824	30		40356.253	−0.0010	0.017	1749.123	6.5	42105.359	5.5
2478.6816	2478.6852	37	as	40331.791	0.0036	−0.059	914.765	4.5	41246.615	4.5
2481.1377	2481.1412	24		40291.868	0.0034	−0.056	289.041	5.5	40580.965	5.5
2484.0042	2484.0095	16		40245.347	0.0054	−0.087	0.000	4.5	40245.434	3.5
2484.6702	2484.6667	41		40234.703	−0.0035	0.057	0.000	4.5	40234.646	5.5
2490.2907	2490.2899	9		40143.856	−0.0009	0.014	914.765	4.5	41058.607	5.5
2491.4292	2491.4330	8		40125.442	0.0037	−0.060	1749.123	6.5	41874.625	6.5
2506.8037	2506.8012	25		39879.462	−0.0025	0.039	914.765	4.5	40794.188	4.5
2512.5746	2512.5784	13		39787.777	0.0038	−0.060	0.000	4.5	39787.837	5.5
2514.7696	2514.7686	19	LA	39753.125	−0.0010	0.016	4420.871	5.5	44173.980	6.5
2518.9755	2518.9760	37		39686.730	0.0005	−0.008	0.000	4.5	39686.738	5.5
2533.2401	2533.2370	42		39463.326	−0.0031	0.049	0.000	4.5	39463.277	5.5
2537.6966	2537.6954	163		39393.998	−0.0012	0.018	289.041	5.5	39683.021	5.5
2538.4329	2538.4355	85		39382.517	0.0026	−0.041	0.000	4.5	39382.558	3.5
2538.7351	2538.7384	33		39377.819	0.0033	−0.051	289.041	5.5	39666.911	4.5
2539.1756	2539.1760	96	as	39371.032	0.0004	−0.006	289.041	5.5	39660.079	6.5
2540.7030	2540.7065	39	c	39347.316	0.0034	−0.053	1749.123	6.5	41096.492	6.5
2541.3669	2541.3655	39	c	39337.112	−0.0014	0.022	0.000	4.5	39337.090	4.5
2554.3761	2554.3725	134	as	39136.819	−0.0035	0.054	1749.123	6.5	40885.888	6.5

Table 9. *Cont.*

wl_{Ritz} in Air (Å)	wl_{exp} in Air (Å)	*Int*	*Note*	wn_{exp} (cm^{-1})	Δwl (Å)	Δwn (cm^{-1})	E_{odd} (cm^{-1})	J_{odd}	E_{even} (cm^{-1})	J_{even}
2556.1928	2556.1946	82	LA	39108.922	0.0018	−0.028	0.000	4.5	39108.950	5.5
2560.1798	2560.1743	20		39048.133	−0.0055	0.084	289.041	5.5	39337.090	4.5
2560.3421	2560.3457	29		39045.519	0.0037	−0.056	0.000	4.5	39045.575	4.5
2561.7992	2561.7934	46		39023.455	−0.0058	0.089	914.765	4.5	39938.131	5.5
2565.4072	2565.4130	104	LA	38968.400	0.0058	−0.088	0.000	4.5	38968.488	5.5
2567.2954	2567.2987	174	as	38939.778	0.0032	−0.049	2294.696	5.5	41234.523	6.5
2567.9515	2567.9578	11		38929.783	0.0063	−0.095	0.000	4.5	38929.878	4.5
2568.9777	2568.9783	26	LA,as	38914.318	0.0006	−0.009	5259.653	7.5	44173.980	6.5
2569.7085	2569.7095	45	LA	38903.246	0.0010	−0.015	0.000	4.5	38903.261	3.5
2575.2266	2575.2291	23	LA	38819.872	0.0025	−0.037	289.041	5.5	39108.950	5.5
2577.3205	2577.3219	20		38788.354	0.0015	−0.022	0.000	4.5	38788.376	4.5
2578.7860	2578.7797	155		38766.427	−0.0063	0.095	1749.123	6.5	40515.455	5.5
2579.5692	2579.5681	29		38754.579	−0.0011	0.017	0.000	4.5	38754.562	4.5
2584.4158	2584.4163	42	LA	38681.882	0.0005	−0.008	0.000	4.5	38681.890	3.5
2584.9012	2584.9028	10	c	38674.602	0.0016	−0.024	0.000	4.5	38674.626	4.5
2586.1972	2586.1965	44		38655.256	−0.0007	0.010	4420.871	5.5	43076.117	4.5
2591.2483	2591.2450	107	as	38579.949	−0.0034	0.050	0.000	4.5	38579.899	4.5
2592.5704	2592.5690	60		38560.247	−0.0014	0.021	0.000	4.5	38560.226	3.5
2593.5699	2593.5698	30		38545.372	−0.0001	0.002	0.000	4.5	38545.370	5.5
2601.4681	2601.4695	72		38428.328	0.0014	−0.020	4420.871	5.5	42849.219	5.5
2604.2985	2604.2993	48	p	38386.572	0.0008	−0.012	0.000	4.5	38386.584	3.5
2606.7253	2606.7266	63		38350.837	0.0013	−0.019	0.000	4.5	38350.856	4.5
2607.3014	2607.3069	65		38342.302	0.0055	−0.081	289.041	5.5	38631.424	5.5
2608.1733	2608.1800	28	p	38329.466	0.0067	−0.099	4420.871	5.5	42750.436	6.5
2609.2426	2609.2457	23		38313.811	0.0031	−0.046	0.000	4.5	38313.857	5.5
2609.8933	2609.8900	253		38304.353	−0.0033	0.049	914.765	4.5	39219.069	5.5
2612.4565	2612.4555	11		38266.741	−0.0010	0.015	0.000	4.5	38266.726	4.5
2613.9584	2613.9578	11		38244.748	−0.0005	0.008	0.000	4.5	38244.740	3.5
2615.9468	2615.9422	24		38215.737	−0.0046	0.067	0.000	4.5	38215.670	4.5
2616.0690	2616.0679	35		38213.901	−0.0012	0.017	0.000	4.5	38213.884	5.5
2620.8611	2620.8670	19		38143.931	0.0059	−0.086	914.765	4.5	39058.782	5.5
2621.4511	2621.4463	21		38135.502	−0.0048	0.070	1749.123	6.5	39884.555	6.5
2623.5499	2623.5514	17		38104.907	0.0015	−0.022	4420.871	5.5	42525.800	5.5
2624.9155	2624.9101	24		38085.183	−0.0054	0.078	4420.871	5.5	42505.976	6.5
2625.2536	2625.2508	21		38080.241	−0.0028	0.041	0.000	4.5	38080.200	5.5
2628.9275	2628.9276	41		38026.982	0.0001	−0.002	0.000	4.5	38026.984	4.5
2632.6555	2632.6570	32		37973.118	0.0015	−0.021	0.000	4.5	37973.139	5.5
2632.9771	2632.9786	42		37968.480	0.0015	−0.021	0.000	4.5	37968.501	4.5
2634.3223	2634.3286	35		37949.022	0.0063	−0.091	2294.696	5.5	40243.809	6.5
2635.1207	2635.1213	26		37937.607	0.0006	−0.008	1749.123	6.5	39686.738	5.5
2635.3792	2635.3781	69	as	37933.914	−0.0011	0.016	1749.123	6.5	39683.021	5.5
2635.5278	2635.5306	102		37931.719	0.0028	−0.041	0.000	4.5	37931.760	4.5
2637.6935	2637.6967	15		37900.569	0.0032	−0.046	4420.871	5.5	42321.486	6.5
2639.5742	2639.5720	20	p	37873.643	−0.0022	0.032	914.765	4.5	38788.376	4.5
2639.8350	2639.8351	26	p	37869.868	0.0001	−0.001	0.000	4.5	37869.869	5.5
2641.5456	2641.5488	20		37845.305	0.0031	−0.045	0.000	4.5	37845.350	3.5
2641.9333	2641.9291	8	p	37839.856	−0.0041	0.059	914.765	4.5	38754.562	4.5
2644.1238	2644.1281	20		37808.391	0.0043	−0.062	0.000	4.5	37808.453	5.5
2645.4716	2645.4749	78	LA	37789.143	0.0033	−0.047	0.000	4.5	37789.190	4.5
2648.7844	2648.7857	9		37741.914	0.0013	−0.018	0.000	4.5	37741.932	4.5
2649.0644	2649.0686	68		37737.884	0.0041	−0.059	289.041	5.5	38026.984	4.5
2650.7354	2650.7392	2		37714.100	0.0038	−0.054	1749.123	6.5	39463.277	5.5
2652.1885	2652.1883	29		37693.494	−0.0003	0.004	1749.123	6.5	39442.613	7.5
2652.8221	2652.8233	83		37684.471	0.0012	−0.017	4420.871	5.5	42105.359	5.5
2656.5889	2656.5910	172		37631.029	0.0021	−0.030	914.765	4.5	38545.824	3.5
2660.1401	2660.1369	20		37580.873	−0.0032	0.045	289.041	5.5	37869.869	5.5
2662.8483	2662.8539	21		37542.527	0.0057	−0.080	4420.871	5.5	41963.478	4.5
2663.2920	2663.2908	4		37536.369	−0.0012	0.017	5526.750	6.5	43063.102	6.5
2664.1581	2664.1519	11	p	37524.237	−0.0062	0.088	4420.871	5.5	41945.020	6.5
2664.4580	2664.4578	23	p	37519.928	−0.0002	0.003	4585.434	6.5	42105.359	5.5
2665.6926	2665.6909	36		37502.572	−0.0016	0.023	4420.871	5.5	41923.420	6.5
2665.8632	2665.8615	6	LA	37500.173	−0.0017	0.024	289.041	5.5	37789.190	4.5
2666.5295	2666.5315	14		37490.754	0.0021	−0.029	5259.653	7.5	42750.436	6.5
2667.8790	2667.8833	25	b,	37471.758	0.0043	−0.061	914.765	4.5	38386.584	3.5
2668.0123	2668.0134	7		37469.931	0.0011	−0.015	1749.123	6.5	39219.069	5.5
2669.1658	2669.1602	28		37453.832	−0.0056	0.078	4420.871	5.5	41874.625	6.5
2669.2273	2669.2230	28		37452.951	−0.0043	0.060	289.041	5.5	37741.932	4.5
2670.5030	2670.5089	49		37434.916	0.0059	−0.083	2294.696	5.5	39729.695	6.5
2672.2712	2672.2736	11		37410.195	0.0024	−0.034	289.041	5.5	37699.270	5.5
2672.4852	2672.4830	182		37407.265	−0.0022	0.031	5259.653	7.5	42666.887	7.5

Table 9. *Cont.*

wl_{Ritz} in Air (Å)	wl_{exp} in Air (Å)	*Int*	*Note*	wn_{exp} (cm^{-1})	Δwl (Å)	Δwn (cm^{-1})	E_{odd} (cm^{-1})	J_{odd}	E_{even} (cm^{-1})	J_{even}
2672.7077	2672.7030	72		37404.185	−0.0047	0.066	0.000	4.5	37404.119	5.5
2675.1142	2675.1087	37		37370.552	−0.0054	0.076	289.041	5.5	37659.517	4.5
2675.8767	2675.8790	35	LA	37359.794	0.0024	−0.033	1749.123	6.5	39108.950	5.5
2676.4154	2676.4115	187	LA	37352.362	−0.0039	0.055	6283.431	6.5	43635.738	6.5
2676.6836	2676.6849	11		37348.546	0.0014	−0.019	1749.123	6.5	39097.688	6.5
2677.4419	2677.4355	23	p	37338.076	−0.0065	0.090	4585.434	6.5	41923.420	6.5
2678.7931	2678.7924	72	p	37319.163	−0.0007	0.010	4585.434	6.5	41904.587	5.5
2683.2766	2683.2723	55		37256.861	−0.0043	0.060	1749.123	6.5	39005.924	5.5
2683.4216	2683.4147	4	c	37254.884	−0.0070	0.097	289.041	5.5	37543.828	4.5
2683.4719	2683.4724	12	c	37254.083	0.0004	−0.006	289.041	5.5	37543.130	5.5
2684.0314	2684.0318	24	as	37246.318	0.0004	−0.005	5259.653	7.5	42505.976	6.5
2685.9761	2685.9705	10	LA,p	37219.443	−0.0056	0.078	1749.123	6.5	38968.488	5.5
2689.1080	2689.1152	13	D	37175.918	0.0072	−0.099	0.000	4.5	37176.017	4.5
2689.1195	2689.1152	13	D	37175.918	−0.0043	0.059	289.041	5.5	37464.900	6.5
2689.6460	2689.6496	8		37168.531	0.0036	−0.050	2294.696	5.5	39463.277	5.5
2691.0334	2691.0336	219	p	37149.415	0.0003	−0.004	4420.871	5.5	41570.290	5.5
2693.7311	2693.7346	55	as	37112.170	0.0036	−0.049	914.765	4.5	38026.984	4.5
2697.3932	2697.3884	20		37061.899	−0.0048	0.066	5259.653	7.5	42321.486	6.5
2697.9173	2697.9129	24	p	37054.694	−0.0044	0.060	1749.123	6.5	38803.757	7.5
2698.4845	2698.4782	148		37046.932	−0.0063	0.087	4585.434	6.5	41632.279	6.5
2700.2512	2700.2548	12	as	37022.562	0.0036	−0.049	4420.871	5.5	41443.482	6.5
2705.7866	2705.7917	13		36946.806	0.0051	−0.070	1749.123	6.5	38695.999	5.5
2706.9739	2706.9728	63		36930.686	−0.0012	0.016	8276.733	6.5	45207.403	7.5
2708.9821	2708.9885	66		36903.206	0.0064	−0.087	4585.434	6.5	41488.727	5.5
2709.5050	2709.5064	30	LA,p	36896.153	0.0013	−0.018	4420.871	5.5	41317.042	5.5
2709.5564	2709.5498	77		36895.562	−0.0066	0.090	0.000	4.5	36895.472	4.5
2711.1029	2711.0998	13	LA,as	36874.468	−0.0032	0.043	914.765	4.5	37789.190	4.5
2711.7043	2711.7061	7		36866.223	0.0018	−0.024	5790.641	5.5	42656.888	5.5
2711.7820	2711.7807	22	b	36865.209	−0.0013	0.018	0.000	4.5	36865.191	5.5
2712.0582	2712.0588	8		36861.429	0.0005	−0.007	4420.871	5.5	41282.307	6.5
2714.5822	2714.5861	7		36827.115	0.0038	−0.052	914.765	4.5	37741.932	4.5
2715.5344	2715.5334	5		36814.267	−0.0010	0.013	2294.696	5.5	39108.950	5.5
2716.4220	2716.4269	9		36802.158	0.0049	−0.067	289.041	5.5	37091.266	4.5
2716.8633	2716.8693	9		36796.166	0.0060	−0.081	1749.123	6.5	38545.370	5.5
2718.0425	2718.0410	39		36780.304	−0.0015	0.020	1749.123	6.5	38529.407	7.5
2718.0444	2718.0410	39		36780.304	−0.0035	0.047	5259.653	7.5	42039.910	7.5
2719.3675	2719.3687	21		36762.350	0.0013	−0.017	1749.123	6.5	38511.490	5.5
2723.1625	2723.1671	139		36711.073	0.0046	−0.062	1749.123	6.5	38460.258	6.5
2725.0668	2725.0738	4	D,c	36685.386	0.0071	−0.095	8521.922	7.5	45207.403	7.5
2725.0752	2725.0738	4	D,c	36685.386	−0.0014	0.019	5259.653	7.5	41945.020	6.5
2725.2686	2725.2662	137	as	36682.796	−0.0024	0.032	6283.431	6.5	42966.195	7.5
2726.6810	2726.6841	27		36663.725	0.0031	−0.042	5259.653	7.5	41923.420	6.5
2727.7730	2727.7792	77	as	36649.007	0.0061	−0.082	4585.434	6.5	41234.523	6.5
2728.4664	2728.4701	7		36639.726	0.0037	−0.050	289.041	5.5	36928.817	4.5
2728.6183	2728.6233	8		36637.669	0.0050	−0.067	4420.871	5.5	41058.607	5.5
2733.9627	2733.9667	45		36566.071	0.0040	−0.054	289.041	5.5	36855.166	4.5
2734.0667	2734.0715	7		36564.670	0.0048	−0.064	1749.123	6.5	38313.857	5.5
2734.2730	2734.2762	285		36561.932	0.0032	−0.043	5401.503	3.5	41963.478	4.5
2735.5783	2735.5728	22	p	36544.602	−0.0055	0.073	4420.871	5.5	40965.400	6.5
2738.9799	2738.9848	35		36499.079	0.0049	−0.065	2294.696	5.5	38793.840	6.5
2739.3900	2739.3921	20	D	36493.652	0.0021	−0.028	2294.696	5.5	38788.376	4.5
2739.3906	2739.3921	20	D,LA	36493.652	0.0015	−0.020	289.041	5.5	36782.713	6.5
2740.6331	2740.6355	6		36477.099	0.0024	−0.032	289.041	5.5	36766.172	5.5
2740.8273	2740.8282	18		36474.534	0.0010	−0.013	289.041	5.5	36763.588	4.5
2740.9305	2740.9325	9		36473.146	0.0020	−0.027	4585.434	6.5	41058.607	5.5
2741.7458	2741.7506	24		36462.264	0.0047	−0.063	914.765	4.5	37377.092	4.5
2742.0571	2742.0563	15		36458.198	−0.0008	0.010	5259.653	7.5	41717.841	7.5
2744.4027	2744.3996	25		36427.069	−0.0032	0.042	914.765	4.5	37341.792	4.5
2745.0627	2745.0659	7		36418.227	0.0032	−0.043	5526.750	6.5	41945.020	6.5
2746.1590	2746.1557	12		36403.775	−0.0033	0.044	1749.123	6.5	38152.854	7.5
2746.6917	2746.6870	179		36396.733	−0.0048	0.063	5526.750	6.5	41923.420	6.5
2747.3598	2747.3547	23		36387.891	−0.0051	0.067	0.000	4.5	36387.824	3.5
2748.4450	2748.4475	7		36373.424	0.0025	−0.033	6283.431	6.5	42656.888	5.5
2748.5078	2748.5044	17		36372.671	−0.0034	0.045	5259.653	7.5	41632.279	6.5
2749.9421	2749.9398	37		36353.685	−0.0023	0.030	8853.748	8.5	45207.403	7.5
2750.3794	2750.3750	15		36347.933	−0.0044	0.058	5526.750	6.5	41874.625	6.5
2750.5536	2750.5520	7		36345.594	−0.0017	0.022	8276.733	6.5	44622.305	7.5

Table 9. *Cont.*

wl_{Ritz} in Air (Å)	wl_{exp} in Air (Å)	*Int*	*Note*	wn_{exp} (cm^{-1})	Δwl (Å)	Δwn (cm^{-1})	E_{odd} (cm^{-1})	J_{odd}	E_{even} (cm^{-1})	J_{even}
2751.2231	2751.2161	21		36336.820	−0.0070	0.092	2294.696	5.5	38631.424	5.5
2752.4357	2752.4349	13		36320.730	−0.0008	0.011	1749.123	6.5	38069.842	5.5
2754.1493	2754.1480	80		36298.143	−0.0013	0.017	914.765	4.5	37212.891	3.5
2756.8379	2756.8307	22		36262.821	−0.0072	0.095	289.041	5.5	36551.767	5.5
2756.9499	2756.9462	9	c	36261.301	−0.0037	0.049	914.765	4.5	37176.017	4.5
2757.5498	2757.5455	32		36253.420	−0.0043	0.056	0.000	4.5	36253.364	5.5
2758.9517	2758.9473	10	as	36235.000	−0.0043	0.057	914.765	4.5	37149.708	4.5
2759.7839	2759.7817	24		36224.045	−0.0022	0.029	1749.123	6.5	37973.139	5.5
2762.7151	2762.7167	12		36185.566	0.0017	−0.022	1749.123	6.5	37934.711	7.5
2762.8494	2762.8471	18		36183.858	−0.0022	0.029	5259.653	7.5	41443.482	6.5
2762.8797	2762.8769	38		36183.468	−0.0028	0.037	0.000	4.5	36183.431	5.5
2763.4090	2763.4131	29		36176.447	0.0041	−0.054	914.765	4.5	37091.266	4.5
2763.6889	2763.6843	14		36172.897	−0.0046	0.060	5790.641	5.5	41963.478	4.5
2764.2397	2764.2400	20	D	36165.625	0.0003	−0.004	5526.750	6.5	41692.379	5.5
2764.2449	2764.2400	20	D	36165.625	−0.0048	0.063	2294.696	5.5	38460.258	6.5
2764.6629	2764.6561	56		36160.182	−0.0067	0.088	4420.871	5.5	40580.965	5.5
2765.3970	2765.3989	49		36150.470	0.0019	−0.025	0.000	4.5	36150.495	3.5
2766.7528	2766.7518	13		36132.792	−0.0010	0.013	5790.641	5.5	41923.420	6.5
2766.8721	2766.8729	28	as	36131.211	0.0008	−0.010	0.000	4.5	36131.221	5.5
2767.6745	2767.6669	314		36120.845	−0.0076	0.099	1749.123	6.5	37869.869	5.5
2768.8587	2768.8516	37		36105.395	−0.0071	0.093	1749.123	6.5	37854.425	5.5
2770.0418	2770.0399	34		36089.906	−0.0019	0.025	0.000	4.5	36089.881	3.5
2770.7417	2770.7376	65		36080.819	−0.0041	0.054	6445.035	4.5	42525.800	5.5
2772.1759	2772.1743	9		36062.120	−0.0016	0.021	4420.871	5.5	40482.970	5.5
2772.3887	2772.3910	9		36059.300	0.0023	−0.030	1749.123	6.5	37808.453	5.5
2772.6325	2772.6313	38		36056.175	−0.0012	0.015	2294.696	5.5	38350.856	4.5
2773.6033	2773.6039	29		36043.532	0.0006	−0.008	5526.750	6.5	41570.290	5.5
2775.0145	2775.0118	6		36025.245	−0.0027	0.035	5526.750	6.5	41551.960	5.5
2775.2114	2775.2079	7		36022.699	−0.0035	0.045	5259.653	7.5	41282.307	6.5
2775.3724	2775.3675	5		36020.628	−0.0049	0.064	5790.641	5.5	41811.205	5.5
2775.8213	2775.8148	11		36014.828	−0.0066	0.085	4420.871	5.5	40435.614	6.5
2776.8169	2776.8205	7		36001.784	0.0036	−0.047	1749.123	6.5	37750.954	5.5
2778.4471	2778.4532	12	p	35980.629	0.0060	−0.078	914.765	4.5	36895.472	4.5
2779.4472	2779.4478	2	D	35967.757	0.0006	−0.008	1749.123	6.5	37716.888	7.5
2779.4508	2779.4478	2	D	35967.757	−0.0029	0.038	1749.123	6.5	37716.842	6.5
2780.0321	2780.0339	11	LA	35960.175	0.0018	−0.023	0.000	4.5	35960.198	4.5
2781.0310	2781.0317	9		35947.273	0.0007	−0.009	289.041	5.5	36236.323	4.5
2781.5634	2781.5684	21		35940.336	0.0050	−0.065	914.765	4.5	36855.166	4.5
2782.0684	2782.0730	5		35933.818	0.0046	−0.059	44357.295	4.5	8423.418	4.5
2783.2065	2783.2076	12		35919.174	0.0011	−0.014	2294.696	5.5	38213.884	5.5
2783.2899	2783.2969	3		35918.021	0.0070	−0.090	0.000	4.5	35918.111	5.5
2783.3968	2783.4034	41	?	35916.647	0.0066	−0.085	5526.750	6.5	41443.482	6.5
2784.4497	2784.4498	16		35903.149	0.0001	−0.001	5526.750	6.5	41429.900	6.5
2784.5592	2784.5533	95	b	35901.815	−0.0060	0.077	5790.641	5.5	41692.379	5.5
2784.6660	2784.6669	11		35900.350	0.0009	−0.011	289.041	5.5	36189.402	5.5
2784.9076	2784.9081	4		35897.241	0.0005	−0.006	8276.733	6.5	44173.980	6.5
2788.5251	2788.5246	11		35850.685	−0.0005	0.007	0.000	4.5	35850.678	5.5
2789.2284	2789.2236	79		35841.700	−0.0048	0.062	5790.641	5.5	41632.279	6.5
2791.2531	2791.2572	3		35815.592	0.0041	−0.052	5259.653	7.5	41075.297	8.5
2793.9333	2793.9363	47		35781.248	0.0030	−0.039	289.041	5.5	36070.328	4.5
2794.0612	2794.0576	8	D,as	35779.695	−0.0036	0.046	5790.641	5.5	41570.290	5.5
2794.0636	2794.0576	8	D,as	35779.695	−0.0060	0.077	8394.362	7.5	44173.980	6.5
2794.9276	2794.9215	37		35768.636	−0.0062	0.079	8853.748	8.5	44622.305	7.5
2795.2282	2795.2335	41		35764.643	0.0053	−0.068	914.765	4.5	36679.476	3.5
2796.2329	2796.2312	5		35751.882	−0.0017	0.022	0.000	4.5	35751.860	5.5
2797.1416	2797.1451	19		35740.201	0.0035	−0.045	914.765	4.5	36655.011	3.5
2800.1004	2800.0975	38		35702.521	−0.0029	0.037	5526.750	6.5	41229.234	7.5
2803.8298	2803.8262	40		35655.042	−0.0036	0.046	1749.123	6.5	37404.119	5.5
2805.2406	2805.2421	14	D	35637.045	0.0015	−0.019	2294.696	5.5	37931.760	4.5
2805.2455	2805.2421	14	D	35637.045	−0.0034	0.043	914.765	4.5	36551.767	5.5
2806.4938	2806.4936	11		35621.158	−0.0002	0.002	6283.431	6.5	41904.587	5.5
2807.1192	2807.1167	69	as	35613.251	−0.0025	0.032	289.041	5.5	35902.260	4.5
2809.0118	2809.0131	34		35589.208	0.0013	−0.017	1749.123	6.5	37338.348	7.5
2809.6382	2809.6426	29		35581.234	0.0044	−0.056	9626.113	6.5	45207.403	7.5
2809.9856	2809.9791	15	p	35576.974	−0.0066	0.083	289.041	5.5	35865.932	4.5
2813.0414	2813.0421	17		35538.240	0.0007	−0.009	4706.273	2.5	40244.522	1.5
2813.5474	2813.5491	7		35531.835	0.0017	−0.022	5526.750	6.5	41058.607	5.5
2814.7037	2814.7027	5		35517.273	−0.0010	0.013	4420.871	5.5	39938.131	5.5
2817.9580	2817.9578	37		35476.246	−0.0002	0.002	914.765	4.5	36391.009	3.5

Table 9. *Cont.*

wl_{Ritz} in Air (Å)	wl_{exp} in Air (Å)	*Int*	*Note*	wn_{exp} (cm^{-1})	Δwl (Å)	Δwn (cm^{-1})	E_{odd} (cm^{-1})	J_{odd}	E_{even} (cm^{-1})	J_{even}
2819.0247	2819.0286	7		35462.770	0.0039	−0.049	289.041	5.5	35751.860	5.5
2819.2845	2819.2778	8		35459.636	−0.0067	0.084	6445.035	4.5	41904.587	5.5
2820.2640	2820.2637	6		35447.240	−0.0003	0.004	2294.696	5.5	37741.932	4.5
2820.5036	2820.4993	13	as	35444.279	−0.0043	0.054	4585.434	6.5	40029.659	6.5
2821.1209	2821.1202	103		35436.482	−0.0006	0.008	914.765	4.5	36351.239	3.5
2826.2615	2826.2551	73	as	35372.099	−0.0064	0.080	0.000	4.5	35372.019	5.5
2826.6653	2826.6723	15		35366.879	0.0070	−0.087	4420.871	5.5	39787.837	5.5
2826.7289	2826.7250	25		35366.219	−0.0039	0.049	6445.035	4.5	41811.205	5.5
2828.9347	2828.9339	37		35338.608	−0.0007	0.009	914.765	4.5	36253.364	5.5
2829.2940	2829.2865	132		35334.205	−0.0075	0.094	5790.641	5.5	41124.752	6.5
2829.3965	2829.4002	53	p	35332.784	0.0038	−0.047	1749.123	6.5	37081.954	7.5
2830.0727	2830.0759	10		35324.349	0.0032	−0.040	0.000	4.5	35324.389	5.5
2831.5587	2831.5603	26	p	35305.831	0.0016	−0.020	5790.641	5.5	41096.492	6.5
2832.0616	2832.0605	44		35299.599	−0.0011	0.014	5259.653	7.5	40559.238	8.5
2832.0988	2832.0965	14		35299.150	−0.0023	0.029	4585.434	6.5	39884.555	6.5
2833.8199	2833.8173	29		35277.715	−0.0026	0.032	2294.696	5.5	37572.379	6.5
2834.0646	2834.0590	57	as	35274.707	−0.0056	0.070	914.765	4.5	36189.402	5.5
2834.5444	2834.5520	13		35268.572	0.0076	−0.094	914.765	4.5	36183.431	5.5
2834.5554	2834.5520	13		35268.572	−0.0035	0.043	6283.431	6.5	41551.960	5.5
2835.5690	2835.5682	10		35255.932	−0.0008	0.010	289.041	5.5	35544.963	4.5
2836.9143	2836.9164	19		35239.182	0.0021	−0.026	4420.871	5.5	39660.079	6.5
2837.1943	2837.1947	18		35235.725	0.0004	−0.005	914.765	4.5	36150.495	3.5
2837.3302	2837.3253	27		35234.103	−0.0049	0.061	0.000	4.5	35234.042	5.5
2839.7944	2839.8005	27		35203.393	0.0061	−0.075	914.765	4.5	36118.233	4.5
2839.8803	2839.8864	34	D	35202.328	0.0061	−0.075	4585.434	6.5	39787.837	5.5
2839.8925	2839.8864	34	D	35202.328	−0.0061	0.076	289.041	5.5	35491.293	5.5
2840.4603	2840.4659	16		35195.146	0.0056	−0.069	1749.123	6.5	36944.338	5.5
2842.4803	2842.4828	54		35170.173	0.0025	−0.031	2294.696	5.5	37464.900	6.5
2842.8541	2842.8515	26		35165.612	−0.0027	0.033	40882.028	5.5	5716.449	4.5
2845.5385	2845.5356	6		35132.445	−0.0028	0.035	1749.123	6.5	36881.533	6.5
2845.9556	2845.9514	9	as	35127.312	−0.0042	0.052	914.765	4.5	36042.025	4.5
2846.1491	2846.1474	11	D	35124.893	−0.0017	0.021	8510.866	5.5	43635.738	6.5
2846.1497	2846.1474	11	D	35124.893	−0.0023	0.028	8276.733	6.5	43401.598	7.5
2846.3700	2846.3683	16		35122.167	−0.0017	0.021	7166.632	4.5	42288.778	5.5
2849.9862	2849.9799	7		35077.659	−0.0063	0.077	5259.653	7.5	40337.235	8.5
2852.7458	2852.7524	9		35043.573	0.0065	−0.080	5526.750	6.5	40570.403	6.5
2853.4221	2853.4200	348		35035.374	−0.0021	0.026	289.041	5.5	35324.389	5.5
2853.5636	2853.5639	12	LA,D	35033.607	0.0003	−0.004	6283.431	6.5	41317.042	5.5
2853.5653	2853.5639	12	LA,D	35033.607	−0.0014	0.017	1749.123	6.5	36782.713	6.5
2854.9132	2854.9129	4		35017.053	−0.0003	0.004	1749.123	6.5	36766.172	5.5
2855.7135	2855.7198	135		35007.158	0.0064	−0.078	8394.362	7.5	43401.598	7.5
2856.0308	2856.0297	182		35003.360	−0.0011	0.014	914.765	4.5	35918.111	5.5
2856.2831	2856.2829	67		35000.257	−0.0002	0.003	2294.696	5.5	37294.950	6.5
2856.6147	2856.6188	13	as	34996.141	0.0042	−0.051	9626.113	6.5	44622.305	7.5
2857.2259	2857.2328	3		34988.621	0.0069	−0.084	5526.750	6.5	40515.455	5.5
2858.9077	2858.9146	124		34968.038	0.0069	−0.085	0.000	4.5	34968.123	5.5
2859.8812	2859.8868	30		34956.151	0.0056	−0.069	5526.750	6.5	40482.970	5.5
2860.4656	2860.4578	141	p	34949.178	−0.0079	0.096	0.000	4.5	34949.082	3.5
2860.7997	2860.8038	48		34944.950	0.0042	−0.051	289.041	5.5	35234.042	5.5
2862.2375	2862.2426	37		34927.384	0.0052	−0.063	7598.353	5.5	42525.800	5.5
2862.4075	2862.4069	69		34925.379	−0.0006	0.007	289.041	5.5	35214.413	4.5
2862.6160	2862.6160	53	LA	34922.828	0.0000	0.000	4585.434	6.5	39508.262	7.5
2863.5279	2863.5306	29	#1	34911.674	0.0027	−0.033	5259.653	7.5	40171.360	8.5
2863.8629	2863.8701	4	c	34907.535	0.0072	−0.088	7598.353	5.5	42505.976	6.5
2864.4082	2864.4097	34	#2	34900.960	0.0015	−0.018	2294.696	5.5	37195.674	6.5
2865.1378	2865.1415	113	#3	34892.046	0.0036	−0.044	4420.871	5.5	39312.961	6.5
2865.6808	2865.6847	558	#4, LA	34885.431	0.0039	−0.048	0.000	4.5	34885.479	5.5
2866.1576	2866.1603	85		34879.643	0.0027	−0.033	8521.922	7.5	43401.598	7.5
2866.7879	2866.7887	24	#5	34871.997	0.0008	−0.010	6445.035	4.5	41317.042	5.5
2868.0074	2868.0134	63	#6	34857.106	0.0060	−0.073	4585.434	6.5	39442.613	7.5
2868.1857	2868.1865	47	#7	34855.003	0.0007	−0.009	2294.696	5.5	37149.708	4.5
2869.3858	2869.3803	62	#8, p	34840.505	−0.0054	0.066	5667.331	3.5	40507.770	3.5
2869.6612	2869.6595	22	#9	34837.116	−0.0017	0.021	914.765	4.5	35751.860	5.5
2870.9740	2870.9721	116	#10	34821.188	−0.0019	0.023	289.041	5.5	35110.206	4.5
2872.5019	2872.5038	25	c	34802.620	0.0020	−0.024	1749.123	6.5	36551.767	5.5
2872.5897	2872.5899	2		34801.577	0.0002	−0.003	6445.035	4.5	41246.615	4.5
2873.0033	2873.0085	44		34796.507	0.0052	−0.063	2294.696	5.5	37091.266	4.5
2873.2953	2873.2939	50	#11	34793.050	−0.0014	0.017	5526.750	6.5	40319.783	5.5
2873.5191	2873.5141	146	#12	34790.384	−0.0050	0.060	5790.641	5.5	40580.965	5.5
2874.0820	2874.0812	86		34783.519	−0.0007	0.009	1749.123	6.5	36532.633	7.5
2874.4694	2874.4633	21		34778.896	−0.0061	0.074	0.000	4.5	34778.822	5.5

Table 9. *Cont.*

wl_{Ritz} in Air (Å)	wl_{exp} in Air (Å)	*Int*	*Note*	wn_{exp} (cm^{-1})	Δwl (Å)	Δwn (cm^{-1})	E_{odd} (cm^{-1})	J_{odd}	E_{even} (cm^{-1})	J_{even}
2874.7708	2874.7635	148		34775.264	−0.0073	0.088	6283.431	6.5	41058.607	5.5
2875.1857	2875.1898	89	T,p	34770.108	0.0041	−0.049	289.041	5.5	35059.198	6.5
2875.1866	2875.1898	89	T,p	34770.108	0.0031	−0.038	8510.866	5.5	43281.012	5.5
2875.1952	2875.1898	89	T,p	34770.108	−0.0055	0.066	914.765	4.5	35684.807	5.5
2876.5188	2876.5190	55		34754.041	0.0002	−0.003	1749.123	6.5	36503.167	5.5
2877.5677	2877.5722	41	LA	34741.325	0.0045	−0.054	0.000	4.5	34741.379	4.5
2877.7302	2877.7226	194		34739.509	−0.0075	0.091	2294.696	5.5	37034.114	5.5
2878.9404	2878.9408	30		34724.810	0.0003	−0.004	5790.641	5.5	40515.455	5.5
2879.0798	2879.0806	118		34723.123	0.0008	−0.010	7598.353	5.5	42321.486	6.5
2879.9719	2879.9729	15	p	34712.365	0.0010	−0.012	43060.067	5.5	8347.690	5.5
2881.7318	2881.7380	18		34691.103	0.0062	−0.075	2294.696	5.5	36985.874	6.5
2881.7944	2881.7925	23		34690.447	−0.0018	0.022	7598.353	5.5	42288.778	5.5
2881.8744	2881.8796	16		34689.399	0.0052	−0.063	8276.733	6.5	42966.195	7.5
2881.9893	2881.9962	28	as	34687.995	0.0070	−0.084	4420.871	5.5	39108.950	5.5
2882.5843	2882.5784	127		34680.989	−0.0059	0.071	0.000	4.5	34680.918	4.5
2882.7370	2882.7381	233		34679.068	0.0012	−0.014	289.041	5.5	34968.123	5.5
2882.9252	2882.9279	165		34676.785	0.0027	−0.032	4420.871	5.5	39097.688	6.5
2885.1866	2885.1884	45		34649.620	0.0018	−0.022	2294.696	5.5	36944.338	5.5
2885.3330	2885.3323	10	c	34647.893	−0.0007	0.009	5667.331	3.5	40315.215	3.5
2885.5754	2885.5836	7		34644.875	0.0082	−0.098	5790.641	5.5	40435.614	6.5
2885.6088	2885.6149	33		34644.499	0.0062	−0.074	7166.632	4.5	41811.205	5.5
2886.0312	2886.0284	32		34639.535	−0.0027	0.033	914.765	4.5	35554.267	3.5
2886.1638	2886.1640	29		34637.908	0.0002	−0.003	4420.871	5.5	39058.782	5.5
2886.4456	2886.4514	28	LA	34634.459	0.0058	−0.070	289.041	5.5	34923.570	6.5
2886.4796	2886.4792	37	D	34634.126	−0.0004	0.005	2294.696	5.5	36928.817	4.5
2886.4824	2886.4792	37	D	34634.126	−0.0033	0.039	0.000	4.5	34634.087	4.5
2886.9223	2886.9234	53		34628.796	0.0012	−0.014	7166.632	4.5	41795.442	3.5
2887.0060	2887.0111	7		34627.745	0.0051	−0.061	40344.255	5.5	5716.449	4.5
2887.2481	2887.2529	165		34624.845	0.0048	−0.057	5259.653	7.5	39884.555	6.5
2887.5908	2887.5910	70	LA	34620.790	0.0003	−0.003	9553.187	5.5	44173.980	6.5
2888.2558	2888.2565	96	LA	34612.813	0.0008	−0.009	0.000	4.5	34612.822	4.5
2888.7371	2888.7399	83		34607.021	0.0028	−0.034	4420.871	5.5	39027.926	6.5
2889.1209	2889.1232	39		34602.430	0.0023	−0.027	6283.431	6.5	40885.888	6.5
2889.2613	2889.2607	29		34600.783	−0.0006	0.007	2294.696	5.5	36895.472	4.5
2889.6236	2889.6258	198	LA	34596.412	0.0022	−0.026	289.041	5.5	34885.479	5.5
2890.4257	2890.4214	43		34586.889	−0.0043	0.052	2294.696	5.5	36881.533	6.5
2891.6259	2891.6265	6	as	34572.478	0.0007	−0.008	8276.733	6.5	42849.219	5.5
2891.6805	2891.6847	19		34571.783	0.0042	−0.050	8394.362	7.5	42966.195	7.5
2891.7924	2891.7926	66	D	34570.493	0.0002	−0.002	2294.696	5.5	36865.191	5.5
2891.8001	2891.7926	66	D	34570.493	−0.0075	0.090	42918.093	5.5	8347.690	5.5
2894.8391	2894.8403	45		34534.101	0.0012	−0.014	1749.123	6.5	36283.238	5.5
2895.5407	2895.5443	47		34525.704	0.0036	−0.043	7166.632	4.5	41692.379	5.5
2895.6254	2895.6257	34		34524.734	0.0003	−0.004	1749.123	6.5	36273.861	6.5
2895.7279	2895.7315	4		34523.472	0.0037	−0.044	4585.434	6.5	39108.950	5.5
2896.0761	2896.0695	46		34519.443	−0.0065	0.078	5526.750	6.5	40046.115	5.5
2896.6728	2896.6710	717	as,IV	34512.275	−0.0018	0.021	4585.434	6.5	39097.688	6.5
2897.4573	2897.4562	47		34502.923	−0.0012	0.014	5526.750	6.5	40029.659	6.5
2898.1286	2898.1254	144	as	34494.955	−0.0032	0.038	5259.653	7.5	39754.570	8.5
2898.3689	2898.3677	51		34492.072	−0.0013	0.015	289.041	5.5	34781.098	4.5
2898.5602	2898.5686	146		34489.681	0.0084	−0.100	289.041	5.5	34778.822	5.5
2898.7085	2898.7080	30		34488.022	−0.0004	0.005	2294.696	5.5	36782.713	6.5
2898.9194	2898.9231	174		34485.463	0.0037	−0.044	42833.197	5.5	8347.690	5.5
2899.9121	2899.9080	19		34473.751	−0.0040	0.048	8276.733	6.5	42750.436	6.5
2899.9419	2899.9443	21		34473.320	0.0024	−0.028	4585.434	6.5	39058.782	5.5
2900.2638	2900.2714	46	D,c	34469.432	0.0076	−0.090	8379.697	4.5	42849.219	5.5
2900.2656	2900.2714	46	D,c	34469.432	0.0058	−0.069	5259.653	7.5	39729.154	7.5
2900.3168	2900.3173	23	c	34468.886	0.0005	−0.006	2294.696	5.5	36763.588	4.5
2900.7128	2900.7164	27	p	34464.144	0.0036	−0.043	4706.273	2.5	39170.460	2.5
2902.3902	2902.3976	39	p	34444.185	0.0074	−0.088	8521.922	7.5	42966.195	7.5
2902.4127	2902.4100	29	p	34444.037	−0.0027	0.032	5790.641	5.5	40234.646	5.5
2902.8069	2902.8073	19	LA	34439.323	0.0004	−0.005	0.000	4.5	34439.328	5.5
2903.7855	2903.7816	121		34427.768	−0.0039	0.046	42775.412	5.5	8347.690	5.5
2904.5041	2904.5065	63	LA	34419.176	0.0024	−0.028	289.041	5.5	34708.245	6.5
2905.8166	2905.8110	46		34403.724	−0.0056	0.066	7166.632	4.5	41570.290	5.5
2906.0896	2906.0976	81		34400.331	0.0080	−0.095	5259.653	7.5	39660.079	6.5
2906.9576	2906.9550	70		34390.184	−0.0025	0.030	8276.733	6.5	42666.887	7.5
2907.0539	2907.0554	41		34388.997	0.0014	−0.017	289.041	5.5	34678.055	6.5
2908.0936	2908.0988	14		34376.658	0.0052	−0.062	6445.035	4.5	40821.755	4.5
2908.4109	2908.4115	89		34372.962	0.0006	−0.007	4420.871	5.5	38793.840	6.5
2909.0748	2909.0674	24		34365.212	−0.0074	0.087	7598.353	5.5	41963.478	4.5

Table 9. *Cont.*

wl_{Ritz} in Air (Å)	wl_{exp} in Air (Å)	*Int*	*Note*	wn_{exp} (cm^{-1})	Δwl (Å)	Δwn (cm^{-1})	E_{odd} (cm^{-1})	J_{odd}	E_{even} (cm^{-1})	J_{even}
2909.6946	2909.6885	63		34357.877	−0.0061	0.072	5526.750	6.5	39884.555	6.5
2910.4278	2910.4339	63		34349.081	0.0061	−0.072	6445.035	4.5	40794.188	4.5
2910.5243	2910.5222	10		34348.039	−0.0021	0.025	5259.653	7.5	39607.667	6.5
2910.6385	2910.6395	32		34346.655	0.0010	−0.012	7598.353	5.5	41945.020	6.5
2911.7385	2911.7334	17		34333.752	−0.0052	0.061	4420.871	5.5	38754.562	4.5
2912.5792	2912.5779	40	LA	34323.796	−0.0013	0.015	289.041	5.5	34612.822	4.5
2913.9646	2913.9679	26		34307.424	0.0032	−0.038	8755.640	6.5	43063.102	6.5
2914.2520	2914.2493	70	D	34304.111	−0.0027	0.032	289.041	5.5	34593.120	5.5
2914.2561	2914.2493	70	D	34304.111	−0.0068	0.080	45044.296	7.5	10740.265	6.5
2914.6285	2914.6235	106		34299.707	−0.0050	0.059	914.765	4.5	35214.413	4.5
2914.7246	2914.7324	82	p	34298.425	0.0078	−0.092	0.000	4.5	34298.517	5.5
2915.4993	2915.4945	97	as	34289.459	−0.0048	0.056	8394.362	7.5	42683.765	8.5
2915.5822	2915.5801	38		34288.453	−0.0021	0.025	1749.123	6.5	36037.551	7.5
2916.7057	2916.7052	57	D	34275.226	−0.0005	0.006	5526.750	6.5	39801.970	6.5
2916.7136	2916.7052	57	D	34275.226	−0.0083	0.098	4420.871	5.5	38695.999	5.5
2916.9351	2916.9366	37		34272.507	0.0015	−0.018	8394.362	7.5	42666.887	7.5
2917.5409	2917.5390	207		34265.431	−0.0020	0.023	5401.503	3.5	39666.911	4.5
2917.9089	2917.9034	26		34261.152	−0.0055	0.065	5526.750	6.5	39787.837	5.5
2938.9919	2938.9908	114		34015.338	−0.0010	0.012	1749.123	6.5	35764.449	7.5
2940.0800	2940.0783	18	p	34002.757	−0.0017	0.020	1749.123	6.5	35751.860	5.5
2940.2834	2940.2880	274	p	34000.331	0.0047	−0.054	9075.732	3.5	43076.117	4.5
2940.4294	2940.4290	46		33998.701	−0.0004	0.005	5401.503	3.5	39400.199	4.5
2941.3079	2941.3068	30		33988.555	−0.0011	0.013	2294.696	5.5	36283.238	5.5
2941.6963	2941.6897	32		33984.131	−0.0067	0.077	8521.922	7.5	42505.976	6.5
2941.9164	2941.9176	213	LA	33981.498	0.0012	−0.014	5526.750	6.5	39508.262	7.5
2942.1196	2942.1204	74		33979.156	0.0008	−0.009	2294.696	5.5	36273.861	6.5
2942.4224	2942.4278	7	D	33975.606	0.0054	−0.062	10198.312	7.5	44173.980	6.5
2942.4268	2942.4278	7	D,LA	33975.606	0.0010	−0.011	4706.273	2.5	38681.890	3.5
2942.7456	2942.7519	100		33971.864	0.0063	−0.073	7598.353	5.5	41570.290	5.5
2942.8515	2942.8516	49	LA	33970.713	0.0001	−0.001	914.765	4.5	34885.479	5.5
2943.8954	2943.8964	160		33958.656	0.0010	−0.012	2294.696	5.5	36253.364	5.5
2944.3342	2944.3300	12	as	33953.655	−0.0042	0.048	7598.353	5.5	41551.960	5.5
2944.5416	2944.5456	34		33951.169	0.0040	−0.046	6283.431	6.5	40234.646	5.5
2945.5252	2945.5297	7		33939.830	0.0045	−0.052	5259.653	7.5	39199.535	7.5
2945.5971	2945.5947	10		33939.081	−0.0023	0.027	5790.641	5.5	39729.695	6.5
2945.8164	2945.8129	13		33936.567	−0.0035	0.040	5526.750	6.5	39463.277	5.5
2945.8896	2945.8919	96	D,LA	33935.658	0.0023	−0.026	1749.123	6.5	35684.807	5.5
2945.8980	2945.8919	96	D	33935.658	−0.0062	0.071	5401.503	3.5	39337.090	4.5
2946.2771	2946.2831	13		33931.152	0.0060	−0.069	4585.434	6.5	38516.655	6.5
2946.6046	2946.6073	32	p	33927.418	0.0027	−0.031	5526.750	6.5	39454.199	6.5
2946.6329	2946.6252	42	p	33927.212	−0.0076	0.088	8394.362	7.5	42321.486	6.5
2947.5118	2947.5119	51		33917.006	0.0001	−0.001	2294.696	5.5	36211.703	6.5
2948.0897	2948.0907	161		33910.347	0.0010	−0.012	289.041	5.5	34199.400	5.5
2949.4511	2949.4501	79	p	33894.718	−0.0010	0.012	2294.696	5.5	36189.402	5.5
2949.6008	2949.6057	38	as	33892.930	0.0049	−0.056	4420.871	5.5	38313.857	5.5
2949.6888	2949.6890	33		33891.973	0.0002	−0.002	7166.632	4.5	41058.607	5.5
2949.8281	2949.8363	23		33890.280	0.0082	−0.094	7598.353	5.5	41488.727	5.5
2949.9708	2949.9735	14		33888.704	0.0027	−0.031	2294.696	5.5	36183.431	5.5
2950.5021	2950.5005	15		33882.651	−0.0017	0.019	4585.434	6.5	38468.066	7.5
2950.5656	2950.5655	26		33881.905	−0.0002	0.002	1749.123	6.5	35631.026	7.5
2951.0563	2951.0646	84	D	33876.174	0.0084	−0.096	5790.641	5.5	39666.911	4.5
2951.0724	2951.0646	84	D	33876.174	−0.0078	0.089	0.000	4.5	33876.085	5.5
2951.9221	2951.9153	23	p	33866.412	−0.0069	0.079	914.765	4.5	34781.098	4.5
2953.0016	2953.0029	105		33853.938	0.0013	−0.015	4706.273	2.5	38560.226	3.5
2953.5797	2953.5870	60		33847.243	0.0073	−0.084	5667.331	3.5	39514.658	2.5
2953.7715	2953.7756	188	p	33845.082	0.0041	−0.047	7598.353	5.5	41443.482	6.5
2954.5230	2954.5233	326	p	33836.521	0.0003	−0.004	2294.696	5.5	36131.221	5.5
2954.6867	2954.6825	143		33834.698	−0.0042	0.048	5259.653	7.5	39094.303	7.5

LA: line already assigned as U II transition in [7], as: asymmetrical line, c: complex line shape, p: line resolved on the plate, but perturbed by a close line, b: broad line, ?: line given by [12] as U III without classification, IV : this line could be blended with a strong U IV line, D: line with double identification, T: line with triple identification, #n: line number in Figure 1.

Table 10. Transitions establishing the newly determined even parity level $5f^36d7p$ $(^4I)^6K(J = 5.5)$ of the U^+ ion at 39113.98 ± 0.1 cm^{-1}. In log(g_lf) , f is the absorption oscillator strength and g_l, the statistical weight of the lower level. gA is the upper level statistical weight g multiplied by the Einstein coefficient of spontaneous emission. CF is the cancellation factor defined by Equation (14.107), p432 in [10].

E_{th} (cm^{-1})	*J*	*Odd Level*	wn_{th} (cm^{-1})	*log(g_lf)*	*gA* (s^{-1})	*CF*	E_{exp} (cm^{-1})	wn_{exp} (cm^{-1})	λ_{exp} in Air (Å)	Int_{exp} (arb.)
−56.8	4.5	$5f^37s^2$ (4I) 4I	38865.8	0.263	1.847E+09	0.63	0. 000	39114.382	2555.8378	545
224.4	5.5	$5f^36d7s$ (4I) 6L	38584.6	−1.518	3.014E+07	0.03	289.041	38824.783	2574.9033	4
1715.5	6.5	$5f^36d7s$ (4I) 6L	37093.5	0.181	1.391E+09	−0.27	1749.123	37364.867	2675.5157	228
2320.7	5.5	$5f^36d7s$ (4I) 6K	36488.3	−0.252	4.974E+08	−0.21	2294.696	36819.292	2715.1628	36
4406.4	5.5	$5f^37s^2$ (4I) 4I	34402.6	−0.877	1.048E+08	0.20	4420.871	34692.797	2881.5973	14
4577.9	6.5	$5f^36d7s$ (4I) 6L	34231.1	−0.160	5.404E+08	−0.16	4585.434	34528.617	2895.3001	33

5. Conclusions

The lowest energy levels of the singly ionized uranium are interpreted following the Racah-Slater parametric method by means of Cowan codes. In the odd parity, the number of interpreted levels is about ten times larger than the number of free parameters. The relatively small *rms* deviation of the energies and the deviations between g_L^{th} and g_L^{exp} Landé factors for many levels show that the present model is robust. Some experimental level energies, although supported by the high accuracy of the observed FTS wave numbers, could not be attributed unambiguously to a theoretical level energy. The limitations of the present theoretical description are even more obvious in the even parity with larger *rms* deviations on the energies for both groups of configurations studied. After 70 years of investigations, the spectrum of U II still deserves further experimental studies for removing uncertain interpretations. The main difficulties are due to the ambiguities on the J values of levels, the determination of which would need a more complete study of Zeeman effect. Furthermore, the description of the strongly mixed CI wave functions could only be confirmed by the value of the Landé factor. By remembering the sentence *Levels without known g values are less certain because of the possibilities of fortuitous coincidences* written in [6], we do consider that the present calculations are satisfactory in spite the uninterpreted levels. A theoretical interpretation of the core configurations $5f^4$ and $5f^3(6d + 7s)$ of U III is presently under way for a better knowledge of appropriate scaling factors of the *HFR* radial integrals to be used in U II. An estimate of the partition function shows that level energies from parametric fit are preferable for its calculation. On the experimental side, a list of 451 ultraviolet spectral lines from high resolution vacuum spark spectra identified as U II transitions is reported, as well as six other transitions establishing a new energy level in the even parity configuration $5f^36d7p$.

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Conflicts of Interest: The authors declare no conflict of interest.

References

1. Cayrel, R.; Hill, V.; Beers, T.; Barbuy, B.; Spite, M.; Spite, F.; Plez, B.; Andersen, J.; Bonifacio, P.; Francois, P.; et al. Measurement of stellar age from uranium decay. *Nature* **2001**, *409*, 691–692.
2. Judd, B. R. Complex atomic spectra. *Rep. Prog. Phys.* **1985**, *48*, 907–954.
3. Blaise, J.; Wyart, J.-F. *Selected Constants Energy Levels and Atomic Spectra of Actinides*; Centre National de la Recherche Scientifique: Paris, France, 1992; Volume 20.

4. Wyart, J.-F.; Blaise, J.; Worden, E.F. Studies of electronic configurations in the emission spectra of lanthanides and actinides: application to the interpretation of Es I and Es II, predictions for Fm I. *J. Sol. State Chem.* **2005**, *178*, 589–602
5. Guyon, F.; Blaise, J.; Wyart, J.-F. Etude paramétrique des configurations impaires profondes dans les spectres de l'uranium UI et UII. *J. Phys.* **1974**, *35*, 929–933.
6. Blaise, J.; Wyart, J.-F.; Vergès, J.; Engleman, R., Jr.; Palmer, B.A.; Radziemski, L.J. Energy levels and isotope shifts for singly ionized uranium (U II). *J. Opt. Soc. Am. B* **1994**, *11*, 1897–1929.
7. Steinhaus, D.W.; Radziemski, L.J., Jr.; Cowan, R.D.; Blaise, J.; Guelachvili, G.; Ben Osman, Z.; Vergès, J. *Present Status of the Analyses of the First and Second Spectra of Uranium (U I and U II) as Derived from Measurements of Optical Spectra*; LASL Report LA-4501; Los Alamos Scientific Lab., N. Mex.: Los Alamos, NM, USA, 1971.
8. Palmer, B.A.; Keller, R.A.; Engleman, R., Jr. *An Atlas of Uranium Emission Intensities in A Hollow Cathode Discharge*; LASL Informal Report LA-8251-MS,UC-34a; Los Alamos Scientific Lab., N. Mex.: Los Alamos, NM, USA, 1980.
9. Brewer, L. Energies of the electronic configurations of the singly, doubly and triply ionized lanthanides and actinides. *J. Opt. Soc. Am.* **1971**, *12*, 1666–1682.
10. Cowan, R.D. *The Theory of Atomic Structure and Spectra*; University of California Press: Berkeley, CA, USA, 1981.
11. Kramida, A. PC Version of Cowan Codes. Available online: http://das101.isan.troitsk.ru (accessed on 21 August 2012).
12. Palmer, B.A.; Engleman, R., Jr. Wavelengths and energy levels of doubly ionized uranium obtained using a Fourier Transform spectrometer. *J. Opt. Soc. Am. B* **1984**, *1*, 609–625.
13. Blaise, J.; Wyart, J.-F.; Palmer, B.A.; Engleman, R., Jr.; Launay, F. Analysis of the spectrum of doubly ionized Uranium (U III). In *19th EGAS, Dublin: European Group for Atomic Spectroscopy: 14–17 July 1987: Abstracts*; European Physical Society: Mulhouse, France, 1987; pp. A3–08.
14. Redman, S.L.; Lawler, J.E.; Nave, G.; Ramsey, L.W.; Mahadevan, S. The infrared spectrum of Uranium Hollow athode Lamps from 850nm to 4000nm. *Astrophys. J. Supp. Ser.* **2011**, *195*, 24.
15. Wyart, J.-F.; Kaufman, V.; Sugar, J. Analysis of the Spectrum of Four-Times-Ionized Uranium (U5). *Phys. Scr.* **1980**, *22*, 389–396.
16. Kaufman, V.; Radziemski, L.F., Jr. The sixth spectrum of Uranium (UVI). *J. Opt. Soc. Am.* **1976**, *66*, 599–600.
17. Meftah, A.; Wyart, J.-F.; Tchang-Brillet, W.-Ü.L.; Blaess, C.; Champion, N. Spectrum and energy levels of the Yb^{4+} free ion (Yb V) *Phys. Scr.* **2013**, *88*, 045305.
18. Tomkins, F.S.; Fred, M. A photoelectric setting device for a spectrum plate comparator. *J. Opt. Soc. Am.* **1951**, *41*, 641.
19. Wyart, J.-F. Theoretical interpretation of the Nd II spectrum: Odd parity energy levels. *Phys. Scr.* **2010**, *82*, 035302.
20. Wyart, J.-F. On the interpretation of complex atomic spectra by means of the parametric Racah-Slater method and Cowan codes. *Can. J. Phys.* **2011**, *89*, 451.
21. Chen, H.-L.; Borzileri, C. Laser induced fluorescence studies of U II produced by photoionization of uranium. *J. Chem. Phys.* **1981**, *74*, 6063–6069.
22. Corliss, C.H. Oscillator strengths for lines of ionized uranium (U II). *J. Res. Nat. Bur. Stand. Sect. A* **1976**, *80*, 429.
23. Nilsson, H.; Ivarsson, S.; Johansson, S.; Lundberg, H. Experimental oscillator strengths in U II of cosmological interest. *Astron. Astrophys.* **2002**, *381*, 1090–1093.
24. Kurucz, R.L. Available online: http://kurucz.harvard.edu/linelists/gfnew/ (accessed on 31 March 2017).