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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  $5f^3 7s^2 + 5f^3 6d 7s + 5f^3 6d^2 + 5f^4 7p + 5f^5$  are interpreted by 24 free parameters and 64 constrained ones, with a root mean square (*rms*) deviation of  $60 \text{ cm}^{-1}$ . In the even parity, the four known configurations  $5f^4 7s, 5f^4 6d, 5f^2 6d^2 7s, 5f^2 6d 7s^2$  and the unknown  $5f^2 6d^3$  form a basis for interpreting 125 levels with a *rms* deviation of  $84 \text{ cm}^{-1}$ . Due to perturbations, the theoretical description of the higher configurations  $5f^3 7s 7p + 5f^3 6d 7p$  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  $2344\text{--}2955 \text{ Å}$ . One new level has been established as  $5f^3 6d 7p (^4I)^6K(J = 5.5)$  at  $39113.98 \pm 0.1 \text{ cm}^{-1}$ .

**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  $^{238}\text{U}$  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  $3859.572 \text{ Å}$  ( $5f^3 6d 7s ^6L_{11/2} - 5f^3 6d 7p ^6M_{13/2}$ ) 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  $5f^3 7s^2 ^4I_{9/2}$ . 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  $E_{\text{exp}}$  should lead to improved predictions of energies  $E_{\text{th}}$  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.

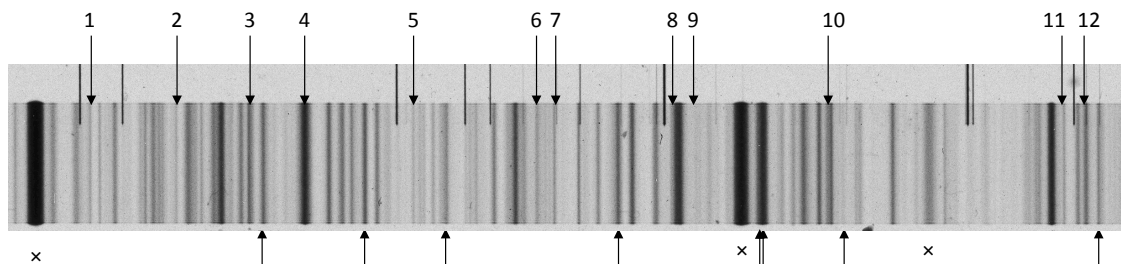
The critical compilation of energy levels and spectra of actinides published in 1992 by Blaise and Wyart [3] provided preliminary tables of energy levels of both parities in U II. The compilation of U II was based on emission data from Steinhaus et al. [7] and on new FTS measurements by Palmer et al. [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  $\pm 0.001$  and  $\pm 0.003$  Å.

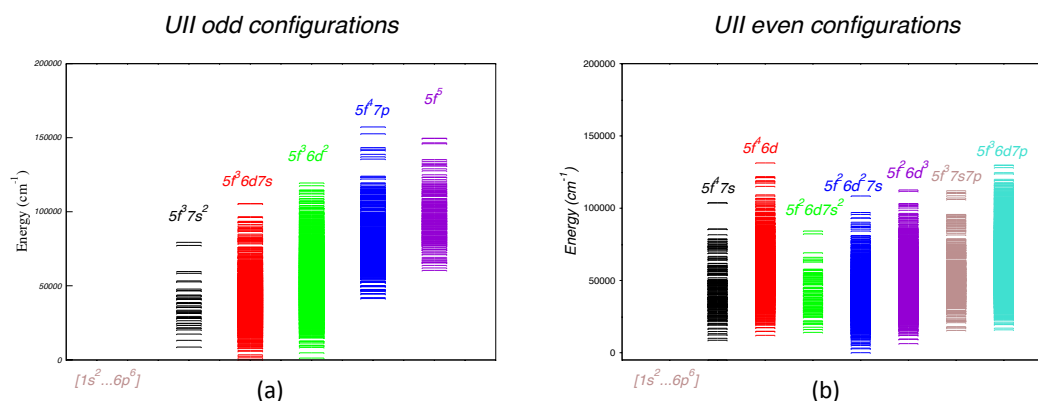
Figure 1 shows a section of the triggered spark spectrum between 2863–2875 Å. The shape of the lines, from relatively sharp (for U II) to hazy (for U IV) may be attributed to Doppler broadening as higher charged ions are produced in hotter part of the sparks. Identified U II lines are numbered. The numbers 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 5*f*, 6*d*, 7*s* and 7*p* 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  $53 \text{ cm}^{-1}$ . 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  $38000 \pm 5000 \text{ cm}^{-1}$  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 RCN2 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  $60 \text{ cm}^{-1}$ . 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  $\alpha$ ,  $\beta$  and  $\gamma$  for the  $5f^n$  core configurations and Slater forbidden parameters for  $5f^n nl$  (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  $E_{exp} = 8379.697 \text{ cm}^{-1}$  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:  $E_{exp} - E_{th} = 22 \text{ cm}^{-1}$  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  $20,000 \text{ cm}^{-1}$ , 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 available [6]. However, a few exceptions have been observed. As an example, the two  $J = 7.5$  levels at  $8394.362$  and  $8521.922 \text{ cm}^{-1}$  were previously [6] assigned respectively as  $f^3d^2 \text{ } ^6M_{15/2}$  and  $f^3ds \text{ } ^6K_{15/2}$ , 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  $8438 \text{ cm}^{-1}$ , 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  $20,000 \text{ cm}^{-1}$  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  $25,726 \text{ cm}^{-1}$  are not reported here.

At an intermediate step of the parametric fitting, the previously assigned  $J$  value,  $J = 11/2$ , of the level  $E_{exp} = 13,695.737 \text{ cm}^{-1}$  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  $13,961.850 \text{ cm}^{-1}$ , and on the other hand, one  $J = 9/2$  level was missing between  $E_{exp} = 13,450.490$  and  $14,265.976 \text{ cm}^{-1}$ . 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  $\Delta E$  value.

**Table 2.** Fitted parameters (in  $\text{cm}^{-1}$ ) 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  $\text{cm}^{-1}$ ). 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  $5f^37s^2$  taken as zero value.

| Param. $P$   | Cstr. | $5f^37s^2$ |      |           |               | $5f^36d7s$ |      |           |               | $5f^36d^2$ |      |           |               |
|--------------|-------|------------|------|-----------|---------------|------------|------|-----------|---------------|------------|------|-----------|---------------|
|              |       | $P_{fit}$  | 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         |
| $\alpha$     | r4    | 36.3       | 1    |           |               | 36.3       | 1    |           |               | 36.3       | 1    |           |               |
| $\beta$      | f     | −600       |      |           |               | −600       |      |           |               | −600       |      |           |               |
| $\gamma$     | 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         |      |           |               |
| $\zeta_f$    | r5    | 1732.4     | 4    | 1868.5    | 0.927         | 1705.7     | 4    | 1839.8    | 0.927         | 1681.2     | 4    | 1813.4    | 0.927         |
| $\zeta_d$    | 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.

| Param. $P$ | Cstr. | $5f^47p$  |      |           |               | Cstr. | $5f^5$    |      |           |               |
|------------|-------|-----------|------|-----------|---------------|-------|-----------|------|-----------|---------------|
|            |       | $P_{fit}$ | Unc. | $P_{HFR}$ | $\Delta E/SF$ |       | $P_{fit}$ | 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         |
| $\alpha$   | r4    | 37.7      | 1    |           |               |       | 36.5      | 1    |           |               |
| $\beta$    | f     | −600      |      |           |               |       | −600      |      |           |               |
| $\gamma$   | f     | 1500      |      |           |               |       | 1500      |      |           |               |
| $\zeta_f$  | r5    | 1550.4    | 4    | 1672.2    | 0.927         |       | 1333.5    | 3    | 1437.9    | 0.927         |
| $\zeta_p$  | 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 |       |           |      |           |               |
| $5f^3 7s^2 - 5f^3 6d 7s$  |       |           |      |           |               |
| $R^2(fs, fd)$             | r15   | −6614     | 71   | −10104    | 0.65          |
| $R^3(fs, df)$             | r15   | −1442     | 15   | −2204     | 0.65          |
| $5f^3 s^2 - 5f^3 d^2$     |       |           |      |           |               |
| $R^2(ss, dd)$             | r15   | 14670     | 157  | 22412     | 0.65          |
| $5f^3 7s^2 - 5f^5$        |       |           |      |           |               |
| $R^3(ss, ff)$             | r15   | 4516      | 48   | 6900      | 0.65          |
| $5f^3 6d 7s - 5f^3 6d^2$  |       |           |      |           |               |
| $R^2(fs, fd)$             | 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          |
| $5f^3 6d 7s - 5f^4 7p$    |       |           |      |           |               |
| $R^1(ds, fp)$             | r15   | −9384     | 101  | −14337    | 0.65          |
| $R^3(ds, pf)$             | r15   | −2805     | 30   | −4286     | 0.65          |
| $5f^3 6d 7s - 5f^5$       |       |           |      |           |               |
| $R^3(ds, ff)$             | r15   | −3507     | 38   | −5357     | 0.65          |
| $5f^3 6d^2 - 5f^4 7p$     |       |           |      |           |               |
| $R^1(dd, fp)$             | r15   | 5580      | 60   | 8526      | 0.66          |
| $R^3(dd, fp)$             | r15   | 2490      | 27   | 3805      | 0.66          |
| $5f^3 6d^2 - 5f^5$        |       |           |      |           |               |
| $R^1(dd, ff)$             | 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          |
| $5f^4 7p - 5f^5$          |       |           |      |           |               |
| $R^2(fp, ff)$             | 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.

| $J$ | $E^{exp}$<br>( $\text{cm}^{-1}$ ) | $E^{th}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{th}$ | $g_L^{exp}$ | % 1 <sup>st</sup> 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.

| $J$ | $E^{exp}$<br>( $\text{cm}^{-1}$ ) | $E^{th}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{th}$ | $g_L^{exp}$ | % 1 <sup>st</sup> 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.

| <i>J</i> | $E^{exp}$<br>(cm <sup>−1</sup> ) | $E^{th}$<br>(cm <sup>−1</sup> ) | $\Delta E$<br>(cm <sup>−1</sup> ) | $g_L^{th}$ | $g_L^{exp}$ | % 1 <sup>st</sup> 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.

| $J$  | $E^{exp}$<br>( $\text{cm}^{-1}$ ) | $E^{th}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{th}$ | $g_L^{exp}$ | % 1 <sup>st</sup> 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.

| $J$ | $E^{exp}$<br>( $\text{cm}^{-1}$ ) | $E^{th}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{th}$ | $g_L^{exp}$ | % 1 <sup>st</sup> 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.

| $J$ | $E^{exp}$<br>( $\text{cm}^{-1}$ ) | $E^{th}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{th}$ | $g_L^{exp}$ | % 1 <sup>st</sup> 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.

| $J$ | $E^{exp}$<br>( $\text{cm}^{-1}$ ) | $E^{th}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{th}$ | $g_L^{exp}$ | % 1 <sup>st</sup> 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.

| $J$ | $E^{exp}$<br>( $\text{cm}^{-1}$ ) | $E^{th}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{th}$ | $g_L^{exp}$ | % 1 <sup>st</sup> 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.

| $J$  | $E^{exp}$<br>( $\text{cm}^{-1}$ ) | $E^{th}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{th}$ | $g_L^{exp}$ | % 1 <sup>st</sup> comp | 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.

| $J$ | $E^{exp}$<br>( $\text{cm}^{-1}$ ) | $E^{th}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{th}$ | $g_L^{exp}$ | % 1 <sup>st</sup> 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  $13695.737 \text{ cm}^{-1}$  with  $J = 4.5$  to even levels of  $J = 3.5$ .

| $wl_{\text{Ritz}}$<br>in Air (Å) | $wn_{\text{Ritz}}$<br>( $\text{cm}^{-1}$ ) | $wn_{exp}$<br>( $\text{cm}^{-1}$ ) | $E_{even}$<br>( $\text{cm}^{-1}$ ) | $J$ | $E_{odd}$<br>( $\text{cm}^{-1}$ ) | $J$ | 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 RCN2 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  $84 \text{ cm}^{-1}$ , i.e., which is less satisfactory than in the odd parity. One of these levels, given at  $E_{exp} = 22917.453 \text{ cm}^{-1}$  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  $\zeta_{5f}$  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  $\text{cm}^{-1}$ ) 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  $\text{cm}^{-1}$ ). 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         |
| $\alpha$     | 19.5      | r4    | 2    |           |               | 19.5         | r4    | 2    |           |               |
| $\beta$      | −600      | f     |      |           |               | −600         | f     |      |           |               |
| $\gamma$     | 1600      | f     |      |           |               | 1600         | f     |      |           |               |
| $\zeta_f$    | 1557      | r5    | 9    | 1661      | 0.938         | 1529         | r5    | 9    | 1631      | 0.938         |
| $\zeta_d$    |           |       |      |           |               | 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         |
| $\alpha$     | 19.5      | r4    | 2    |           |               | 19.5         | r4    | 2    |           |               |
| $\beta$      | −600      | f     |      |           |               | −600         | f     |      |           |               |
| $\gamma$     | 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     |      |           |               |
| $\zeta_f$    | 1908      | r5    | 11   | 2036      | 0.937         | 1884         | r5    | 11   | 2010      | 0.937         |
| $\zeta_d$    | 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.

| $5f^2 6d^3$                   |           |       |       |           |               |
|-------------------------------|-----------|-------|-------|-----------|---------------|
| 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         |
| $\alpha$                      | 19.5      | r4    | 2     |           |               |
| $\beta$                       | −600      | f     |       |           |               |
| $\gamma$                      | 1600      | f     |       |           |               |
| $F^2(dd)$                     | 22416     | r13   | 1488  | 36319     | 0.617         |
| $F^4(dd)$                     | 14359     | r16   | 2926  | 24013     | 0.598         |
| $\alpha(dd)$                  | 10        | f     |       |           |               |
| $\zeta_f$                     | 1860      | r5    | 11    | 1986      | 0.937         |
| $\zeta_d$                     | 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     |           |       |       |           |               |
| $5f^4 7s - 5f^4 6d$           |           |       |       |           |               |
| $R^2(fs, fd)$                 | −6216     | r14   | 357   | −10574    | 0.588         |
| $R^3(fs, df)$                 | −1875     | r14   | 108   | −3189     | 0.588         |
| $5f^4 7s - 5f^2 6d 7s^2$      |           |       |       |           |               |
| $R^3(ff, ds)$                 | −2310     | r14   | 133   | −3930     | 0.588         |
| $5f^4 7s - 5f^2 6d^2 7s$      |           |       |       |           |               |
| $R^1(ff, dd)$                 | 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         |
| $5f^4 6d - 5f^2 6d 7s^2$      |           |       |       |           |               |
| $R^3(ff, ss)$                 | 3556      | r14   | 204   | 6050      | 0.588         |
| $5f^4 6d - 5f^2 6d^2 7s$      |           |       |       |           |               |
| $R^3(ff, ds)$                 | −2385     | r14   | 137   | −4056     | 0.588         |
| $5f^4 6d - 5f^2 6d^3$         |           |       |       |           |               |
| $R^1(ff, dd)$                 | 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         |
| $5f^2 6d 7s^2 - 5f^2 6d^2 7s$ |           |       |       |           |               |
| $R^2(fs, fd)$                 | −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         |
| $5f^2 6d 7s^2 - 5f^2 6d^3$    |           |       |       |           |               |
| $R^2(ss, dd)$                 | 13119     | r14   | 752   | 22316     | 0.588         |
| $5f^2 6d^2 7s - 5f^2 6d^3$    |           |       |       |           |               |
| $R^2(fs, fd)$                 | −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.  $\Delta E = E^{exp} - E^{th}$ . The percentage, the configuration and the *LS* name of the leading component in the corresponding configuration are given in the last three columns.

| <i>J</i> | $E^{exp}$<br>( $\text{cm}^{-1}$ ) | $E^{th}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{th}$ | $g_L^{exp}$ | % 1 <sup>st</sup> 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.

| $J$ | $E^{\text{exp}}$<br>( $\text{cm}^{-1}$ ) | $E^{\text{th}}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{\text{th}}$ | $g_L^{\text{exp}}$ | % 1 <sup>st</sup> 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.

| $J$ | $E^{\text{exp}}$<br>( $\text{cm}^{-1}$ ) | $E^{\text{th}}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{\text{th}}$ | $g_L^{\text{exp}}$ | % 1 <sup>st</sup> 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.

| $J$  | $E^{\text{exp}}$<br>( $\text{cm}^{-1}$ ) | $E^{\text{th}}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{\text{th}}$ | $g_L^{\text{exp}}$ | % 1 <sup>st</sup> 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.

| $J$ | $E^{\text{exp}}$<br>( $\text{cm}^{-1}$ ) | $E^{\text{th}}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{\text{th}}$ | $g_L^{\text{exp}}$ | % 1 <sup>st</sup> 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.

| $J$ | $E^{\text{exp}}$<br>( $\text{cm}^{-1}$ ) | $E^{\text{th}}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{\text{th}}$ | $g_L^{\text{exp}}$ | % 1 <sup>st</sup> 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  $\text{cm}^{-1}$  has a leading component belonging to the  $5f^26d7s^2$  configuration but the dominant configuration is  $5f^26d^27s$ .

**Table 7.** Adopted parameters (in  $\text{cm}^{-1}$ ) for even parity configurations  $5f^37s7p$  and  $5f^36d7p$  of U II compared with HFR radial integrals. The scaling factors are  $SF(P) = P_{\text{fit}}/P_{\text{HFR}}$ . 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  $E_{\text{av}}$  parameters are relative to the lowest even configuration  $5f^47s$  taken as zero value.

| $5f^37s7p$                |                  |       |        |                  |               | $5f^36d7p$       |       |      |                  |               |
|---------------------------|------------------|-------|--------|------------------|---------------|------------------|-------|------|------------------|---------------|
| Param. $P$                | $P_{\text{fit}}$ | Cstr. | Unc.   | $P_{\text{HFR}}$ | $\Delta E/SF$ | $P_{\text{fit}}$ | Cstr. | Unc. | $P_{\text{HFR}}$ | $\Delta E/SF$ |
| $E_{\text{av}}$           | 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         |
| $\alpha$                  | 36.5             | f     |        |                  |               | 36.5             | f     |      |                  |               |
| $\beta$                   | −600             | f     |        |                  |               | −600             | f     |      |                  |               |
| $\gamma$                  | 1500             | f     |        |                  |               | 1500             | f     |      |                  |               |
| $\zeta_f$                 | 1809             | r1    | 102    | 1875             | 0.965         | 1781             | r1    | 100  | 1846             | 0.965         |
| $\zeta_d$                 |                  |       |        |                  |               | 1624             | f     |      | 1902             | 0.854         |
| $\zeta_p$                 | 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.

| $J$ | $E^{exp}$<br>( $\text{cm}^{-1}$ ) | $E^{th}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{th}$ | $g_L^{exp}$ | % 1 <sup>st</sup> 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.

| $J$ | $E^{\text{exp}}$<br>( $\text{cm}^{-1}$ ) | $E^{\text{th}}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{\text{th}}$ | $g_L^{\text{exp}}$ | % 1 <sup>st</sup> comp | Conf         | Term    |
|-----|------------------------------------------|-----------------------------------------|------------------------------------|-------------------|--------------------|------------------------|--------------|---------|
| 2.5 |                                          | 35093                                   |                                    | 0.837             |                    | 17                     | $5f^3 7s 7p$ | (4F)4Ga |
| 3.5 |                                          | 35149                                   |                                    | 0.908             |                    | 9                      | $5f^3 7s 7p$ | (4I)6H  |
| 7.5 |                                          | 35301                                   |                                    | 1.085             |                    | 17                     | $5f^3 6d 7p$ | (4I)6I  |
| 4.5 |                                          | 35338                                   |                                    | 0.895             |                    | 10                     | $5f^3 6d 7p$ | (4I)6K  |
| 2.5 |                                          | 35498                                   |                                    | 1.074             |                    | 17                     | $5f^3 7s 7p$ | (4F)6F  |
| 6.5 |                                          | 35514                                   |                                    | 0.990             |                    | 31                     | $5f^3 6d 7p$ | (4I)6Kb |
| 7.5 |                                          | 35529                                   |                                    | 1.051             |                    | 27                     | $5f^3 6d 7p$ | (4I)6La |
| 3.5 |                                          | 35552                                   |                                    | 0.873             |                    | 12                     | $5f^3 6d 7p$ | (4I)6H  |
| 3.5 |                                          | 35666                                   |                                    | 0.834             |                    | 6                      | $5f^3 6d 7p$ | (4I)6H  |
| 4.5 |                                          | 35696                                   |                                    | 0.811             |                    | 13                     | $5f^3 6d 7p$ | (4I)6H  |
| 5.5 |                                          | 35744                                   |                                    | 0.966             |                    | 19                     | $5f^3 7s 7p$ | (4I)2I  |
| 4.5 |                                          | 35780                                   |                                    | 0.867             |                    | 11                     | $5f^3 6d 7p$ | (4I)4Ia |
| 5.5 |                                          | 35804                                   |                                    | 0.901             |                    | 14                     | $5f^3 6d 7p$ | (4I)4Ke |
| 6.5 |                                          | 35809                                   |                                    | 1.064             |                    | 30                     | $5f^3 7s 7p$ | (4I)2K  |
| 7.5 |                                          | 35892                                   |                                    | 1.196             |                    | 34                     | $5f^3 7s 7p$ | (4I)6H  |
| 3.5 |                                          | 35906                                   |                                    | 1.009             |                    | 9                      | $5f^3 6d 7p$ | (4F)6G  |
| 5.5 |                                          | 35985                                   |                                    | 0.961             |                    | 13                     | $5f^3 6d 7p$ | (4I)6Ka |
| 1.5 |                                          | 36046                                   |                                    | 0.867             |                    | 14                     | $5f^3 7s 7p$ | (4F)6F  |
| 3.5 |                                          | 36064                                   |                                    | 1.089             |                    | 10                     | $5f^3 7s 7p$ | (4F)6D  |
| 4.5 |                                          | 36137                                   |                                    | 0.865             |                    | 10                     | $5f^3 6d 7p$ | (4I)6Ib |
| 2.5 |                                          | 36149                                   |                                    | 1.444             |                    | 33                     | $5f^3 7s 7p$ | (4S)6P  |
| 8.5 |                                          | 36364                                   |                                    | 1.210             |                    | 31                     | $5f^3 7s 7p$ | (4I)6I  |
| 7.5 |                                          | 36389                                   |                                    | 1.059             |                    | 29                     | $5f^3 6d 7p$ | (4I)6Lb |
| 6.5 |                                          | 36410                                   |                                    | 1.019             |                    | 14                     | $5f^3 6d 7p$ | (4I)6I  |
| 2.5 |                                          | 36417                                   |                                    | 0.607             |                    | 17                     | $5f^3 6d 7p$ | (4F)6Ha |
| 1.5 |                                          | 36462                                   |                                    | 1.200             |                    | 14                     | $5f^3 7s 7p$ | (4S)2P  |
| 5.5 |                                          | 36516                                   |                                    | 0.934             |                    | 39                     | $5f^3 6d 7p$ | (4I)6Ka |
| 0.5 |                                          | 36680                                   |                                    | 1.812             |                    | 15                     | $5f^3 6d 7p$ | (4S)4Pa |
| 3.5 |                                          | 36721                                   |                                    | 0.935             |                    | 9                      | $5f^3 7s 7p$ | (4F)6I  |
| 4.5 |                                          | 36849                                   |                                    | 0.904             |                    | 18                     | $5f^3 6d 7p$ | (4I)4Hf |
| 2.5 |                                          | 36946                                   |                                    | 1.020             |                    | 5                      | $5f^3 6d 7p$ | (4F)4Fa |
| 4.5 |                                          | 37004                                   |                                    | 1.163             |                    | 34                     | $5f^3 7s 7p$ | (4F)6G  |
| 3.5 |                                          | 37008                                   |                                    | 0.949             |                    | 10                     | $5f^3 6d 7p$ | (4I)6Ia |
| 1.5 |                                          | 37053                                   |                                    | 0.995             |                    | 12                     | $5f^3 6d 7p$ | (4I)6Ga |
| 0.5 |                                          | 37112                                   |                                    | 2.063             |                    | 27                     | $5f^3 7s 7p$ | (4F)6D  |
| 2.5 |                                          | 37313                                   |                                    | 0.864             |                    | 6                      | $5f^3 6d 7p$ | (4I)6Ga |
| 3.5 |                                          | 37369                                   |                                    | 0.935             |                    | 16                     | $5f^3 7s 7p$ | (4G)6H  |
| 2.5 |                                          | 37477                                   |                                    | 0.897             |                    | 13                     | $5f^3 6d 7p$ | (4G)6H  |
| 1.5 |                                          | 37537                                   |                                    | 0.695             |                    | 14                     | $5f^3 6d 7p$ | (4F)4Ff |
| 7.5 |                                          | 37620                                   |                                    | 1.065             |                    | 13                     | $5f^3 7s 7p$ | (4I)4Ka |
| 6.5 |                                          | 37789                                   |                                    | 1.127             |                    | 26                     | $5f^3 7s 7p$ | (4I)4Ha |
| 3.5 |                                          | 37822                                   |                                    | 0.986             |                    | 8                      | $5f^3 7s 7p$ | (4F)4Ga |
| 1.5 |                                          | 37855                                   |                                    | 1.172             |                    | 15                     | $5f^3 6d 7p$ | (4F)6F  |
| 5.5 |                                          | 37879                                   |                                    | 0.929             |                    | 11                     | $5f^3 6d 7p$ | (4I)6Kb |
| 7.5 |                                          | 37917                                   |                                    | 0.996             |                    | 18                     | $5f^3 6d 7p$ | (4I)4Mb |
| 2.5 |                                          | 37960                                   |                                    | 0.861             |                    | 9                      | $5f^3 6d 7p$ | (4G)6H  |
| 8.5 | 37308.326                                | 37991                                   | −683                               | 1.062             | 1.070              | 18                     | $5f^3 6d 7p$ | (4I)6M  |
| 4.5 |                                          | 38040                                   |                                    | 0.895             |                    | 18                     | $5f^3 6d 7p$ | (4I)6I  |
| 3.5 |                                          | 38063                                   |                                    | 0.821             |                    | 10                     | $5f^3 6d 7p$ | (4F)6I  |
| 1.5 |                                          | 38080                                   |                                    | 0.578             |                    | 23                     | $5f^3 6d 7p$ | (4G)6G  |
| 6.5 |                                          | 38156                                   |                                    | 0.931             |                    | 15                     | $5f^3 6d 7p$ | (4I)4Ld |
| 5.5 |                                          | 38183                                   |                                    | 0.896             |                    | 13                     | $5f^3 6d 7p$ | (4I)6K  |
| 4.5 |                                          | 38205                                   |                                    | 0.863             |                    | 12                     | $5f^3 6d 7p$ | (4I)6I  |
| 2.5 |                                          | 38217                                   |                                    | 0.816             |                    | 9                      | $5f^3 6d 7p$ | (4I)6Hb |
| 0.5 |                                          | 38228                                   |                                    | 2.117             |                    | 26                     | $5f^3 7s 7p$ | (4F)6D  |

Table 8. Cont.

| $J$ | $E^{\text{exp}}$<br>( $\text{cm}^{-1}$ ) | $E^{\text{th}}$<br>( $\text{cm}^{-1}$ ) | $\Delta E$<br>( $\text{cm}^{-1}$ ) | $g_L^{\text{th}}$ | $g_L^{\text{exp}}$ | % 1 <sup>st</sup> comp | Conf         | Term    |
|-----|------------------------------------------|-----------------------------------------|------------------------------------|-------------------|--------------------|------------------------|--------------|---------|
| 3.5 |                                          | 38436                                   |                                    | 0.941             |                    | 9                      | $5f^3 6d 7p$ | (4F)4Hd |
| 2.5 |                                          | 38452                                   |                                    | 0.879             |                    | 17                     | $5f^3 7s 7p$ | (4G)2F  |
| 7.5 |                                          | 38497                                   |                                    | 1.029             |                    | 25                     | $5f^3 6d 7p$ | (4I)4Lc |
| 2.5 |                                          | 38554                                   |                                    | 0.760             |                    | 11                     | $5f^3 6d 7p$ | (4I)6Gb |
| 4.5 |                                          | 38630                                   |                                    | 1.028             |                    | 10                     | $5f^3 6d 7p$ | (4G)6H  |
| 6.5 |                                          | 38721                                   |                                    | 0.974             |                    | 15                     | $5f^3 6d 7p$ | (4I)6Kb |
| 1.5 |                                          | 38794                                   |                                    | 1.134             |                    | 8                      | $5f^3 6d 7p$ | (4F)6D  |
| 5.5 |                                          | 38809                                   |                                    | 0.916             |                    | 22                     | $5f^3 6d 7p$ | (4I)6K  |
| 8.5 |                                          | 38835                                   |                                    | 1.187             |                    | 29                     | $5f^3 7s 7p$ | (4I)6K  |
| 2.5 |                                          | 38916                                   |                                    | 1.074             |                    | 12                     | $5f^3 6d 7p$ | (4F)6F  |
| 4.5 |                                          | 38931                                   |                                    | 1.064             |                    | 7                      | $5f^3 6d 7p$ | (4I)6I  |
| 4.5 |                                          | 38975                                   |                                    | 0.830             |                    | 20                     | $5f^3 6d 7p$ | (4G)6K  |
| 3.5 |                                          | 38993                                   |                                    | 0.936             |                    | 8                      | $5f^3 7s 7p$ | (4I)4Ha |
| 2.5 |                                          | 39000                                   |                                    | 0.891             |                    | 14                     | $5f^3 7s 7p$ | (4G)6G  |
| 1.5 |                                          | 39006                                   |                                    | 0.407             |                    | 30                     | $5f^3 6d 7p$ | (4I)6Gb |
| 9.5 | 39809.365                                | 39050                                   | 758                                | 1.111             | 1.105              | 48                     | $5f^3 6d 7p$ | (4I)6M  |
| 5.5 |                                          | 39065                                   |                                    | 1.092             |                    | 5                      | $5f^3 6d 7p$ | (4I)6Kb |
| 6.5 |                                          | 39122                                   |                                    | 1.038             |                    | 14                     | $5f^3 6d 7p$ | (4I)6Ka |
| 4.5 |                                          | 39161                                   |                                    | 1.136             |                    | 14                     | $5f^3 6d 7p$ | (4F)6D  |

### 3.3. Partition Function

To get an idea of how semi-empirical parametric calculations could influence the value of the partition function  $Q(T) = \sum_i (2J_i + 1) \exp(-E_i/k_B T)$  ( $k_B$ : Boltzmann constant), we made an estimation of the partition function of U II for a typical stellar temperature. The temperature chosen is 4825 K ( $k_B T = 3353.54 \text{ cm}^{-1}$ ), 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  $46\,000 \text{ cm}^{-1}$  of both parities. The result is:  $Q_{\text{exp/LSF}}(T) = 122.99$ , 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:  $Q_{\text{LSF}}(T) = 120.99$ , which agrees with  $Q_{\text{exp/LSF}}(T)$  within 2%. When *ab initio* HFR energy values are used, we have  $Q_{\text{HFR}}(T) = 89.19$ , 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  $2.8 \times 10^8 \text{ s}^{-1}$ , to be compared with previous measurement  $1.1 \times 10^8 \text{ s}^{-1}$  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  $26191 \text{ cm}^{-1}$  to find a  $gIf$  value of 0.856 for the oscillator strength weighted by the lower level degeneracy. The corresponding  $gA$  value (Equation (1) of [23]) is  $3.8 \times 10^8 \text{ s}^{-1}$  in agreement with the

value of  $3.5 \times 10^8 \text{ s}^{-1}$  calculated by Kurucz [24]. Our calculations lead to  $gA = 1.53 \times 10^9 \text{ s}^{-1}$ , four times larger, but they confirm the order of magnitude. However, the parametric study for the high even levels of  $5f^3 7s 7p + 5f^3 6d 7p$  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  $\pm 0.003 \text{ \AA}$ . Thus the corresponding uncertainty on wave numbers should be less than  $\pm 0.05 \text{ cm}^{-1}$ . To take into account any possible perturbations in the spark spectrum, we chose a tolerance of  $\pm 0.1 \text{ cm}^{-1}$  for a criterion of identification. Indeed, according to [14], the level energies in [6], therefore the Ritz wave numbers, have negligible uncertainties of about  $\pm 0.01 \text{ cm}^{-1}$ . 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  $5f^3 6d 7p$  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  $5f^3 6d 7p (^4I)^6K$  with  $J = 5.5$  at  $39113.98 \pm 0.1 \text{ cm}^{-1}$ . Table 10 lists the six transitions that establish this level.

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

| $wl_{\text{Ritz}}$<br>in Å | $wl_{\text{exp}}$<br>in Å | Int | Note | $wn_{\text{exp}}$<br>( $\text{cm}^{-1}$ ) | $\Delta wl$<br>(Å) | $\Delta wn$<br>( $\text{cm}^{-1}$ ) | $E_{\text{odd}}$<br>( $\text{cm}^{-1}$ ) | $J_{\text{odd}}$ | $E_{\text{even}}$<br>( $\text{cm}^{-1}$ ) | $J_{\text{even}}$ |
|----------------------------|---------------------------|-----|------|-------------------------------------------|--------------------|-------------------------------------|------------------------------------------|------------------|-------------------------------------------|-------------------|
| 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.

| $wl_{Ritz}$<br>in Air (Å) | $wl_{exp}$<br>in Air (Å) | <i>Int</i> | <i>Note</i> | $wl_{exp}$<br>(cm <sup>−1</sup> ) | $\Delta wl$<br>(Å) | $\Delta wn$<br>(cm <sup>−1</sup> ) | $E_{odd}$<br>(cm <sup>−1</sup> ) | <i>J</i> <sub>odd</sub> | <i>Even</i><br>(cm <sup>−1</sup> ) | <i>J</i> <sub>even</sub> |
|---------------------------|--------------------------|------------|-------------|-----------------------------------|--------------------|------------------------------------|----------------------------------|-------------------------|------------------------------------|--------------------------|
| 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.

| $wl_{\text{Ritz}}$<br>in Air (Å) | $wl_{\text{exp}}$<br>in Air (Å) | Int | Note  | $wl_{\text{exp}}$<br>(cm <sup>-1</sup> ) | $\Delta wl$<br>(Å) | $\Delta wn$<br>(cm <sup>-1</sup> ) | $E_{\text{odd}}$<br>(cm <sup>-1</sup> ) | $J_{\text{odd}}$ | Even<br>(cm <sup>-1</sup> ) | $J_{\text{even}}$ |
|----------------------------------|---------------------------------|-----|-------|------------------------------------------|--------------------|------------------------------------|-----------------------------------------|------------------|-----------------------------|-------------------|
| 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  |       | 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.

| $wl_{Ritz}$<br>in Air (Å) | $wl_{exp}$<br>in Air (Å) | <i>Int</i> | <i>Note</i> | $wl_{exp}$<br>(cm <sup>−1</sup> ) | $\Delta wl$<br>(Å) | $\Delta wn$<br>(cm <sup>−1</sup> ) | $E_{odd}$<br>(cm <sup>−1</sup> ) | <i>J</i> <sub>odd</sub> | $E_{even}$<br>(cm <sup>−1</sup> ) | <i>J</i> <sub>even</sub> |
|---------------------------|--------------------------|------------|-------------|-----------------------------------|--------------------|------------------------------------|----------------------------------|-------------------------|-----------------------------------|--------------------------|
| 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.

| $wl_{Ritz}$<br>in Air (Å) | $wl_{exp}$<br>in Air (Å) | $Int$ | $Note$ | $w_{nexp}$<br>( $cm^{-1}$ ) | $\Delta wl$<br>(Å) | $\Delta wn$<br>( $cm^{-1}$ ) | $E_{odd}$<br>( $cm^{-1}$ ) | $J_{odd}$ | $E_{even}$<br>( $cm^{-1}$ ) | $J_{even}$ |
|---------------------------|--------------------------|-------|--------|-----------------------------|--------------------|------------------------------|----------------------------|-----------|-----------------------------|------------|
| 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.

| $wl_{Ritz}$<br>in Air (Å) | $wl_{exp}$<br>in Air (Å) | <i>Int</i> | <i>Note</i> | $wl_{exp}$<br>(cm <sup>−1</sup> ) | $\Delta wl$<br>(Å) | $\Delta wn$<br>(cm <sup>−1</sup> ) | $E_{odd}$<br>(cm <sup>−1</sup> ) | $J_{odd}$ | $E_{even}$<br>(cm <sup>−1</sup> ) | $J_{even}$ |
|---------------------------|--------------------------|------------|-------------|-----------------------------------|--------------------|------------------------------------|----------------------------------|-----------|-----------------------------------|------------|
| 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.

| $wl_{Ritz}$<br>in Air (Å) | $wl_{exp}$<br>in Air (Å) | Int | Note | $wn_{exp}$<br>(cm <sup>-1</sup> ) | $\Delta wl$<br>(Å) | $\Delta wn$<br>(cm <sup>-1</sup> ) | $E_{odd}$<br>(cm <sup>-1</sup> ) | $J_{odd}$ | $E_{even}$<br>(cm <sup>-1</sup> ) | $J_{even}$ |
|---------------------------|--------------------------|-----|------|-----------------------------------|--------------------|------------------------------------|----------------------------------|-----------|-----------------------------------|------------|
| 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                         | 7.5        |
| 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  $5f^3 6d 7p$  ( $^4I$ ) $^6K(J = 5.5)$  of the  $U^+$  ion at  $39113.98 \pm 0.1 \text{ cm}^{-1}$ . In  $\log(g_L f)$ ,  $f$  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].

| $E_{th}$<br>( $\text{cm}^{-1}$ ) | $J$ | Odd Level            | $wn_{th}$<br>( $\text{cm}^{-1}$ ) | $\log(g_L f)$ | $gA$<br>( $\text{s}^{-1}$ ) | $CF$  | $E_{exp}$<br>( $\text{cm}^{-1}$ ) | $wn_{exp}$<br>( $\text{cm}^{-1}$ ) | $\lambda_{exp}$<br>in Air ( $\text{\AA}$ ) | $Int_{exp}$<br>(arb.) |
|----------------------------------|-----|----------------------|-----------------------------------|---------------|-----------------------------|-------|-----------------------------------|------------------------------------|--------------------------------------------|-----------------------|
| −56.8                            | 4.5 | $5f^3 7s^2$ (4I) 4I  | 38865.8                           | 0.263         | $1.847\text{E}+09$          | 0.63  | 0.000                             | 39114.382                          | 2555.8378                                  | 545                   |
| 224.4                            | 5.5 | $5f^3 6d 7s$ (4I) 6L | 38584.6                           | −1.518        | $3.014\text{E}+07$          | 0.03  | 289.041                           | 38824.783                          | 2574.9033                                  | 4                     |
| 1715.5                           | 6.5 | $5f^3 6d 7s$ (4I) 6L | 37093.5                           | 0.181         | $1.391\text{E}+09$          | −0.27 | 1749.123                          | 37364.867                          | 2675.5157                                  | 228                   |
| 2320.7                           | 5.5 | $5f^3 6d 7s$ (4I) 6K | 36488.3                           | −0.252        | $4.974\text{E}+08$          | −0.21 | 2294.696                          | 36819.292                          | 2715.1628                                  | 36                    |
| 4406.4                           | 5.5 | $5f^3 7s^2$ (4I) 4I  | 34402.6                           | −0.877        | $1.048\text{E}+08$          | 0.20  | 4420.871                          | 34692.797                          | 2881.5973                                  | 14                    |
| 4577.9                           | 6.5 | $5f^3 6d 7s$ (4I) 6L | 34231.1                           | −0.160        | $5.404\text{E}+08$          | −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  $5f^3 6d 7p$ .

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