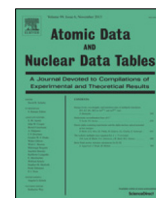




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# Multiconfiguration Dirac–Hartree–Fock energy levels, weighted oscillator strengths, transitions probabilities, lifetimes, hyperfine constants, Landé $g$ -factors and isotope shifts of Xe *LIII*

Dhia Elhak Salhi<sup>a,b,c</sup>, Pascal Quinet<sup>d,e</sup>, Haikel Jelassi<sup>a,b,\*</sup><sup>a</sup> Laboratory on Energy and Matter for Nuclear Sciences Development, LR16CNS TN 02, Tunisia<sup>b</sup> National Centre for Nuclear Sciences and Technologies, Sidi Thabet Technopark, 2020 Ariana, Tunisia<sup>c</sup> Faculty of Sciences of Tunis, University Tunis El Manar Tunis, Tunisia<sup>d</sup> Physique Atomique et Astrophysique, Université de Mons, 7000 Mons, Belgium<sup>e</sup> IPNAS, Université de Liège, 4000 Liège, Belgium

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## ABSTRACT

Energy levels, weighted oscillator strengths and transition probabilities, lifetimes, hyperfine interaction constants, Landé  $g$  factors and isotope shifts are calculated for all levels of  $1s^2$  and  $1snl$  ( $n = 2 - 7$ ) configurations of He-like xenon ion (Xe *LIII*). Multiconfigurational Dirac–Hartree–Fock (MCDHF) method is adopted for calculating these spectroscopic data. Comparisons are made with similar data obtained with FAC (Flexible Atomic Code) to assess the accuracy of the results. Transition probabilities are reported for all  $E1$ ,  $E2$ ,  $M1$  and  $M2$  transitions from the ground level. Breit interactions and quantum electrodynamics effects are estimated in extensive Relativistic Configuration Interaction (RCI) calculations. Comparisons were made with the available data in the literature and good agreement was found which confirms the reliability of our results. The accuracy of the present calculations is high enough to facilitate identification of many observed spectral lines. Almost all atomic data of He-like xenon ion presented in this paper are calculated for the first time.

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\* Correspondence to: National Centre for Nuclear Sciences and Technologies, Sidi Thabet Technopark, 2020 Ariana, Tunisia.  
E-mail address: [haikel.jelassi@cnstn.rnrt.tn](mailto:haikel.jelassi@cnstn.rnrt.tn) (H. Jelassi).

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## 1. Introduction

In recent years, there have been extensive spectroscopic studies, both experimental and theoretical, of helium isoelectronic sequence. An analysis of the spectra of solar, stellar and other astrophysical plasmas by many space missions, such as SOHO, Chandra and XMM Newton shows the presence of highly ionized atoms [1]. In addition, they are injected as impurities into tokamak plasmas [2,3]. In particular, high  $Z$  elements of the fifth period are being increasingly used as injected impurities for tokamak fusion plasmas. Also, the inert gas atoms show a significant importance in the diagnostics of laboratory plasmas. Furthermore, atomic data (namely energy levels, weighted oscillator strengths, radiative rates, lifetimes, hyperfine structure and Landé  $g_j$  factors and isotope shifts) are required for many ions in order to estimate the power loss from the impurities in the forthcoming fusion reactors, such as ITER project [4].

In the last few years, various theoretical and experimental research for providing atomic data for He-like ions have been carried out. But for He-like Xe, a limited number of studies has been carried out for providing atomic data for higher levels. In a recent review, Saloman [5] has listed energy levels for many ions of xenon, but unfortunately there is a paucity of data for this ion of interest.

These data are available at the National Institute of Standards and Technology (NIST) [6] database. Energy levels were calculated for the ground state and  $n = 2$  singlet states of heliumlike ions with nuclear charges in the range  $4 \leq Z \leq 92$  by Cheng et al. [7]. Plante et al. [8] performed relativistic all-order many-body calculations on the He-isoelectronic sequence in the range  $Z = 5-100$  and included Breit energy and other higher order correction terms in their calculations. Drake [9] carried out extensive two-electron quantum electrodynamics (QED) calculations using a unified method. Indelicato [10] adopted the multi-configuration Dirac-Fock (MCDHF) formalism to study the properties of He-like ions. Recently, energies and rates from  $2s3p-1s2s$  transitions were calculated for 23 ions (He-like) in the range  $Z = 14-54$  using multi-configuration Dirac-Fock wave functions by L. Natarajan et al. [11].

For correct interpretation of the experimentally observed spectra in the stellar and laboratory induced high-temperature plasmas, accurate theoretical data regarding the atomic transitions of highly ionized atoms are needed [12].

As previously published [13-15], we continue to focus on He-like ions. We report in this work the hereabove mentioned parameters for a comparatively larger number of levels/transitions by performing a large-scale multiconfiguration Dirac-Hartree-Fock

(MCDHF) [16] method to calculate the 97 lowest fine-structure levels for Xe *LIII*, in an effort to offer complete and consistent data sets of high accuracy. The calculations have been divided into two main groups, with even and odd parity. Also, wavelengths, weighted oscillator strengths, transition probabilities for the *E1*, *E2*, *M1* and *M2* radiations have been computed. Accurate interpretation of stellar spectra requires the knowledge not only of weighted oscillator strengths, but also of isotope shifts and hyperfine structures, since they cause an asymmetry and splitting of atomic transitions. So, hyperfine structures, Landé  $g_j$  factors and isotope shifts are also presented in this work.

We employ the FAC code [17] to compare some of these atomic data. The present MCDHF and FAC results are compared with each other and previous experimental and theoretical results, where available.

The configurations  $1s^2$  and  $1snl$  ( $n = 2-7, l \leq n-1$ ) are included in this calculation. Breit interactions and quantum electrodynamic (QED) effects have been added. This computational approach enables us to present a consistent and improved data set of all important transitions of the Xe *LIII* spectrum, which are useful for identifying transition lines in further investigations.

## 2. Theoretical method

### 2.1. MCDHF/RCI approach

Our calculations are performed by means of two numerical Codes. First, we employ the GRASP2K code. This is a fully relativistic code based on the Multiconfiguration Dirac–Hartree–Fock (MCDHF) method in *jj*-coupling. This method is fully described in detail by Grant [18]. Therefore, we only introduce the essential features here.

The atom is represented by an atomic state functions (ASF), which is a linear combination of configuration state functions (CSFs),

$$\psi(\gamma PJM) = \sum_{j=1}^{N_{CSF}} c_j \Phi(\gamma_j PJM), \quad (1)$$

where  $c_j$  are the mixing coefficients for the configuration  $j$ ,  $J$  and  $M$  are the angular quantum numbers and  $P$  is the parity. The label  $\gamma_j$  denotes appropriate information about the configuration state function  $j$ , such as parity, orbital occupancy and angular coupling scheme.

For the CSF, as  $\Phi(\gamma_j PJM)$ , it is an antisymmetrized linear combination of products of relativistic orbitals. One relativistic orbital can be expressed as,

$$\Phi(r) = \frac{1}{r} \begin{pmatrix} P_{n\kappa}(r) & \chi_{\kappa m}(r) \\ iQ_{n\kappa}(r) & \chi_{-\kappa m}(r) \end{pmatrix}, \quad (2)$$

where  $\kappa$  is the relativistic spherical symmetry quantum number,  $m$  is the magnetic quantum number,  $n$  is the principal quantum number,  $P_{n\kappa}(r)$  and  $Q_{n\kappa}(r)$  are the large and small component radial wavefunctions, and  $\chi_{\kappa m}(r)$  is the spinor spherical harmonic in the *lsj* coupling scheme.

These relativistic orbitals can be generated by using an appropriate Hamiltonian. In our MCDHF calculations, the Dirac–Coulomb Hamiltonian can be described as,

$$H_{DC} = \sum_{i=1}^N (c\alpha_i \cdot \mathbf{p}_i + (\beta_i - 1)c^2 + V(r_i)) + \sum_{i>j}^N \frac{1}{r_{ij}}, \quad (3)$$

where  $V(r_i)$  is the nuclear potential at radius  $r$ ,  $\alpha$  and  $\beta$  are the  $4 \times 4$  Dirac matrices,  $\mathbf{p}_i$  is the momentum operator of the electron  $i$  and  $c$  is the speed of light in atomic units. The first term describes the electron kinetic energy and the electron–nucleus interaction, and

the second term is the two-body Coulomb interactions between the electrons.

Once a set of radial orbitals like  $P_{n\kappa}(r)$  and  $Q_{n\kappa}(r)$  has been obtained by self-consistent field procedure, they are used to determine the expansion coefficients of the CSFs by diagonalizing the Hamiltonian matrix.

The transverse interaction in the low-frequency limit, or the Breit interaction [19],

$$H_{Breit} = - \sum_{i<j}^N \frac{1}{2r_{ij}} \left[ \alpha_i \cdot \alpha_j + \frac{(\alpha_i \cdot r_{ij})(\alpha_j \cdot r_{ij})}{r_{ij}^2} \right], \quad (4)$$

and leading quantum electrodynamic (QED) effects (vacuum polarization and self-energy) have been included in subsequent configuration interaction (RCI) calculations, where optimization is on a weighted sum of energies. At the end, a transformation from *jj*- to *LS*-coupling [20] can be done for practical purposes.

### 2.2. Transition parameters

Transition parameters, such as transition rates or weighted oscillator strengths, between two states  $\gamma PJ$  and  $\gamma' P' J'$  can be described in terms of the reduced transition matrix element,

$$\langle \psi(\gamma PJ) \| Q_k^{(\lambda)} \| \psi(\gamma' P' J') \rangle, \quad (5)$$

where  $Q_k^{(\lambda)}$  is the electromagnetic multipole operator of order  $k$  in Coulomb or Babushkin gauges [21]. The superscript designates the type of multipole:  $\lambda = 1$  for electric multipoles and  $\lambda = 0$  for magnetic multipoles. In cases where the wave functions of the two states  $\gamma' P' J'$  and  $\gamma PJ$  have been separately determined, the radial orbitals are not orthogonal. To deal with this complication, a transformation to a biorthonormal orbital basis was applied [22]. In the new representation, the evaluation of the matrix element has been done using standard Racah algebra techniques.

In order to ensure a rigorous accuracy assessment of results of energy levels and transition probabilities, we have performed another calculation with the widely used FAC code of Gu [17]. It is also a fully relativistic code which has higher efficiency. It enables user to carry out large-scale computations and allows finding various atomic parameters. It uses a modified Dirac–Fock–Slater central-field potential that includes an approximate treatment of the exchange interaction.

### 2.3. Hyperfine structure and Landé $g_j$ factors

The hyperfine interaction is caused by the interaction between the electrons and the electromagnetic multipole moments of the nucleus, and its Hamiltonian can be represented using the spherical tensor operators  $\mathbf{T}^{(k)}$  and  $\mathbf{M}^{(k)}$  [23],

$$H_{\text{hfs}} = \sum_{k \geq 1} \mathbf{T}^{(k)} \cdot \mathbf{M}^{(k)}. \quad (6)$$

Here,  $k = 1$  and  $k = 2$  represent the magnetic dipole and electric quadrupole interactions, respectively. For a  $N$ -electron atom, the electronic tensor operators  $\mathbf{T}^{(1)}$  and  $\mathbf{T}^{(2)}$  are the sums of the one-electron operators  $t^{(k)}$ ,

$$\mathbf{T}^{(1)} = \sum_{j=1}^N \mathbf{t}^{(1)}(j) = \sum_{j=1}^N -i\alpha \left( \alpha_j \cdot \mathbf{l}_j \mathbf{c}^{(1)}(j) \right) r_j^{-2} \quad (7)$$

and

$$\mathbf{T}^{(2)} = \sum_{j=1}^N \mathbf{t}^{(2)}(j) = \sum_{j=1}^N -\mathbf{c}^{(2)}(j) r_j^{-3}. \quad (8)$$

Here,  $i$  is the imaginary unit,  $\alpha$  is the fine-structure constant,  $\mathbf{C}^{(1)}$  and  $\mathbf{C}^{(2)}$  are spherical tensor operators, and  $\mathbf{L}$  is the orbital angular momentum operator. The nuclear tensor operators  $\mathbf{M}^{(1)}$  and  $\mathbf{M}^{(2)}$  are related to magnetic dipole moment  $\mu_I$  and electronic quadrupole moment  $Q_I$  of the nucleus with spin  $I$  through [24]

$$\mu_I = \langle IM_I(=I) | \mathbf{M}_0^{(1)} | IM_I(=I) \rangle \quad (9)$$

and

$$Q_I = \langle IM_I(=I) | \mathbf{M}_0^{(2)} | IM_I(=I) \rangle. \quad (10)$$

The nuclear magnetic dipole moments  $\mu_I$  and the nuclear quadrupole moments  $Q_I$  for the different isotopes have been taken from a compilation by Stone [25].

According to perturbation theory, the magnetic dipole and the electric quadrupole  $A_J$  and  $B_J$  are [24]

$$A_J = \frac{\mu_I}{I} \frac{1}{[J(J+1)]^{1/2}} \langle \Psi(PJ) | \mathbf{T}^{(1)} | \Psi(PJ) \rangle \quad (11)$$

and

$$B_J = 2Q \left[ \frac{J(2J-1)}{(J+1)(2J+3)} \right]^{1/2} \langle \Psi(PJ) | \mathbf{T}^{(2)} | \Psi(PJ) \rangle. \quad (12)$$

The Landé  $g_j$  factors are given by

$$g_j = \frac{2}{\sqrt{J(J+1)}} \langle \gamma J | \sum_{j=1}^N -i \frac{\sqrt{2}}{2\alpha^2} r_j (\alpha_j \mathbf{C}_j^{(1)})^{(1)} + \frac{g_s - 2}{2} \beta_j \Sigma_j | \gamma J \rangle, \quad (13)$$

where  $i$  is the imaginary unit,  $\Sigma$  the relativistic spin-matrix and  $g_s = 2.00232$  the  $g$ -factor of the electron spin corrected for QED effects. The Landé  $g_j$  factors determine the splitting of magnetic sub-levels in external magnetic fields. In addition they give information about the coupling conditions in the system [26].

#### 2.4. Isotope shift

The isotope shift (IS) for an atomic energy level is composed of the field shift (FS) and the mass shift (MS). The field shift, arising from the difference in the charge distribution between two isotopes with mass number  $A$  and  $A'$  ( $A > A'$ ), is given in the approximation of the first-order perturbation theory by [27,28]

$$\Delta E_{FS}^{A,A'} = \langle \Psi(PJM) | \sum_i \delta V_i^{N,AA'} | \Psi(PJM) \rangle. \quad (14)$$

Here,  $\delta V^{N,AA'} = V^{N,A} - V^{N,A'}$  and the nuclear potential  $V^N$  for each isotope is produced by a two-parameter Fermi nuclear model [29,30]. Neglecting the higher-order nuclear moments [31], Eq. (14) is further simplified to

$$\Delta E_{FS}^{A,A'} = F \delta \langle r^2 \rangle^{A,A'}, \quad (15)$$

where

$$F_k = \frac{2\pi}{3} \left( \frac{Ze^2}{4\pi\epsilon_0} \right) \Delta |\Psi(\mathbf{0})|_k^2 \quad (16)$$

is the field-shift factor proportional to the total electron probability density at the origin between the levels  $l$  and  $u$ ,

$$\Delta |\Psi(\mathbf{0})|_k^2 = \Delta \rho_k^e(0) = \rho_u^e(0) - \rho_l^e(0) \quad (17)$$

and  $\delta \langle r^2 \rangle^{A,A'}$  is the difference of the nuclear charge mean square radius between these two isotopes.

The mass shift between two isotopes  $A$  and  $A'$ , caused by the motion of nucleus with the finite mass, is expressed as [32,33]

$$\Delta E_{MS}^{A,A'} = \frac{M' - M}{MM'} K_{MS}. \quad (18)$$

Here,  $M$  and  $M'$  are the nuclear masses for isotopes  $A$  and  $A'$ , respectively. The electronic factor  $K_{MS}$  is defined by

$$\frac{K_{MS}}{M} \equiv \langle \Psi(PJM) | H_{MS} | \Psi(PJM) \rangle, \quad (19)$$

where

$$H_{MS} = \frac{1}{2M} \sum_{i,j} \mathbf{p}_i \cdot \mathbf{p}_j. \quad (20)$$

The mass shift operator (Eq. (20)) can be split into two parts, that is, the one-body and the two-body mass shift operators

$$H_{NMS} = \frac{1}{2M} \sum_i p_i^2 \quad (21)$$

$$H_{SMS} = \frac{1}{2M} \sum_{i \neq j} \mathbf{p}_i \cdot \mathbf{p}_j, \quad (22)$$

which are also called the normal mass shift (NMS) and the specific mass shift (SMS) operator, respectively.

### 3. Method of calculations

The MCDHF/RCI calculations have been performed in the extended optimal level (EOL) scheme for each group of atomic states using configuration expansions including all lower states of the same parity and symmetry. For the optimization of the orbitals, Dirac-Coulomb version has been used, including Breit corrections in a final configuration interaction calculation.

To build a CSF expansion, the restrictive active space methods have been also used. The idea of the active space methods is to consider only electrons from the active space and to excite them from the occupied orbitals to unoccupied ones. The orbital has been increased systematically in order to monitor the convergence of the calculation. Since the orbitals with the same principal quantum number  $n$  often have similar energies, the active set is usually enlarged in steps of orbital layers. It is convenient to refer to the  $\{1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f\}$  set of orbitals as the  $n = 4$  orbital layer,  $\{1s, 2s, 2p, \dots, 5s, 5p, 5d, 5f, 5g\}$  as the  $n = 5$  layer, etc. We increase the AS in a systematic way to ensure the convergence of the atomic parameters under consideration. Only the outermost  $nl$ -orbitals are optimized while the inside ones are fixed. For example, the total number of CSF in the active set of  $n = 8$  is 3896 for even configurations and 3560 for odd configurations. For the active set of  $n = 9$ , the number of CSF increases to 6104 and 5490 for even and odd, respectively. For the last active set of consideration  $n = 10$ , the number will be 8824 and 7854 for even and odd, respectively. So, we can deduce that larger orbital sets can result in a considerable increase of computational time required for the problem, and appropriate restrictions may be necessary.

We have divided up the calculations into two parts, one where we optimized a set of orbitals for the even states and one for the odd states, i.e. the upper and lower states have been described by two independently optimized sets of orbitals. Because of this, we have to use biorthogonal transformation of the atomic state functions ASF to calculate the transition parameters. Radiative transition characteristics have been calculated for  $E1$ ,  $M1$ ,  $E2$  and  $M2$  transitions, following the relativistic configuration-interaction RCI calculation in which both the Breit interaction and the other corrections to the DC Hamiltonian are included.

### 4. Results and data evaluation

In the following subsections, the results of the calculations are presented, and compared with values available from the literature. The identification of the levels is based on the LS composition obtained by transforming from  $jj$ - to  $LS$ -coupling schemes using the  $jj2lsj$  tool integrated in the new release of GRASP2K [16].

#### 4.1. Energy levels

The calculated energy levels of  $1s^2$ ,  $1s2l$ ,  $1s3l$ ,  $1s4l$ ,  $1s5l$ ,  $1s6l$  and  $1s7l$  configurations for the He-like xenon have been tabulated in Table 1, which generate up to 97 levels. These calculations are performed by means of two codes FAC and GRASP2K. The first column of results show the results from the FAC code. The other columns of GRASP1, GRASP2 and GRASP3 show the results from the GRASP2K code. The former results are calculated as function of increasing active sets with single excitations. All the calculated energy levels have been compared with experimental values. It is obvious that, when the active space is expanded to  $n = 8$  (GRASP1) and  $n = 9$  (GRASP2), the energy levels deviate very largely from experimental values taken from the National Institute of Standards and Technology NIST compilation [6], which is entirely based on the data listed by Ref [5]. When the active space set is expanded to  $n = 10$  (GRASP3), the calculated energy levels are substantially improved. So, we can clearly find that, with the increasing of active space set, the calculated energy levels are closer to experimental values.

The average difference between the GRASP3 values and NIST is 0.002% for the 8 states listed in the NIST database. The average difference between the calculated FAC and GRASP3 level energies is within 0.006% for all 97 states in *Xe LIII* while the average difference between the calculated FAC and NIST database level energies is 0.007%. Small discrepancies can be observed in the GRASP and FAC energies mainly arise due to the different ways of calculations of electron wave-functions for radial orbitals and recoupling schemes of angular parts. Since some of energy levels are not available on NIST, our energy levels GRASP3 should be adopted in modelling applications. We may state that overall there is no discrepancy between theory and experiment and the results of GRASP3 are in good agreement with the experimental values for the energy levels of *Xe LIII*.

We compare also the lifetimes from the two calculations from the FAC and GRASP2K codes. Some large discrepancies have found for some levels like  $1s2s^1S_0$ ,  $1s2p^3P_2^o$ ,  $1s2p^1P_1^o$  when the differences are 14.54%, 6.62% and 7.00% respectively. For the others values the percentage do not exceed 2% for the almost levels.

We list in Table 2, the LSJ coupling percentage compositions for all levels of interest. The level composition in LSJ coupling values show that, the major contributions to the total wave function of a given level are those coming from the same configuration.

#### 4.2. Radiative rates

The weighted oscillator strengths  $g_{ifij}$  are related to the transition probabilities  $A_{ji}$  for a transition from  $i$  to  $j$  by the following expression

$$g_{ifij} = \frac{mc}{8\pi^2 e^2} \lambda_{ji}^2 g_i A_{ji} = 1.49 \times 10^{-16} \lambda_{ji}^2 g_i A_{ji}, \quad (23)$$

where  $m$  and  $e$  are the electron mass and charge, respectively,  $c$  is the velocity of light,  $\lambda_{ji}$  is the wavelength in Å,  $g_i$  and  $g_j$  are the statistical weights of the lower ( $i$ ) and upper ( $j$ ) levels, respectively. Similarly, the weighted oscillator strength  $g_{ifij}$  and the line strength  $S$  are related by the standard equation for the electric dipole  $E1$ -transitions,

$$A_{ji} = \frac{2.0261 \times 10^{18}}{g_j \lambda_{ji}^3} S^{E1} \quad \text{and} \quad g_{ifij} = \frac{303.75}{\lambda_{ji}} S^{E1} \quad (24)$$

for the magnetic dipole  $M1$ -transitions,

$$A_{ji} = \frac{2.6974 \times 10^{13}}{g_j \lambda_{ji}^3} S^{M1} \quad \text{and} \quad g_{ifij} = \frac{4.044 \times 10^{-3}}{\lambda_{ji}} S^{M1} \quad (25)$$

for the electric quadrupole  $E2$ -transitions,

$$A_{ji} = \frac{1.1199 \times 10^{18}}{g_j \lambda_{ji}^5} S^{E2} \quad \text{and} \quad g_{ifij} = \frac{167.89}{\lambda_{ji}^3} S^{E2} \quad (26)$$

and for the magnetic quadrupole  $M2$ -transitions,

$$A_{ji} = \frac{1.4910 \times 10^{13}}{g_j \lambda_{ji}^5} S^{M2} \quad \text{and} \quad g_{ifij} = \frac{2.236 \times 10^{-3}}{\lambda_{ji}^3} S^{M2}. \quad (27)$$

Below, we present and discuss our determined  $gf$ -values and  $A$ -values for transitions in *Xe LIII* for all types of transitions  $E1$ ,  $E2$ ,  $M1$  and  $M2$  of all levels of energies in interest  $1s^2$  and  $1snl$  ( $n = 2-7$ ). The effects of Breit and QED corrections are assessed by our calculations. We should mention that for the GRASP2K calculation, the active set is expanded to  $n = 10$  (GRASP3) and only the length form for transition probabilities has tabulated in Tables 3–6. We present in these tables the wavelengths, weighted oscillator strengths  $g_{ifij}$  and radiative rates  $A_{ji}$  for 1054 electric dipole  $E1$ , 1389 electric quadrupole  $E2$ , 1012 magnetic dipole  $M1$  and 1430 magnetic quadrupole  $M2$  transitions among the 97 levels of *Xe LIII* calculated with GRASP2K and FAC codes. However, for these transitions only the  $gf$ -values and  $A$ -values are listed and the corresponding results for  $S$ -values can be easily obtained. We also present the uncertainty of the electric transitions  $dT$  to provide an additional indicator of the accuracy of our GRASP2K results in Tables 3 and 4.

We compare our calculated transition energy of the  $1s2s^3S_1-1s2p^3P_2^o$  ( $3756964 \text{ cm}^{-1}$ ) transition with the experimental value measured by S. Martin [34] ( $3750937 \text{ cm}^{-1}$ ) and other theoretical results elaborated by Indelicato [35] ( $3752138 \text{ cm}^{-1}$ ) and Drake [9] ( $3751576 \text{ cm}^{-1}$ ). Moreover, the calculated wavelength of the former transition is  $26.617 \text{ Å}$  where the experimental value is  $26.66 \text{ Å}$ . We state that the differences are minor. Furthermore, our calculated wavelengths compared to the data from the NIST database shows a good agreement such as the case of transitions  $1s^2^1S_0-1s2p^3P_2^o$  ( $0.4104 \text{ Å}$ ) and  $1s^2^1S_0-1s2p^1P_1^o$  ( $0.4047 \text{ Å}$ ).

For almost, all strong transitions (those with  $gf \geq 0.01$ ), the  $gf$  values and  $A$ -values from GRASP2K agree to better than 10% with those of FAC, which is satisfactory. Moreover, for many strong transitions, the difference between both velocity and length forms, does not exceed 2%, giving its credit to the accuracy of calculations of wave functions from GRASP2K. To confirm that, we have plotted in Fig. 1, the uncertainty  $dT$  as a function of transition rates of type  $E1$ .

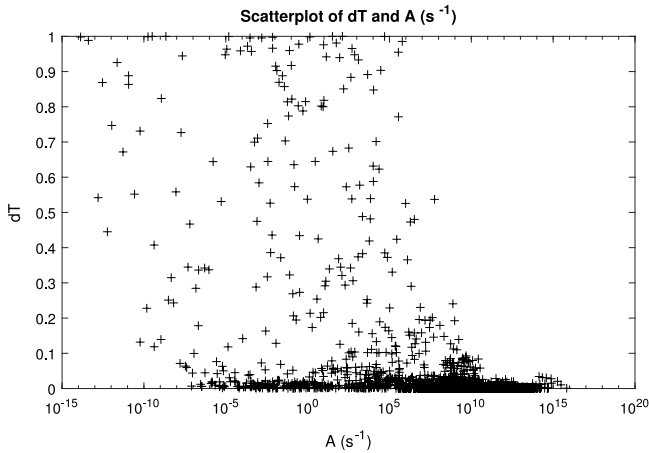
We remind that the uncertainty  $dT$  is generated by only the GRASP2K code and it is expressed by

$$dT = \frac{|A_l - A_v|}{\max(A_l, A_v)}, \quad (28)$$

where  $A_l$  and  $A_v$  are the transition rates calculated in length and velocity gauges, respectively.

However, for some weak transitions ( $gf < 0.01$ ), the situation is more unclear such as the  $1s2s^3S_1-1s4f^3F_2^o$  transition ( $gf = 3.265 \times 10^{-09}$ ) for the transition of type  $E1$ , the difference between two sets of  $A$ -values is large. We note also that we have large difference in some transitions because their transition energy is very small, such as  $1s3p^3P_1^o-1s3s^1S_0$ ,  $1s4p^3P_1^o-1s4s^1S_0$  and  $1s5p^3P_1^o-1s5s^1S_0$  for the type of  $E1$  transitions and the same case for  $E2$ ,  $M1$  and  $M2$  transitions. Hence, a slight variation in  $\Delta E$  has a considerable effect on the values of  $A$ . Moreover, the contribution of the  $A$ -values for weak transitions that required in modelling applications is (generally) small in comparison to the stronger transitions.

Therefore, on the basis of these comparisons and the above discussion, we may state that for a majority of strong  $E1$ ,  $E2$ ,  $M1$  and  $M2$  transitions, our radiative rates are accurate to better than 10%. However, for the weak transitions, this assessment of accuracy is not applied.



**Fig. 1.** The uncertainty  $dT$  by the GRASP2K code between the velocity and length forms of E1 transition rates as function of E1 transition rates  $A$ .

### 4.3. Lifetimes

The lifetime  $\tau$  for a level  $j$  is defined as follows

$$\tau_j = \frac{1}{\sum_i A_{ji}}. \quad (29)$$

Since this is a measurable parameter. It provides a check on the accuracy of the calculations. Therefore, in Table 1 we have also listed our calculated lifetimes from the GRASP2K code, which include the contributions from four types of transitions:  $E1$ ,  $E2$ ,  $M1$  and  $M2$ . To our knowledge, neither calculations nor measurements were determined for  $Xe\ LIII$  ion. We hope the present results will be useful for future comparisons and may encourage experimentalists to measure their lifetimes.

### 4.4. Hyperfine structure and Landé $g_j$ factors

The calculation of the hyperfine interaction constants and Landé  $g_j$  factors have been performed only with the GRASP2K code. In the case of our ion  $Xe\ LIII$ , the constants for the spin  $I$ , magnetic dipole moments  $\mu_I$  and the nuclear quadrupole moment  $Q_I$  were taken 1.5,  $0.691 \times \mu_N$  and  $-0.1$  barn, respectively.  $\mu_N$  is the nuclear magneton.

The active set (AS) is considered up to  $n = 10$  and  $l = 7$  for all the configurations of interest  $1snl$  ( $n = 1-7$ ). We list in Table A some of results of calculation of the magnetic dipole  $A$  and electric quadrupole  $B$  hyperfine interaction constants and Landé  $g_j$  factors for the four lowest states  $1s2s\ ^3S_1$ ,  $1s2p\ ^3P_1^o$ ,  $1s2p\ ^3P_2^o$  and  $1s2p\ ^1P_1^o$  to study the effect of increasing the AS in the hyperfine structure and the Landé  $g_j$  factors. We observe that the variation is minor. We can state that no influence of increasing set in the calculation of these hyperfine interaction constants.

In Table 7, we tabulate the hyperfine structure and Landé  $g_j$  factors for all levels of interest.

We have been unable to compare our predicted results of the hyperfine structure and Landé  $g_j$  factors with any other experimental or theoretical results because the required results are missing. However, our accurate values of Landé  $g_j$  factors and hyperfine structure constants are of great interest for atomic spectroscopy researchers.

### 4.5. Isotope shifts

The isotope shift and the electron densities at the nucleus parameters are calculated in a first-order perturbation theory using

**Table A**

Calculated values using the GRASP2K code of magnetic dipole  $A$ , electric quadrupole  $B$  and Landé  $g$ -factors with increasing the active set to  $n = 10$  (GRASP3).

| AS   | $1s2s\ ^3S_1$ | $1s2p\ ^3P_1^o$ | $1s2p\ ^3P_2^o$ | $1s2p\ ^1P_1^o$ |
|--|---------------|-----------------|-----------------|-----------------|
| <b>Magnetic dipole <math>A</math> (in MHz)</b>     |               |                 |                 |                 |
| $n = 3$  | 1.328E7       | 1.218E7         | 5.963E6         | -5.633E6        |
| $n = 4$  | 1.328E7       | 1.218E7         | 5.963E6         | -5.633E6        |
| $n = 5$  | 1.328E7       | 1.218E7         | 5.963E6         | -5.633E6        |
| $n = 6$  | 1.328E7       | 1.218E7         | 5.963E6         | -5.633E6        |
| $n = 7$  | 1.328E7       | 1.218E7         | 5.963E6         | -5.633E6        |
| $n = 8$  | 1.328E7       | 1.218E7         | 5.964E6         | -5.629E6        |
| $n = 9$  | 1.328E7       | 1.218E7         | 5.965E6         | -5.633E6        |
| $n = 10$   | 1.329E7       | 1.218E7         | 5.965E6         | -5.636E6        |
| <b>Electric quadrupole <math>B</math> (in MHz)</b> |               |                 |                 |                 |
| $n = 3$  | -2.062        | 4603            | -64830          | -34880          |
| $n = 4$  | -1.8          | 4614            | -64830          | -34820          |
| $n = 5$  | -1.048        | 4615            | -64830          | -34810          |
| $n = 6$  | -0.7197       | 4550            | -64810          | -34820          |
| $n = 7$  | -0.5684       | 4561            | -64810          | -34820          |
| $n = 8$  | -0.4849       | 4475            | -65310          | -35650          |
| $n = 9$  | 5.223         | 4480            | -64910          | -35320          |
| $n = 10$   | 1.941         | 4527            | -64660          | -34880          |
| <b>Landé <math>g</math>-factors</b>                |               |                 |                 |                 |
| $n = 3$  | 1.93514       | 1.28539         | 1.459           | 1.15044         |
| $n = 4$  | 1.93515       | 1.28538         | 1.45899         | 1.15047         |
| $n = 5$  | 1.93515       | 1.28538         | 1.45899         | 1.15047         |
| $n = 6$  | 1.93515       | 1.28539         | 1.45899         | 1.15047         |
| $n = 7$  | 1.93515       | 1.28539         | 1.45899         | 1.15047         |
| $n = 8$  | 1.93515       | 1.28532         | 1.45904         | 1.15036         |
| $n = 9$  | 1.93516       | 1.28523         | 1.45905         | 1.15054         |
| $n = 10$   | 1.93517       | 1.28519         | 1.45897         | 1.15063         |

the MCDHF/RCI atomic state functions as the zero-order wavefunctions. In Table B, we start by studying the effect of increasing the active set (AS) up to  $n = 10$ . For that, seven lowest levels  $1s^2\ ^1S_0$ ,  $1s2s\ ^3S_1$ ,  $1s2p\ ^3P_1^o$ ,  $1s2p\ ^3P_2^o$ ,  $1s2s\ ^1S_0$ ,  $1s2p\ ^3P_2^o$  and  $1s2p\ ^1P_1^o$  are chosen for consideration. No major effect is observed with increasing the active set. All calculations are performed with increasing the reference configurations up to  $n = 7$  when the active set AS is enlarged step by step up to  $n = 10$  and  $l = 7$ . Moreover, all these parameters are displayed in Table 8 for all the known levels belonging to the configurations  $1s^2$  and  $1snl$  with  $n = 2-7$ ,  $l \leq 6$ .

We plot the calculated specific mass shifts (SMS) using the GRASP2K code, only for the ground state  $1s^2$  with increasing the active set AS up to  $n = 10$  in Fig. 2. The result is compared with previous works, MCDHF [36], MCHF [36] and Drake [9]. Our result matches well with the result of the MCDHF work which proves the reliability of results. The difference with the other results can be explained by the different ways of calculation of codes. The GRASP2K and MCDHF are considered as relativistic codes while MCHF is a non relativistic one. The difference between the results of the two relativistic codes does not exceed 2.2% but the differences with the MCHF and Drake are approximately 15%.

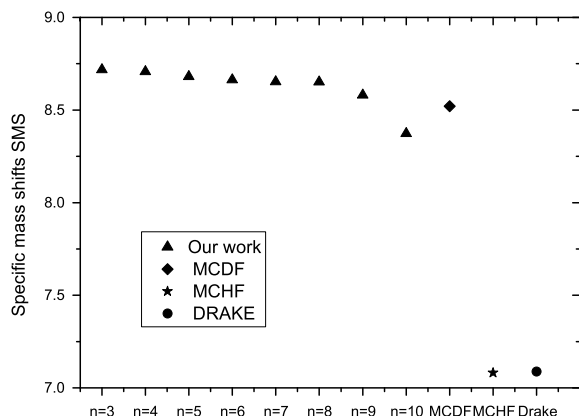
## 5. Conclusion

In the present study, fine structure energy levels, wavelengths, weighted oscillator strengths, transition probabilities for  $E1$ ,  $E2$ ,  $M1$  and  $M2$  transitions among 97 energy levels belonging to He-like xenon are presented. Additionally, lifetimes, hyperfine structure constants, Landé  $g_j$  factors and isotope shifts have been reported, although no measurements or other theoretical results are available for comparison except one work treating the calculation of only the ground state  $1s^2\ ^1S_0$ . The self-consistent field approximation and the Breit interaction Hamiltonian as well as QED effects have been included in the calculations to improve the generated wave functions. The calculated energy levels, weighted

**Table B**

Calculated values using the GRASP2K code of normal, specific mass shifts and electron densities at the nucleus for the seven lowest levels with increasing active set AS up to  $n = 10$ .

| AS                                       | $1s^2 \ ^1S_0$ | $1s2s \ ^3S_1$ | $1s2p \ ^3P_1^o$ | $1s2p \ ^3P_0^o$ | $1s2s \ ^1S_0$ | $1s2p \ ^3P_2^o$ | $1s2p \ ^1P_1^o$ |
|--|----------------|----------------|------------------|------------------|----------------|------------------|------------------|
| Normal mass shift NMS (a.u.)             |                |                |                  |                  |                |                  |                  |
| $n = 3$                                  | 2862.371       | 1818.908       | 1816.760         | 1815.086         | 1816.736       | 1803.102         | 1802.086         |
| $n = 4$                                  | 2862.365       | 1819.197       | 1816.720         | 1815.010         | 1815.793       | 1803.182         | 1801.819         |
| $n = 5$                                  | 2862.337       | 1819.261       | 1816.695         | 1814.981         | 1815.592       | 1803.179         | 1801.750         |
| $n = 6$                                  | 2862.332       | 1819.284       | 1816.689         | 1814.974         | 1815.522       | 1803.185         | 1801.726         |
| $n = 7$                                  | 2862.328       | 1819.295       | 1816.686         | 1814.971         | 1815.488       | 1803.186         | 1801.717         |
| $n = 8$                                  | 2862.349       | 1819.317       | 1818.194         | 1816.601         | 1815.483       | 1804.312         | 1803.566         |
| $n = 9$                                  | 2862.115       | 1819.47        | 1817.501         | 1815.864         | 1815.214       | 1803.816         | 1802.661         |
| $n = 10$                                 | 2862.115       | 1819.58        | 1817             | 1815.49          | 1815.192       | 1803.659         | 1802.099         |
| Specific mass shift SMS (a.u.)           |                |                |                  |                  |                |                  |                  |
| $n = 3$                                  | 8.717903       | 0.5995701      | −80.16853        | −195.2675        | 2.357866       | −205.907         | 83.54837         |
| $n = 4$                                  | 8.70804        | 0.6207144      | −80.2113         | −195.2448        | 2.119602       | −205.9269        | 83.36892         |
| $n = 5$                                  | 8.680987       | 0.6271347      | −80.20777        | −195.2282        | 2.042898       | −205.9166        | 83.34515         |
| $n = 6$                                  | 8.663317       | 0.6302334      | −80.15193        | −195.1577        | 2.007405       | −205.89          | 83.36138         |
| $n = 7$                                  | 8.65289        | 0.6318741      | −80.15315        | −195.1561        | 1.988378       | −205.8906        | 83.35634         |
| $n = 8$                                  | 8.651809       | 0.6336825      | −80.89982        | −197.0734        | 1.980105       | −207.2639        | 84.04787         |
| $n = 9$                                  | 8.580615       | 0.65771        | −80.56291        | −196.2107        | 1.67668        | −206.4653        | 83.54352         |
| $n = 10$                                 | 8.37281        | 0.65445        | −80.2194         | −195.3285        | 1.61861        | −205.8238        | 83.21168         |
| Electron densities at the nucleus (a.u.) |                |                |                  |                  |                |                  |                  |
| $n = 3$                                  | 235656.3       | 136365.8       | 120103           | 119991.8         | 136038.1       | 119543.4         | 119715.1         |
| $n = 4$                                  | 235660.7       | 136377.1       | 120099.6         | 119989.3         | 136019.9       | 119540.7         | 119710.3         |
| $n = 5$                                  | 235658.2       | 136379.7       | 120096.3         | 119986.4         | 136016         | 119537.7         | 119706.4         |
| $n = 6$                                  | 235657.7       | 136380.8       | 120095.9         | 119986           | 136015.2       | 119537.4         | 119705.8         |
| $n = 7$                                  | 235657.2       | 136381.3       | 120095.5         | 119985.7         | 136014.9       | 119537           | 119705.2         |
| $n = 8$                                  | 235659.3       | 136382.9       | 120102.9         | 119998           | 136016.1       | 119534.3         | 119697.6         |
| $n = 9$                                  | 235598.7       | 136395.2       | 120130           | 120023.1         | 136025.1       | 119570.9         | 119733.3         |
| $n = 10$                                 | 235581.5       | 136426.2       | 120162.2         | 120117.3         | 136014.9       | 119664.2         | 119832.8         |



**Fig. 2.** Comparison of specific mass shifts (in a.u.) for the ground state  $1s^2 \ ^1S_0$  with previous works MCDF [36], MCHF [36], Drake [9].

oscillator strengths and all radiative transitions show a good agreement with other published results from the literature. In addition, we have obtained some new data for the hyperfine structure constants, Landé  $g_j$  factors and isotope shifts for this ion. The present data sets are believed to be the most comprehensive and accurate ones to date for *Xe LIII*. Our results are expected to be useful for many applications such as controlled thermonuclear fusion, laser and plasma physics as well as astrophysics.

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## Explanation of Tables

|                                   |   |
|-----------------------------------|---|
| <b>Table 1.</b>                   | <b>Energies (<math>E</math> in <math>\text{cm}^{-1}</math>) relative to the ground state for the lowest 97 levels arising from the <math>1s^2</math> and <math>1snl</math> with <math>n = 2-7</math> configurations of Xe LIII. Two calculations are performed using FAC and GRASP2K and compared with data from NIST database. The GRASP1, GRASP2 and GRASP3 are determined respectively with increasing the active set (AS) up to <math>n = 8</math>, <math>n = 9</math> and <math>n = 10</math>. The last two columns denote the lifetimes (in <math>\text{s}^{-1}</math>) obtained from our FAC and GRASP2K calculations.</b> |
| Configuration                     | Configuration of energy level   |
| Level                             | Configuration of energy level   |
| FAC                               | Energy levels calculated with the FAC code  |
| GRASP1                            | Energy levels calculated with the GRASP2K code up to $n = 8$  |
| GRASP2                            | Energy levels calculated with the GRASP2K code up to $n = 9$  |
| GRASP3                            | Energy levels calculated with the GRASP2K code up to $n = 10$   |
| NIST                              | Energy levels compiled by the NIST database   |
| Lifetimes (GRASP2K)               | compilation or from current literature  |
| Lifetimes (FAC)                   | Lifetimes calculated with the FAC code  |
| Lifetimes (GRASP2K)               | Lifetimes calculated with the GRASP2K code  |
| <b>Table 2.</b>                   | <b>Calculated values using the GRASP2K code of the composition in LSJ coupling for all levels of interest with increasing the active set to <math>n = 10</math> (GRASP3).</b>   |
| Level                             | Configuration of the level of energy  |
| Composition in LSJ coupling       | Composition in LSJ coupling for each level of energy  |
| <b>Table 3.</b>                   | <b>Electric dipole transitions <math>E1</math> calculated with GRASP2K and FAC for all <math>n = 1-7</math> configurations. For the GRASP2K calculation, the active set is expanded to <math>n = 10</math> (GRASP3) and only the length form is considered. A comparison between the wavelengths, weighted oscillator strengths and transition probabilities is given. The relative difference between transition rates in the velocity and length gauge is given in the last column by <math>dT</math>.</b>  |
| Lower                             | Lower state of energy   |
| Upper                             | Upper state of energy   |
| $\lambda$ (Å)                     | Wavelengths calculated with the GRASP2K and FAC codes   |
| $gf$                              | Weighted oscillator strengths calculated with the GRASP2K and FAC codes   |
| $A$ ( $\text{s}^{-1}$ )           | Electric dipole transitions $E1$ calculated with the GRASP2K and FAC codes  |
| $dT$                              | Uncertainty between the transition rates in the velocity and length gauge   |
| <b>Table 4.</b>                   | <b>Electric quadrupole transitions <math>E2</math> calculated with GRASP2K and FAC for all <math>n = 1-7</math> configurations. For the GRASP2K calculation, the active set is expanded to <math>n = 10</math> (GRASP3) and only the length form is considered. A comparison between the wavelengths, weighted oscillator strengths and transition probabilities is given. The relative difference between transition probabilities in the velocity and length gauge is given in the last column by <math>dT</math>.</b>  |
| Lower                             | Lower state of energy   |
| Upper                             | Upper state of energy   |
| $\lambda$ (Å)                     | Wavelengths calculated with the GRASP2K and FAC codes   |
| $gf$                              | Weighted oscillator strengths calculated with the GRASP2K and FAC codes   |
| $A$ ( $\text{s}^{-1}$ )           | Electric dipole transitions $E2$ calculated with the GRASP2K and FAC codes  |
| $dT$                              | Uncertainty between the transition rates in the velocity and length gauge   |
| <b>Table 5.</b>                   | <b>Magnetic dipole transitions <math>M1</math> calculated with GRASP2K and FAC for all <math>n = 1-7</math> configurations. For the GRASP2K calculation, the active set is expanded to <math>n = 10</math> (GRASP3) and only the length form is considered. A comparison between the wavelengths, weighted oscillator strengths and transition probabilities is given.</b>  |
| Lower                             | Lower state of energy   |
| Upper                             | Upper state of energy   |
| $\lambda$ (Å)                     | Wavelengths calculated with the GRASP2K and FAC codes   |
| $gf$                              | Weighted oscillator strengths calculated with the GRASP2K and FAC codes   |
| $A$ ( $\text{s}^{-1}$ )           | Electric dipole transitions $E1$ calculated with the GRASP2K and FAC codes  |
| <b>Table 6.</b>                   | <b>Magnetic quadrupole transitions <math>M2</math> calculated with GRASP2K and FAC for all <math>n = 1-7</math> configurations. For the GRASP2K calculation, the active set is expanded to <math>n = 10</math> (GRASP3) and only the length form is considered. A comparison between the wavelengths, weighted oscillator strengths and transition probabilities is given.</b>  |
| Lower                             | Lower state of energy   |
| Upper                             | Upper state of energy   |
| $\lambda$ (Å)                     | Wavelengths calculated with the GRASP2K and FAC codes   |
| $gf$                              | Weighted oscillator strengths calculated with the GRASP2K and FAC codes   |
| $A$ ( $\text{s}^{-1}$ )           | Electric dipole transitions $E1$ calculated with the GRASP2K and FAC codes  |
| <b>Table 7.</b>                   | <b>Calculated values using the GRASP2K code of the magnetic dipole <math>A</math>, electric quadrupole <math>B</math> and Landé <math>g</math>-factors for all levels of interest. For this calculation, the active set expanded to <math>n = 10</math> (GRASP3) has been considered.</b>   |
| Configuration                     | Configuration of the level of energy  |
| $A$ (MHz)                         | Magnetic dipole $A$   |
| $B$ (MHz)                         | Electric quadrupole $B$   |
| $g_j$                             | Landé $g$ -factors  |
| <b>Table 8.</b>                   | <b>Calculated values using the GRASP2K code of normal, specific mass shifts and electron densities at the nucleus for the all singly excited levels up to <math>n = 7</math> with increasing the active set to <math>n = 10</math> (GRASP3).</b>  |
| Index                             | Index of the level of energy  |
| Configuration                     | Configuration of the level of energy  |
| $K_{NMS}$                         | Normal mass shifts  |
| $K_{SMS}$                         | Specific mass shifts  |
| Electron densities at the nucleus | Electron densities at the nucleus   |

**Table 1**

Energies ( $E$  in  $\text{cm}^{-1}$ ) relative to the ground state for the lowest 97 levels arising from the  $1s^2$  and  $1snl$  with  $n = 2-7$  configurations of Xe *LIII*. Two calculations are performed using FAC and GRASP2K and compared with data from NIST database. The GRASP1, GRASP2 and GRASP3 are determined respectively with increasing the active set (AS) up to  $n = 8$ ,  $n = 9$  and  $n = 10$ . The last two columns denote the lifetimes (in  $\text{s}^{-1}$ ) obtained from our FAC and GRASP2K calculations.

| Configuration   | Level                                    | FAC        | GRASP1    | GRASP2    | GRASP3    | NIST      | Lifetimes (FAC) | Lifetimes (GRASP2K) |
|-----------------|--|------------|-----------|-----------|-----------|-----------|-----------------|---------------------|
| 1s <sup>2</sup> | <sup>1</sup> S <sub>0</sub>              | 0          | 0         | 0         | 0         | 0         |                 |                     |
| 1s 2s           | <sup>3</sup> S <sub>1</sub>              | 242981032  | 242992840 | 242996188 | 242999633 | 243004900 | 2.6569E–12      | 2.6101E–12          |
| 1s 2p           | <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 243610281  | 243619151 | 243620649 | 243622562 | 243626600 | 3.3975E–16      | 3.3084E–16          |
| 1s 2p           | <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 243656320  | 243667841 | 243669210 | 243670879 | 243674700 | 5.7419E–10      | 5.8607E–10          |
| 1s 2s           | <sup>1</sup> S <sub>0</sub>              | 243677020  | 243680822 | 243683119 | 243685687 | 243691200 | 6.5427E–07      | 7.6560E–07          |
| 1s 2p           | <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 246740070  | 246751551 | 246753838 | 246756598 | 246756600 | 3.2404E–13      | 3.4703E–13          |
| 1s 2p           | <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 247026227  | 247036525 | 247037250 | 247038566 | 247044900 | 1.3777E–16      | 1.4814E–16          |
| 1s 3s           | <sup>3</sup> S <sub>1</sub>              | 288924950  | 288935786 | 288939203 | 288942662 |           | 1.4006E–14      | 1.3954E–14          |
| 1s 3p           | <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 2890965210 | 289106563 | 289109120 | 289112287 |           | 1.0612E–15      | 1.0241E–15          |
| 1s 3s           | <sup>1</sup> S <sub>0</sub>              | 289108182  | 289117871 | 289120773 | 289123953 |           | 1.4184E–14      | 1.4470E–14          |
| 1s 3p           | <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 289107415  | 289119367 | 289121868 | 289124969 |           | 4.9927E–15      | 5.1073E–15          |
| 1s 3p           | <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 290026737  | 290038530 | 290041366 | 290044705 |           | 5.7548E–15      | 5.9395E–15          |
| 1s 3d           | <sup>3</sup> D <sub>2</sub>              | 290093250  | 290105217 | 290108667 | 290112235 |           | 1.8090E–15      | 1.8193E–15          |
| 1s 3d           | <sup>3</sup> D <sub>1</sub>              | 290105192  | 290117231 | 290120677 | 290124145 |           | 1.8379E–15      | 1.8516E–15          |
| 1s 3p           | <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 290107569  | 290119473 | 290121577 | 290124581 |           | 4.6643E–16      | 4.9660E–16          |
| 1s 3d           | <sup>3</sup> D <sub>3</sub>              | 290385275  | 290397902 | 290401352 | 290404821 | 290413200 | 1.9104E–15      | 1.9570E–15          |
| 1s 3d           | <sup>1</sup> D <sub>2</sub>              | 290396539  | 290409015 | 290412465 | 290415933 |           | 1.8837E–15      | 1.9162E–15          |
| 1s 4s           | <sup>3</sup> S <sub>1</sub>              | 304797684  | 304810015 | 304813454 | 304816918 |           | 2.0732E–14      | 2.0635E–14          |
| 1s 4p           | <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 304866150  | 304879429 | 304882766 | 304886176 |           | 2.4379E–15      | 2.3464E–15          |
| 1s 4s           | <sup>1</sup> S <sub>0</sub>              | 304871588  | 304883666 | 304886805 | 304890134 |           | 2.0958E–14      | 2.1245E–14          |
| 1s 4p           | <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 304871052  | 304884541 | 304887868 | 304891257 |           | 8.6891E–15      | 8.7915E–15          |
| 1s 4p           | <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 305258024  | 305271468 | 305274839 | 305278274 |           | 9.7044E–15      | 9.9498E–15          |
| 1s 4d           | <sup>3</sup> D <sub>2</sub>              | 305287622  | 305299503 | 305302961 | 305306431 |           | 4.1830E–15      | 4.1928E–15          |
| 1s 4d           | <sup>3</sup> D <sub>1</sub>              | 305292454  | 305304374 | 305307831 | 305311301 |           | 4.2748E–15      | 4.2838E–15          |
| 1s 4p           | <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 305291458  | 305304769 | 305307957 | 305311348 |           | 1.1013E–15      | 1.1689E–15          |
| 1s 4d           | <sup>3</sup> D <sub>3</sub>              | 305410833  | 305423127 | 305426585 | 305430056 |           | 4.4651E–15      | 4.5484E–15          |
| 1s 4f           | <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 305411941  | 305425949 | 305428640 | 305431982 |           | 8.8845E–15      | 8.9144E–15          |
| 1s 4f           | <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 305414511  | 305428553 | 305431218 | 305434552 |           | 8.8976E–15      | 8.9207E–15          |
| 1s 4d           | <sup>1</sup> D <sub>2</sub>              | 305415952  | 305428167 | 305431625 | 305435095 |           | 4.3461E–15      | 4.4234E–15          |
| 1s 4f           | <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 305472935  | 305486462 | 305489675 | 305493125 |           | 9.0070E–15      | 9.0807E–15          |
| 1s 4f           | <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 305474843  | 305488377 | 305491581 | 305495030 |           | 9.0252E–15      | 9.0870E–15          |
| 1s 5s           | <sup>3</sup> S <sub>1</sub>              | 312072452  | 312085468 | 312088918 | 312092385 |           | 3.2951E–14      | 3.2811E–14          |
| 1s 5p           | <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 312106783  | 312120509 | 312123852 | 312127291 |           | 4.6828E–15      | 4.5019E–15          |
| 1s 5s           | <sup>1</sup> S <sub>0</sub>              | 312109421  | 312122408 | 312125671 | 312129058 |           | 3.3281E–14      | 3.3582E–14          |
| 1s 5p           | <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 312109229  | 312123048 | 312126394 | 312129823 |           | 1.4960E–14      | 1.5067E–14          |
| 1s 5p           | <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 312306662  | 312320496 | 312323875 | 312327320 |           | 1.6453E–14      | 1.6819E–14          |
| 1s 5d           | <sup>3</sup> D <sub>2</sub>              | 312322459  | 312334715 | 312338177 | 312341649 |           | 8.0273E–15      | 8.0351E–15          |
| 1s 5p           | <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 312323602  | 312337225 | 312340644 | 312344087 |           | 2.1439E–15      | 2.2719E–15          |
| 1s 5d           | <sup>3</sup> D <sub>1</sub>              | 312324883  | 312337162 | 312340623 | 312344095 |           | 8.2220E–15      | 8.2189E–15          |
| 1s 5d           | <sup>3</sup> D <sub>3</sub>              | 312385482  | 312397978 | 312401440 | 312404912 |           | 8.6074E–15      | 8.7460E–15          |
| 1s 5f           | <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 312385818  | 312400664 | 312402591 | 312405985 |           | 1.7108E–14      | 1.7138E–14          |
| 1s 5f           | <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 312387134  | 312402027 | 312403912 | 312407300 |           | 1.7127E–14      | 1.7149E–14          |
| 1s 5d           | <sup>1</sup> D <sub>2</sub>              | 312388183  | 312400635 | 312404097 | 312407568 |           | 8.3320E–15      | 8.4797E–15          |
| 1s 5f           | <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 312417093  | 312430652 | 312433874 | 312437344 |           | 1.7355E–14      | 1.7476E–14          |
| 1s 5g           | <sup>3</sup> G <sub>4</sub>              | 312417177  | 312430463 | 312433929 | 312437402 |           | 2.9246E–14      | 2.9310E–14          |
| 1s 5g           | <sup>3</sup> G <sub>3</sub>              | 312417930  | 312431215 | 312434682 | 312438155 |           | 2.9267E–14      | 2.9320E–14          |
| 1s 5f           | <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 312418079  | 312431645 | 312434859 | 312438328 |           | 1.7385E–14      | 1.7489E–14          |
| 1s 5g           | <sup>3</sup> G <sub>5</sub>              | 312435809  | 312449135 | 312452602 | 312456074 |           | 2.9431E–14      | 2.9553E–14          |
| 1s 5g           | <sup>1</sup> G <sub>4</sub>              | 312436404  | 312449730 | 312453197 | 312456669 |           | 2.9447E–14      | 2.9560E–14          |
| 1s 6s           | <sup>3</sup> S <sub>1</sub>              | 315993781  | 316009270 | 316012725 | 316016194 |           | 5.0842E–14      | 5.0676E–14          |
| 1s 6p           | <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 316015359  | 316030311 | 316032803 | 316036253 |           | 8.2030E–15      | 7.6967E–15          |
| 1s 6s           | <sup>1</sup> S <sub>0</sub>              | 316011643  | 316030412 | 316033745 | 316037162 |           | 5.1360E–14      | 5.1446E–14          |
| 1s 6p           | <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 316011594  | 316031770 | 316034252 | 316037693 |           | 2.4183E–14      | 2.4286E–14          |
| 1s 6p           | <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 316130593  | 316145514 | 316148194 | 316151654 |           | 2.6341E–14      | 2.6886E–14          |
| 1s 6d           | <sup>3</sup> D <sub>2</sub>              | 316140922  | 316152973 | 316156437 | 316159909 |           | 1.4049E–14      | 1.3705E–14          |
| 1s 6p           | <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 316139182  | 316155139 | 316157859 | 316161294 |           | 3.6568E–15      | 3.9123E–15          |
| 1s 6d           | <sup>3</sup> D <sub>1</sub>              | 316140582  | 316154374 | 316157837 | 316161309 |           | 1.3703E–14      | 1.4021E–14          |
| 1s 6d           | <sup>3</sup> D <sub>3</sub>              | 316177189  | 316189550 | 316193014 | 316196486 |           | 1.4721E–14      | 1.4943E–14          |
| 1s 6f           | <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 316177224  | 316192482 | 316193664 | 316197135 |           | 2.9214E–14      | 2.9210E–14          |
| 1s 6f           | <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 316177216  | 316193297 | 316194426 | 316197896 |           | 2.9180E–14      | 2.9224E–14          |
| 1s 6d           | <sup>1</sup> D <sub>2</sub>              | 316177743  | 316191110 | 316194574 | 316198045 |           | 1.4208E–14      | 1.4457E–14          |
| 1s 6f           | <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 316195254  | 316208405 | 316211819 | 316215291 |           | 2.9614E–14      | 2.9805E–14          |
| 1s 6g           | <sup>3</sup> G <sub>4</sub>              | 316195229  | 316208388 | 316211855 | 316215327 |           | 5.0068E–14      | 5.0144E–14          |
| 1s 6g           | <sup>3</sup> G <sub>3</sub>              | 316195229  | 316208825 | 316212291 | 316215764 |           | 5.0109E–14      | 5.0158E–14          |
| 1s 6f           | <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 316195267  | 316208980 | 316212392 | 316215864 |           | 2.9665E–14      | 2.9824E–14          |
| 1s 6g           | <sup>3</sup> G <sub>5</sub>              | 316205987  | 316219204 | 316222671 | 316226143 |           | 5.0397E–14      | 5.0581E–14          |
| 1s 6h           | <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 316205987  | 316219251 | 316222682 | 316226155 |           | 7.6145E–14      | 7.6271E–14          |
| 1s 6h           | <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 316205987  | 316219534 | 316222964 | 316226437 |           | 7.6189E–14      | 7.6284E–14          |
| 1s 6g           | <sup>1</sup> G <sub>4</sub>              | 316205987  | 316219549 | 316223016 | 316226488 |           | 5.0429E–14      | 5.0591E–14          |
| 1s 6h           | <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 316213134  | 316226435 | 316229866 | 316233339 |           | 7.6403E–14      | 7.6606E–14          |

(continued on next page)

Table 1 (continued)

| Configuration | Level     | FAC       | GRASP1    | GRASP2    | GRASP3    | NIST | Lifetimes (FAC) | Lifetimes (GRASP2K) |
|---------------|-----------|-----------|-----------|-----------|-----------|------|-----------------|---------------------|
| 1s6h          | $^1H_5^0$ | 316213134 | 316226670 | 316230099 | 316233572 |      | 7.6438E-14      | 7.6616E-14          |
| 1s7s          | $^3S_1$   | 318347824 | 318362488 | 318365947 | 318369417 |      | 7.5196E-14      | 7.5428E-14          |
| 1s7p          | $^3P_1^0$ | 318361378 | 318379168 | 318379301 | 318382488 |      | 1.2935E-14      | 1.2034E-14          |
| 1s7s          | $^1S_0$   | 318358961 | 318375742 | 318379117 | 318382551 |      | 7.5936E-14      | 7.4869E-14          |
| 1s7p          | $^3P_0^0$ | 318359030 | 318380144 | 318380220 | 318383393 |      | 3.6841E-14      | 3.6655E-14          |
| 1s7p          | $^3P_2^0$ | 318433740 | 318451061 | 318451711 | 318454952 |      | 3.9905E-14      | 4.0394E-14          |
| 1s7d          | $^3D_2$   | 318440253 | 318452794 | 318456259 | 318459731 |      | 2.1567E-14      | 2.1568E-14          |
| 1s7d          | $^3D_1$   | 318440035 | 318453670 | 318457135 | 318460607 |      | 2.2119E-14      | 2.2062E-14          |
| 1s7p          | $^1P_1^0$ | 318439121 | 318457447 | 318457914 | 318461036 |      | 5.7984E-15      | 6.1365E-15          |
| 1s7d          | $^3D_3$   | 318463080 | 318475804 | 318479269 | 318482741 |      | 2.3193E-14      | 2.3579E-14          |
| 1s7f          | $^3F_3^0$ | 318463096 | 318479601 | 318479839 | 318483171 |      | 4.5885E-14      | 4.5872E-14          |
| 1s7f          | $^3F_2^0$ | 318463090 | 318480145 | 318480317 | 318483651 |      | 4.5848E-14      | 4.5866E-14          |
| 1s7d          | $^1D_2$   | 318463439 | 318476795 | 318480260 | 318483731 |      | 2.2348E-14      | 2.2705E-14          |
| 1s7f          | $^3F_4^0$ | 318474448 | 318487999 | 318491154 | 318494599 |      | 4.6540E-14      | 4.6813E-14          |
| 1s7g          | $^3G_4$   | 318474415 | 318487681 | 318491148 | 318494620 |      | 7.8748E-14      | 7.8818E-14          |
| 1s7g          | $^3G_3$   | 318474415 | 318487956 | 318491423 | 318494895 |      | 7.8784E-14      | 7.8824E-14          |
| 1s7f          | $^1F_3^0$ | 318474457 | 318488359 | 318491517 | 318494961 |      | 4.6606E-14      | 4.6830E-14          |
| 1s7g          | $^3G_5$   | 318481193 | 318494494 | 318497961 | 318501433 |      | 7.9274E-14      | 7.9533E-14          |
| 1s7h          | $^3H_5^0$ | 318481193 | 318494511 | 318497969 | 318501442 |      | 1.2015E-13      | 1.2028E-13          |
| 1s7h          | $^3H_4^0$ | 318481192 | 318494689 | 318498147 | 318501620 |      | 1.2018E-13      | 1.2030E-13          |
| 1s7g          | $^1G_4$   | 318481192 | 318494712 | 318498178 | 318501651 |      | 7.9303E-14      | 7.9537E-14          |
| 1s7h          | $^3H_6^0$ | 318485697 | 318499038 | 318502496 | 318505969 |      | 1.2057E-13      | 1.2083E-13          |
| 1s7i          | $^3I_6$   | 318485696 | 318499030 | 318502497 | 318505969 |      | 1.6971E-13      | 1.6989E-13          |
| 1s7i          | $^3I_5$   | 318485696 | 318499155 | 318502621 | 318506094 |      | 1.6971E-13      | 1.6990E-13          |
| 1s7h          | $^1H_5^0$ | 318485697 | 318499185 | 318502643 | 318506116 |      | 1.2059E-13      | 1.2084E-13          |
| 1s7i          | $^3I_7$   | 318488907 | 318502254 | 318505721 | 318509193 |      | 1.7004E-13      | 1.7033E-13          |
| 1s7i          | $^1I_6$   | 318488907 | 318502361 | 318505827 | 318509300 |      | 1.7004E-13      | 1.7034E-13          |

**Table 2**  
Calculated values using the GRASP2K code of the composition in LSJ coupling for all levels of interest with increasing the active set to  $n = 10$  (GRASP3).

| Level             | Composition in LSJ coupling   |
|-------------------|---|
| $1s^2 \ ^1S_0$    | $1s^2 \ ^1S_0$ 99.98%   |
| $1s 2s \ ^3S_1$   | $1s 2s \ ^3S_1$ 99.98%  |
| $1s 2s \ ^1S_0$   | $1s 2s \ ^1S_0$ 99.94%  |
| $1s 2p \ ^3P_1^0$ | $1s 2p \ ^3P_1^0$ 70.31% + $1s 2p \ ^1P_1^0$ 29.64%   |
| $1s 2p \ ^3P_2^0$ | $1s 2p \ ^3P_2^0$ 99.97%  |
| $1s 2p \ ^3P_0^0$ | $1s 2p \ ^3P_0^0$ 99.96%  |
| $1s 2p \ ^1P_1^0$ | $1s 2p \ ^1P_1^0$ 70.29% + $1s 2p \ ^3P_1^0$ 29.65%   |
| $1s 3s \ ^3S_1$   | $1s 3s \ ^3S_1$ 99.95%  |
| $1s 3s \ ^1S_0$   | $1s 3s \ ^1S_0$ 99.88%  |
| $1s 3p \ ^3P_1^0$ | $1s 3p \ ^3P_1^0$ 70.04% + $1s 3p \ ^1P_1^0$ 29.84%   |
| $1s 3p \ ^3P_2^0$ | $1s 3p \ ^3P_2^0$ 99.90%  |
| $1s 3p \ ^3P_0^0$ | $1s 3p \ ^3P_0^0$ 99.88%  |
| $1s 3d \ ^3D_2$   | $1s 3d \ ^3D_2$ 60.30% + $1s 3d \ ^1D_2$ 39.67%   |
| $1s 3d \ ^3D_1$   | $1s 3d \ ^3D_1$ 99.97%  |
| $1s 3p \ ^1P_1^0$ | $1s 3p \ ^1P_1^0$ 70.01% + $1s 3p \ ^3P_1^0$ 29.85%   |
| $1s 3d \ ^3D_3$   | $1s 3d \ ^3D_3$ 99.90%  |
| $1s 3d \ ^1D_2$   | $1s 3d \ ^1D_2$ 60.26% + $1s 3d \ ^3D_2$ 39.64%   |
| $1s 4s \ ^3S_1$   | $1s 4s \ ^3S_1$ 99.90%  |
| $1s 4s \ ^1S_0$   | $1s 4s \ ^1S_0$ 99.81%  |
| $1s 4p \ ^3P_1^0$ | $1s 4p \ ^3P_1^0$ 69.90% + $1s 4p \ ^1P_1^0$ 29.88%   |
| $1s 4p \ ^3P_0^0$ | $1s 4p \ ^3P_0^0$ 99.77% + $1s 5p \ ^3P_0^0$ 00.10%   |
| $1s 4p \ ^3P_2^0$ | $1s 4p \ ^3P_2^0$ 99.81%  |
| $1s 4d \ ^3D_2$   | $1s 4d \ ^3D_2$ 60.45% + $1s 4d \ ^1D_2$ 39.45%   |
| $1s 4d \ ^3D_1$   | $1s 4d \ ^3D_1$ 99.90%  |
| $1s 4p \ ^1P_1^0$ | $1s 4p \ ^1P_1^0$ 69.86% + $1s 4p \ ^3P_1^0$ 29.89%   |
| $1s 4d \ ^3D_3$   | $1s 4d \ ^3D_3$ 99.82%  |
| $1s 4d \ ^3D_1$   | $1s 4d \ ^3D_1$ 99.90%  |
| $1s 4f \ ^3F_3^0$ | $1s 4f \ ^3F_3^0$ 56.88% + $1s 4f \ ^1F_3^0$ 43.04%   |
| $1s 4f \ ^3F_2^0$ | $1s 4f \ ^3F_2^0$ 99.93%  |
| $1s 4d \ ^1D_2$   | $1s 4d \ ^1D_2$ 60.39% + $1s 4d \ ^3D_2$ 39.42%   |
| $1s 4f \ ^3F_4^0$ | $1s 4f \ ^3F_4^0$ 99.93%  |
| $1s 4f \ ^1F_3^0$ | $1s 4f \ ^1F_3^0$ 56.88% + $1s 4f \ ^3F_3^0$ 43.04%   |
| $1s 5s \ ^3S_1$   | $1s 5s \ ^3S_1$ 99.84%  |
| $1s 5s \ ^1S_0$   | $1s 5s \ ^1S_0$ 99.74% + $1s 6s \ ^1S_0^0$ 00.13%   |
| $1s 5p \ ^3P_1^0$ | $1s 5p \ ^3P_1^0$ 69.79% + $1s 5p \ ^1P_1^0$ 29.87%   |
| $1s 5p \ ^3P_2^0$ | $1s 5p \ ^3P_2^0$ 99.71% + $1s 6p \ ^3P_2^0$ 00.13%   |
| $1s 5d \ ^3D_2$   | $1s 5d \ ^3D_2$ 60.48% + $1s 5d \ ^1D_2$ 39.34%   |
| $1s 5p \ ^1P_1^0$ | $1s 5p \ ^1P_1^0$ 69.74% + $1s 5p \ ^3P_1^0$ 29.89% + $1s 6p \ ^1P_1^0$ 00.11%                            |
| $1s 5p \ ^3P_0^0$ | $1s 5p \ ^3P_0^0$ 99.66% + $1s 6p \ ^3P_0^0$ 00.15%   |
| $1s 5d \ ^3D_1$   | $1s 5d \ ^3D_1$ 99.82%  |
| $1s 5d \ ^3D_3$   | $1s 5d \ ^3D_3$ 99.79%  |
| $1s 5f \ ^3F_3^0$ | $1s 5f \ ^3F_3^0$ 56.83% + $1s 5f \ ^1F_3^0$ 42.98%   |
| $1s 5f \ ^3F_2^0$ | $1s 5f \ ^3F_2^0$ 99.81% + $1s 6f \ ^3F_2^0$ 00.10%   |
| $1s 5d \ ^1D_2$   | $1s 5d \ ^1D_2$ 60.45% + $1s 5d \ ^3D_2$ 39.32%   |
| $1s 5f \ ^3F_4^0$ | $1s 5f \ ^3F_4^0$ 99.82%  |
| $1s 5g \ ^3G_4$   | $1s 5g \ ^3G_4$ 55.34% + $1s 5g \ ^1G_4$ 44.61%   |
| $1s 5g \ ^3G_3$   | $1s 5g \ ^3G_3$ 99.95%  |
| $1s 5f \ ^1F_3^0$ | $1s 5f \ ^1F_3^0$ 56.83% + $1s 5f \ ^3F_3^0$ 42.98%   |
| $1s 5g \ ^3G_5$   | $1s 5g \ ^3G_5$ 99.90%  |
| $1s 5g \ ^1G_4$   | $1s 5g \ ^1G_4$ 55.31% + $1s 5g \ ^3G_4$ 44.59%   |
| $1s 6s \ ^3S_1$   | $1s 6s \ ^3S_1$ 99.79% + $1s 7s \ ^3S_1$ 00.11%   |
| $1s 6s \ ^1S_0$   | $1s 6s \ ^1S_0$ 99.68% + $1s 7s \ ^1S_0$ 00.16% + $1s 5s \ ^1S_0$ 00.12%                                  |
| $1s 6p \ ^3P_1^0$ | $1s 6p \ ^3P_1^0$ 69.70% + $1s 6p \ ^1P_1^0$ 29.85% + $1s 7p \ ^3P_1^0$ 00.12%                            |
| $1s 6p \ ^3P_0^0$ | $1s 6p \ ^3P_0^0$ 99.54% + $1s 7p \ ^3P_0^0$ 00.19% + $1s 5p \ ^3P_0^0$ 00.13%                            |
| $1s 6p \ ^3P_2^0$ | $1s 6p \ ^3P_2^0$ 99.60% + $1s 7p \ ^3P_2^0$ 00.17% + $1s 5p \ ^3P_2^0$ 00.12%                            |
| $1s 6d \ ^3D_2$   | $1s 6d \ ^3D_2$ 60.48% + $1s 6d \ ^1D_2$ 39.27%   |
| $1s 6p \ ^1P_1^0$ | $1s 6p \ ^1P_1^0$ 69.64% + $1s 6p \ ^3P_1^0$ 29.88% + $1s 7p \ ^1P_1^0$ 00.15% + $1s 5p \ ^1P_1^0$ 00.10% |
| $1s 6d \ ^3D_1$   | $1s 6d \ ^3D_1$ 99.75% + $1s 7d \ ^3D_1$ 00.13%   |
| $1s 6d \ ^3D_3$   | $1s 6d \ ^3D_3$ 99.76% + $1s 7d \ ^3D_3$ 00.12%   |
| $1s 6f \ ^3F_3^0$ | $1s 6f \ ^3F_3^0$ 56.77% + $1s 6f \ ^1F_3^0$ 42.92%   |
| $1s 6f \ ^3F_2^0$ | $1s 6f \ ^3F_2^0$ 99.69% + $1s 7f \ ^3F_2^0$ 00.14%   |
| $1s 6d \ ^1D_2$   | $1s 6d \ ^1D_2$ 60.48% + $1s 6d \ ^3D_2$ 39.27%   |
| $1s 6f \ ^3F_4^0$ | $1s 6f \ ^3F_4^0$ 99.70% + $1s 7f \ ^3F_4^0$ 00.14%   |
| $1s 6g \ ^3G_4$   | $1s 6g \ ^3G_4$ 55.29% + $1s 6g \ ^1G_4$ 44.57%   |
| $1s 6g \ ^3G_3$   | $1s 6g \ ^3G_3$ 99.87%  |
| $1s 6f \ ^1F_3^0$ | $1s 6f \ ^1F_3^0$ 56.77% + $1s 6f \ ^3F_3^0$ 42.92%   |
| $1s 6g \ ^3G_5$   | $1s 6g \ ^3G_5$ 99.84%  |
| $1s 6h \ ^3H_5^0$ | $1s 6h \ ^3H_5^0$ 54.35% + $1s 6h \ ^1H_5^0$ 45.57%   |
| $1s 6h \ ^3H_4^0$ | $1s 6h \ ^3H_4^0$ 99.93%  |
| $1s 6g \ ^1G_4$   | $1s 6g \ ^1G_4$ 55.28% + $1s 6g \ ^3G_4$ 44.56%   |
| $1s 6h \ ^3H_6^0$ | $1s 6h \ ^3H_6^0$ 99.93%  |

(continued on next page)

Table 2 (continued)

| Level           | Composition in LSJ coupling  |
|-----------------|--|
| 1s 6h $^1H_5^0$ | 1s 6h $^1H_5^0$ 54.35% + 1s 6h $^3H_5^0$ 45.57%                          |
| 1s 7s $^3S_1$   | 1s 7s $^3S_1$ 99.86% + 1s 6s $^3S_1$ 00.10%                              |
| 1s 7s $^1S_0$   | 1s 7s $^1S_0$ 99.80% + 1s 6s $^1S_0$ 00.15%                              |
| 1s 7p $^3P_1^0$ | 1s 7p $^3P_1^0$ 69.68% + 1s 7p $^1P_1^0$ 29.83% + 1s 6p $^3P_1^0$ 00.11% |
| 1s 7p $^3P_2^0$ | 1s 7p $^3P_2^0$ 99.57% + 1s 6p $^3P_2^0$ 00.15%                          |
| 1s 7p $^3P_0^0$ | 1s 7p $^3P_0^0$ 99.51% + 1s 6p $^3P_0^0$ 00.17%                          |
| 1s 7d $^3D_2$   | 1s 7d $^3D_2$ 60.56% + 1s 7d $^1D_2$ 39.28%                              |
| 1s 7d $^3D_1$   | 1s 7d $^3D_1$ 99.84% + 1s 6d $^3D_1$ 00.13%                              |
| 1s 7p $^1P_1^0$ | 1s 7p $^1P_1^0$ 69.63% + 1s 7p $^3P_1^0$ 29.86% + 1s 6p $^1P_1^0$ 00.13% |
| 1s 7d $^3D_3$   | 1s 7d $^3D_3$ 99.84% + 1s 6d $^3D_3$ 00.12%                              |
| 1s 7f $^3F_3^0$ | 1s 7f $^3F_3^0$ 56.72% + 1s 7f $^1F_3^0$ 42.87%                          |
| 1s 7f $^3F_2^0$ | 1s 7f $^3F_2^0$ 99.58% + 1s 6f $^3F_2^0$ 00.13%                          |
| 1s 7d $^1D_2$   | 1s 7d $^1D_2$ 60.56% + 1s 7d $^3D_2$ 39.28%                              |
| 1s 7f $^3F_4^0$ | 1s 7f $^3F_4^0$ 99.59% + 1s 6f $^3F_4^0$ 00.13%                          |
| 1s 7g $^3G_4$   | 1s 7g $^3G_4$ 55.31% + 1s 7g $^1G_4$ 44.59%                              |
| 1s 7g $^3G_3$   | 1s 7g $^3G_3$ 99.91%   |
| 1s 7f $^1F_3^0$ | 1s 7f $^1F_3^0$ 56.72% + 1s 7f $^3F_3^0$ 42.87%                          |
| 1s 7g $^3G_5$   | 1s 7g $^3G_5$ 99.91%   |
| 1s 7h $^3H_5^0$ | 1s 7h $^3H_5^0$ 54.29% + 1s 7h $^1H_5^0$ 45.52%                          |
| 1s 7h $^3H_4^0$ | 1s 7h $^3H_4^0$ 99.81%   |
| 1s 7g $^1G_4$   | 1s 7g $^1G_4$ 55.32% + 1s 7g $^3G_4$ 44.59%                              |
| 1s 7h $^3H_6^0$ | 1s 7h $^3H_6^0$ 99.81%   |
| 1s 7i $^3I_6$   | 1s 7i $^3I_6$ 53.71% + 1s 7i $^1I_6$ 46.28%                              |
| 1s 7i $^3I_5$   | 1s 7i $^3I_5$ 99.99%   |
| 1s 7h $^1H_5^0$ | 1s 7h $^1H_5^0$ 54.29% + 1s 7h $^3H_5^0$ 45.52%                          |
| 1s 7i $^3I_7$   | 1s 7i $^3I_7$ 99.99%   |
| 1s 7i $^1I_6$   | 1s 7i $^1I_6$ 53.71% + 1s 7i $^3I_6$ 46.28%                              |

**Table 3**

Electric dipole transitions  $E1$  calculated with GRASP2K and FAC for all  $n = 1-7$  configurations. For the GRASP2K calculation, the active set is expanded to  $n = 10$  (GRASP3) and only the length form is considered. A comparison between the wavelengths, weighted oscillator strengths and transition probabilities is given. The relative difference between transition rates in the velocity and length gauge is given in the last column by  $dT$ .

| Lower                             | Upper                             | GRASP2K       |           |                  | FAC           |           |                  | $dT$  |
|-----------------------------------|-----------------------------------|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|                                   |                                   | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |       |
| 1s <sup>2</sup> 1S <sub>0</sub>   | 1s2p 3P <sub>1</sub> <sup>o</sup> | 4.1040E-01    | 2.290E-01 | 3.023E+15        | 4.0874E-01    | 2.230E-01 | 2.943E+15        | 0.010 |
| 1s2s 3S <sub>1</sub>              | 1s2p 3P <sub>0</sub> <sup>o</sup> | 1.6053E+02    | 1.112E-02 | 9.593E+08        | 1.5824E+02    | 1.129E-02 | 9.944E+08        | 0.193 |
| 1s2s 3S <sub>1</sub>              | 1s2p 3P <sub>0</sub> <sup>o</sup> | 1.4898E+02    | 5.677E-03 | 1.706E+09        | 1.4745E+02    | 5.725E-03 | 1.741E+09        | 0.139 |
| 1s2p 3P <sub>0</sub> <sup>o</sup> | 1s2s 1S <sub>0</sub>              | 1.5842E+03    | 4.752E-04 | 1.263E+06        | 1.4920E+03    | 4.997E-04 | 1.484E+06        | 0.365 |
| 1s2s 3S <sub>1</sub>              | 1s2p 3P <sub>2</sub> <sup>o</sup> | 2.6617E+01    | 1.713E-01 | 3.226E+11        | 2.6489E+01    | 1.725E-01 | 3.252E+11        | 0.028 |
| 1s <sup>2</sup> 1S <sub>0</sub>   | 1s2p 1P <sub>1</sub> <sup>o</sup> | 4.0470E-01    | 4.975E-01 | 6.750E+15        | 4.0309E-01    | 5.349E-01 | 7.257E+15        | 0.001 |
| 1s2s 3S <sub>1</sub>              | 1s2p 1P <sub>1</sub> <sup>o</sup> | 2.4759E+01    | 3.299E-02 | 1.196E+11        | 2.4615E+01    | 3.310E-02 | 1.204E+11        | 0.014 |
| 1s2s 1S <sub>0</sub>              | 1s2p 1P <sub>1</sub> <sup>o</sup> | 2.9825E+01    | 6.507E-02 | 1.626E+11        | 2.9731E+01    | 6.480E-02 | 1.616E+11        | 0.019 |
| 1s2p 3P <sub>0</sub> <sup>o</sup> | 1s3s 3S <sub>1</sub>              | 2.2065E+00    | 3.037E-02 | 1.387E+13        | 2.1974E+00    | 3.067E-02 | 1.400E+13        | 0.001 |
| 1s2p 3P <sub>0</sub> <sup>o</sup> | 1s3s 3S <sub>1</sub>              | 2.2089E+00    | 1.488E-02 | 6.779E+12        | 2.1996E+00    | 1.466E-02 | 6.681E+12        | 0.001 |
| 1s2p 3P <sub>0</sub> <sup>o</sup> | 1s3s 3S <sub>1</sub>              | 2.3705E+00    | 1.089E-01 | 4.309E+13        | 2.3604E+00    | 1.085E-01 | 4.294E+13        | 0.000 |
| 1s2p 1P <sub>1</sub> <sup>o</sup> | 1s3s 3S <sub>1</sub>              | 2.3864E+00    | 1.988E-02 | 7.761E+12        | 2.3765E+00    | 1.946E-02 | 7.596E+12        | 0.002 |
| 1s <sup>2</sup> 1S <sub>0</sub>   | 1s3p 3P <sub>1</sub> <sup>o</sup> | 3.4580E-01    | 4.196E-02 | 7.798E+14        | 3.4443E-01    | 4.008E-02 | 7.449E+14        | 0.015 |
| 1s2s 3S <sub>1</sub>              | 1s3p 3P <sub>1</sub> <sup>o</sup> | 2.1686E+00    | 2.902E-01 | 1.372E+14        | 2.1593E+00    | 2.946E-01 | 1.393E+14        | 0.003 |
| 1s2s 1S <sub>0</sub>              | 1s3p 3P <sub>1</sub> <sup>o</sup> | 2.2014E+00    | 1.285E-01 | 5.894E+13        | 2.1924E+00    | 1.253E-01 | 5.750E+13        | 0.006 |
| 1s3s 3S <sub>1</sub>              | 1s3p 3P <sub>1</sub> <sup>o</sup> | 5.8954E+02    | 1.889E-02 | 1.208E+08        | 5.8484E+02    | 1.901E-02 | 1.225E+08        | 0.179 |
| 1s2p 3P <sub>1</sub> <sup>o</sup> | 1s3s 3S <sub>1</sub>              | 2.1977E+00    | 1.194E-02 | 1.649E+13        | 2.1885E+00    | 1.243E-02 | 1.717E+13        | 0.005 |
| 1s2p 1P <sub>1</sub> <sup>o</sup> | 1s3s 1S <sub>0</sub>              | 2.3761E+00    | 4.454E-02 | 5.262E+13        | 2.3662E+00    | 4.514E-02 | 5.332E+13        | 0.002 |
| 1s3p 3P <sub>0</sub> <sup>o</sup> | 1s3s 3S <sub>0</sub>              | 8.5719E+03    | 5.545E-04 | 5.034E+04        | 7.6765E+03    | 6.142E-04 | 6.893E+04        | 1.000 |
| 1s2s 3S <sub>1</sub>              | 1s3p 3P <sub>0</sub> <sup>o</sup> | 2.1680E+00    | 1.376E-01 | 1.953E+14        | 2.1587E+00    | 1.407E-01 | 1.997E+14        | 0.003 |
| 1s3s 3S <sub>1</sub>              | 1s3p 3P <sub>0</sub> <sup>o</sup> | 5.4853E+02    | 9.695E-03 | 2.149E+08        | 5.4572E+02    | 9.712E-03 | 2.156E+08        | 0.148 |
| 1s2s 3S <sub>1</sub>              | 1s3p 3P <sub>2</sub> <sup>o</sup> | 2.1256E+00    | 5.650E-01 | 1.668E+14        | 2.1165E+00    | 5.828E-01 | 1.721E+14        | 0.003 |
| 1s3s 3S <sub>1</sub>              | 1s3p 3P <sub>2</sub> <sup>o</sup> | 9.0741E+01    | 3.059E-01 | 4.957E+10        | 9.0375E+01    | 3.069E-01 | 4.970E+10        | 0.026 |
| 1s2p 3P <sub>1</sub> <sup>o</sup> | 1s3d 3D <sub>2</sub>              | 2.1510E+00    | 1.556E+00 | 4.485E+14        | 2.1422E+00    | 1.568E+00 | 4.520E+14        | 0.001 |
| 1s2p 3P <sub>1</sub> <sup>o</sup> | 1s3d 3D <sub>2</sub>              | 2.3065E+00    | 3.054E-01 | 7.659E+13        | 2.2968E+00    | 3.049E-01 | 7.645E+13        | 0.001 |
| 1s2p 1P <sub>1</sub> <sup>o</sup> | 1s3d 3D <sub>2</sub>              | 2.3216E+00    | 5.348E-02 | 1.324E+13        | 2.3121E+00    | 5.146E-02 | 1.273E+13        | 0.002 |
| 1s3p 3P <sub>1</sub> <sup>o</sup> | 1s3d 3D <sub>2</sub>              | 1.0002E+02    | 1.760E-01 | 2.348E+10        | 9.9770E+01    | 1.757E-01 | 2.335E+10        | 0.002 |
| 1s3p 3P <sub>1</sub> <sup>o</sup> | 1s3d 3D <sub>2</sub>              | 1.4830E+03    | 2.141E-03 | 1.298E+06        |               |           |                  | 0.003 |
| 1s2p 3P <sub>1</sub> <sup>o</sup> | 1s3d 3D <sub>1</sub>              | 2.1505E+00    | 3.325E-01 | 1.598E+14        | 2.1416E+00    | 3.373E-01 | 1.621E+14        | 0.001 |
| 1s2p 3P <sub>1</sub> <sup>o</sup> | 1s3d 3D <sub>1</sub>              | 2.1527E+00    | 6.302E-01 | 3.024E+14        | 2.1437E+00    | 6.350E-01 | 3.046E+14        | 0.001 |
| 1s2p 3P <sub>2</sub> <sup>o</sup> | 1s3d 3D <sub>1</sub>              | 2.3059E+00    | 3.362E-02 | 1.406E+13        | 2.2962E+00    | 3.352E-02 | 1.401E+13        | 0.001 |
| 1s2p 1P <sub>1</sub> <sup>o</sup> | 1s3d 3D <sub>1</sub>              | 2.3210E+00    | 1.511E-01 | 6.236E+13        | 2.3114E+00    | 1.497E-01 | 6.179E+13        | 0.002 |
| 1s3p 3P <sub>1</sub> <sup>o</sup> | 1s3d 3D <sub>1</sub>              | 9.8828E+01    | 3.812E-02 | 8.679E+09        | 9.8590E+01    | 3.804E-02 | 8.628E+09        | 0.006 |
| 1s3p 3P <sub>1</sub> <sup>o</sup> | 1s3d 3D <sub>1</sub>              | 1.0008E+02    | 7.109E-02 | 1.578E+10        | 9.9796E+01    | 7.095E-02 | 1.570E+10        | 0.006 |
| 1s3p 3P <sub>2</sub> <sup>o</sup> | 1s3d 3D <sub>1</sub>              | 1.2588E+03    | 2.725E-04 | 3.823E+05        |               |           |                  | 0.053 |
| 1s <sup>2</sup> 1S <sub>0</sub>   | 1s3p 3P <sub>1</sub> <sup>o</sup> | 3.4460E-01    | 9.869E-02 | 1.847E+15        | 3.4323E-01    | 1.055E-01 | 1.975E+15        | 0.020 |
| 1s2s 3S <sub>1</sub>              | 1s3p 1P <sub>1</sub> <sup>o</sup> | 2.1220E+00    | 9.943E-02 | 4.910E+13        | 2.1129E+00    | 1.031E-01 | 5.095E+13        | 0.004 |
| 1s2s 1S <sub>0</sub>              | 1s3p 1P <sub>1</sub> <sup>o</sup> | 2.1534E+00    | 2.439E-01 | 1.170E+14        | 2.1446E+00    | 2.435E-01 | 1.167E+14        | 0.004 |
| 1s3s 3S <sub>1</sub>              | 1s3p 1P <sub>1</sub> <sup>o</sup> | 8.4608E+01    | 5.893E-02 | 1.830E+10        | 8.4198E+01    | 5.901E-02 | 1.835E+10        | 0.020 |
| 1s3s 1S <sub>0</sub>              | 1s3p 1P <sub>1</sub> <sup>o</sup> | 9.9937E+01    | 1.175E-01 | 2.616E+10        | 9.9635E+01    | 1.170E-01 | 2.599E+10        | 0.026 |
| 1s3d 3D <sub>2</sub>              | 1s3p 1P <sub>1</sub> <sup>o</sup> | 8.0349E+03    | 6.680E-05 | 2.301E+03        |               |           |                  | 0.383 |
| 1s3d 3D <sub>1</sub>              | 1s3p 1P <sub>1</sub> <sup>o</sup> | 2.2947E+05    | 6.878E-06 | 2.904E-01        |               |           |                  | 0.978 |
| 1s2p 3P <sub>2</sub> <sup>o</sup> | 1s3d 3D <sub>3</sub>              | 2.2910E+00    | 2.807E+00 | 5.095E+14        | 2.2814E+00    | 2.875E+00 | 5.219E+14        | 0.001 |
| 1s3p 3P <sub>2</sub> <sup>o</sup> | 1s3d 3D <sub>3</sub>              | 2.7769E+02    | 1.088E-01 | 1.345E+09        | 2.7772E+02    | 1.082E-01 | 1.326E+09        | 0.004 |
| 1s2p 3P <sub>1</sub> <sup>o</sup> | 1s3d 1D <sub>2</sub>              | 2.1371E+00    | 2.237E-03 | 6.534E+11        | 2.1283E+00    | 2.733E-03 | 7.982E+11        | 0.001 |
| 1s2p 3P <sub>2</sub> <sup>o</sup> | 1s3d 1D <sub>2</sub>              | 2.2905E+00    | 1.988E-01 | 5.056E+13        | 2.2809E+00    | 2.036E-01 | 5.177E+13        | 0.001 |
| 1s2p 1P <sub>1</sub> <sup>o</sup> | 1s3d 1D <sub>2</sub>              | 2.3053E+00    | 1.814E+00 | 4.553E+14        | 2.2959E+00    | 1.836E+00 | 4.607E+14        | 0.001 |
| 1s3p 3P <sub>1</sub> <sup>o</sup> | 1s3d 1D <sub>2</sub>              | 7.6708E+01    | 2.981E-04 | 6.759E+07        | 7.6517E+01    | 2.967E-04 | 6.704E+07        | 0.000 |
| 1s3p 3P <sub>2</sub> <sup>o</sup> | 1s3d 1D <sub>2</sub>              | 2.6938E+02    | 7.955E-03 | 1.463E+08        | 2.6926E+02    | 7.908E-03 | 1.442E+08        | 0.018 |
| 1s3p 1P <sub>1</sub> <sup>o</sup> | 1s3d 1D <sub>2</sub>              | 3.4323E+02    | 5.654E-02 | 6.403E+08        | 3.4458E+02    | 5.610E-02 | 6.249E+08        | 0.015 |
| 1s2p 3P <sub>1</sub> <sup>o</sup> | 1s4s 3S <sub>1</sub>              | 1.6341E+00    | 6.721E-03 | 5.596E+12        | 1.6274E+00    | 6.812E-03 | 5.671E+12        | 0.003 |
| 1s2p 3P <sub>0</sub> <sup>o</sup> | 1s4s 3S <sub>1</sub>              | 1.6354E+00    | 3.290E-03 | 2.735E+12        | 1.6286E+00    | 3.273E-03 | 2.721E+12        | 0.000 |
| 1s2p 3P <sub>0</sub> <sup>o</sup> | 1s4s 3S <sub>1</sub>              | 1.7223E+00    | 2.273E-02 | 1.703E+13        | 1.7151E+00    | 2.261E-02 | 1.694E+13        | 0.001 |
| 1s2p 1P <sub>1</sub> <sup>o</sup> | 1s4s 3S <sub>1</sub>              | 1.7308E+00    | 4.129E-03 | 3.065E+12        | 1.7236E+00    | 4.044E-03 | 3.001E+12        | 0.002 |
| 1s3p 3P <sub>0</sub> <sup>o</sup> | 1s4s 3S <sub>1</sub>              | 6.3675E+00    | 7.121E-02 | 3.905E+12        | 6.3413E+00    | 7.108E-02 | 3.897E+12        | 0.000 |
| 1s3p 3P <sub>0</sub> <sup>o</sup> | 1s4s 3S <sub>1</sub>              | 6.3727E+00    | 3.469E-02 | 1.899E+12        | 6.3462E+00    | 3.391E-02 | 1.856E+12        | 0.001 |
| 1s3p 3P <sub>2</sub> <sup>o</sup> | 1s4s 3S <sub>1</sub>              | 6.7695E+00    | 2.464E-01 | 1.195E+13        | 6.7412E+00    | 2.453E-01 | 1.190E+13        | 0.001 |
| 1s3p 1P <sub>1</sub> <sup>o</sup> | 1s4s 3S <sub>1</sub>              | 6.8063E+00    | 4.518E-02 | 2.169E+12        | 6.7783E+00    | 4.436E-02 | 2.128E+12        | 0.001 |
| 1s <sup>2</sup> 1S <sub>0</sub>   | 1s4p 3P <sub>1</sub> <sup>o</sup> | 3.2790E-01    | 1.510E-02 | 3.121E+14        | 3.2662E-01    | 1.433E-02 | 2.962E+14        | 0.013 |
| 1s2s 3S <sub>1</sub>              | 1s4p 3P <sub>1</sub> <sup>o</sup> | 1.6159E+00    | 6.856E-02 | 5.839E+13        | 1.6090E+00    | 6.888E-02 | 5.866E+13        | 0.002 |
| 1s2s 1S <sub>0</sub>              | 1s4p 3P <sub>1</sub> <sup>o</sup> | 1.6340E+00    | 2.993E-02 | 2.492E+13        | 1.6273E+00    | 2.929E-02 | 2.438E+13        | 0.006 |
| 1s3s 3S <sub>1</sub>              | 1s4p 3P <sub>1</sub> <sup>o</sup> | 6.2721E+00    | 3.224E-01 | 1.822E+13        | 6.2463E+00    | 3.272E-01 | 1.849E+13        | 0.002 |
| 1s3s 1S <sub>0</sub>              | 1s4p 3P <sub>1</sub> <sup>o</sup> | 6.3443E+00    | 1.439E-01 | 7.951E+12        | 6.3190E+00    | 1.408E-01 | 7.778E+12        | 0.003 |
| 1s3d 3D <sub>2</sub>              | 1s4p 3P <sub>1</sub> <sup>o</sup> | 6.7686E+00    | 7.309E-02 | 3.547E+12        | 6.7403E+00    | 7.330E-02 | 3.557E+12        | 0.000 |
| 1s3d 3D <sub>1</sub>              | 1s4p 3P <sub>1</sub> <sup>o</sup> | 6.7741E+00    | 1.585E-02 | 7.680E+11        | 6.7458E+00    | 1.555E-02 | 7.537E+11        | 0.002 |
| 1s3d 1D <sub>2</sub>              | 1s4p 3P <sub>1</sub> <sup>o</sup> | 6.9107E+00    | 1.013E-04 | 4.717E+09        |               |           |                  | 0.003 |
| 1s4s 3S <sub>1</sub>              | 1s4p 3P <sub>1</sub> <sup>o</sup> | 1.4439E+03    | 2.625E-02 | 2.800E+07        | 1.4544E+03    | 2.601E-02 | 2.711E+07        | 0.173 |
| 1s2p 3P <sub>1</sub> <sup>o</sup> | 1s4s 1S <sub>0</sub>              | 1.6322E+00    | 2.684E-03 | 6.721E+12        | 1.6254E+00    | 2.783E-03 | 6.967E+12        | 0.005 |

(continued on next page)

Table 3 (continued)

| Lower                   | Upper          | GRASP2K       |           |                  | FAC           |           |                  | dT    |
|-------------------------|----------------|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|                         |                | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) |       |
| 1s2p $^1P_1^o$          | 1s4s $^1S_0$   | 1.7286E+00    | 9.390E-03 | 2.096E+13        | 1.7214E+00    | 9.412E-03 | 2.100E+13        | 0.002 |
| 1s3p $^3P_1^o$          | 1s4s $^1S_0$   | 6.3380E+00    | 2.847E-02 | 4.727E+12        | 6.3116E+00    | 2.931E-02 | 4.867E+12        | 0.002 |
| 1s3p $^1P_1^o$          | 1s4s $^1S_0$   | 6.7725E+00    | 1.006E-01 | 1.463E+13        | 6.7444E+00    | 1.020E-01 | 1.484E+13        | 0.001 |
| 1s4p $^3P_1^o$          | 1s4s $^1S_0$   | 2.5265E+04    | 6.429E-04 | 6.718E+03        | 1.8312E+04    | 8.806E-04 | 1.736E+04        | 0.482 |
| 1s2s $^3S_1$            | 1s4p $^3P_0^o$ | 1.6157E+00    | 3.257E-02 | 8.322E+13        | 1.6089E+00    | 3.284E-02 | 8.391E+13        | 0.003 |
| 1s3s $^3S_1$            | 1s4p $^3P_0^o$ | 6.2701E+00    | 1.531E-01 | 2.598E+13        | 6.2444E+00    | 1.569E-01 | 2.661E+13        | 0.003 |
| 1s3d $^3D_1$            | 1s4p $^3P_0^o$ | 6.7718E+00    | 2.941E-02 | 4.278E+12        | 6.7435E+00    | 2.941E-02 | 4.277E+12        | 0.002 |
| 1s4s $^3S_1$            | 1s4p $^3P_0^o$ | 1.3452E+03    | 1.349E-02 | 4.973E+07        | 1.3572E+03    | 1.332E-02 | 4.783E+07        | 0.146 |
| 1s2s $^3S_1$            | 1s4p $^3P_2^o$ | 1.6057E+00    | 1.450E-01 | 7.505E+13        | 1.5989E+00    | 1.491E-01 | 7.718E+13        | 0.003 |
| 1s3s $^3S_1$            | 1s4p $^3P_2^o$ | 6.1216E+00    | 6.028E-01 | 2.146E+13        | 6.0965E+00    | 6.147E-01 | 2.187E+13        | 0.003 |
| 1s3d $^3D_2$            | 1s4p $^3P_2^o$ | 6.5936E+00    | 8.587E-03 | 2.635E+11        | 6.5661E+00    | 8.500E-03 | 2.607E+11        | 0.000 |
| 1s3d $^3D_1$            | 1s4p $^3P_2^o$ | 6.5989E+00    | 9.266E-04 | 2.839E+10        | 6.5713E+00    | 9.191E-04 | 2.815E+10        | 0.003 |
| 1s3d $^3D_3$            | 1s4p $^3P_2^o$ | 6.7234E+00    | 9.374E-02 | 2.766E+12        | 6.6951E+00    | 9.195E-02 | 2.713E+12        | 0.001 |
| 1s3d $^1D_2$            | 1s4p $^3P_2^o$ | 6.7284E+00    | 6.658E-03 | 1.962E+11        | 6.7001E+00    | 6.480E-03 | 1.909E+11        | 0.003 |
| 1s4s $^3S_1$            | 1s4p $^3P_2^o$ | 2.1675E+02    | 4.308E-01 | 1.223E+10        | 2.1631E+02    | 4.309E-01 | 1.218E+10        | 0.025 |
| 1s2p $^3P_0^o$          | 1s4d $^3D_2$   | 1.6212E+00    | 2.941E-01 | 1.493E+14        | 1.6144E+00    | 2.954E-01 | 1.499E+14        | 0.001 |
| 1s2p $^3P_1^o$          | 1s4d $^3D_2$   | 1.7079E+00    | 5.276E-02 | 2.413E+13        | 1.7070E+00    | 5.191E-02 | 2.374E+13        | 0.001 |
| 1s2p $^1P_1^o$          | 1s4d $^3D_2$   | 1.7162E+00    | 8.902E-03 | 4.032E+12        | 1.7091E+00    | 8.758E-03 | 3.966E+12        | 0.002 |
| 1s3p $^3P_0^o$          | 1s4d $^3D_2$   | 6.1751E+00    | 1.295E+00 | 4.531E+13        | 6.1494E+00    | 1.301E+00 | 4.554E+13        | 0.001 |
| 1s3p $^3P_1^o$          | 1s4d $^3D_2$   | 6.5523E+00    | 2.758E-01 | 8.571E+12        | 6.5248E+00    | 2.781E-01 | 8.643E+12        | 0.001 |
| 1s3p $^1P_1^o$          | 1s4d $^3D_2$   | 6.5868E+00    | 4.612E-02 | 1.418E+12        | 6.5595E+00    | 4.379E-02 | 1.346E+12        | 0.001 |
| 1s4p $^3P_1^o$          | 1s4d $^3D_2$   | 2.3795E+02    | 3.169E-01 | 7.465E+09        | 2.3625E+02    | 3.177E-01 | 7.531E+09        | 0.000 |
| 1s4p $^3P_2^o$          | 1s4d $^3D_2$   | 3.5515E+03    | 3.857E-03 | 4.079E+05        |               |           |                  | 0.046 |
| 1s2p $^3P_1^o$          | 1s4d $^3D_1$   | 1.6210E+00    | 6.298E-02 | 5.329E+13        | 1.6143E+00    | 6.329E-02 | 5.354E+13        | 0.001 |
| 1s2p $^3P_0^o$          | 1s4d $^3D_1$   | 1.6223E+00    | 1.192E-01 | 1.007E+14        | 1.6155E+00    | 1.195E-01 | 1.009E+14        | 0.001 |
| 1s2p $^3P_2^o$          | 1s4d $^3D_1$   | 1.7078E+00    | 5.792E-03 | 4.416E+12        | 1.7006E+00    | 5.679E-03 | 4.329E+12        | 0.001 |
| 1s2p $^1P_1^o$          | 1s4d $^3D_1$   | 1.7161E+00    | 2.583E-02 | 1.950E+13        | 1.7090E+00    | 2.527E-02 | 1.907E+13        | 0.002 |
| 1s3p $^3P_0^o$          | 1s4d $^3D_1$   | 6.1732E+00    | 2.754E-01 | 1.607E+13        | 6.1476E+00    | 2.797E-01 | 1.631E+13        | 0.001 |
| 1s3p $^3P_1^o$          | 1s4d $^3D_1$   | 6.1781E+00    | 5.239E-01 | 3.052E+13        | 6.1522E+00    | 5.268E-01 | 3.068E+13        | 0.001 |
| 1s3p $^3P_2^o$          | 1s4d $^3D_1$   | 6.5502E+00    | 3.014E-02 | 1.562E+12        | 6.5227E+00    | 3.037E-02 | 1.573E+12        | 0.001 |
| 1s3p $^1P_1^o$          | 1s4d $^3D_1$   | 6.5847E+00    | 1.379E-01 | 7.069E+12        | 6.5574E+00    | 1.381E-01 | 7.082E+12        | 0.001 |
| 1s4p $^3P_0^o$          | 1s4d $^3D_1$   | 2.3523E+02    | 6.848E-02 | 2.752E+09        | 2.3358E+02    | 6.867E-02 | 2.774E+09        | 0.006 |
| 1s4p $^3P_1^o$          | 1s4d $^3D_1$   | 2.3807E+02    | 1.279E-01 | 5.016E+09        | 2.3629E+02    | 1.282E-01 | 5.063E+09        | 0.005 |
| 1s4p $^3P_2^o$          | 1s4d $^3D_1$   | 3.0279E+03    | 4.889E-04 | 1.186E+05        |               |           |                  | 0.032 |
| 1s <sup>2</sup> $^1S_0$ | 1s4p $^1P_1^o$ | 3.2750E-01    | 3.647E-02 | 7.559E+14        | 3.2616E-01    | 3.896E-02 | 8.074E+14        | 0.028 |
| 1s2s $^3S_1$            | 1s4p $^1P_1^o$ | 1.6048E+00    | 2.578E-02 | 2.226E+13        | 1.5980E+00    | 2.662E-02 | 2.298E+13        | 0.003 |
| 1s2s $^1S_0$            | 1s4p $^1P_1^o$ | 1.6227E+00    | 6.199E-02 | 5.234E+13        | 1.6161E+00    | 6.223E-02 | 5.253E+13        | 0.004 |
| 1s3s $^3S_1$            | 1s4p $^1P_1^o$ | 6.1092E+00    | 1.059E-01 | 6.309E+12        | 6.0840E+00    | 1.087E-01 | 6.475E+12        | 0.003 |
| 1s3s $^1S_0$            | 1s4p $^1P_1^o$ | 6.1776E+00    | 2.605E-01 | 1.518E+13        | 6.1529E+00    | 2.580E-01 | 1.502E+13        | 0.002 |
| 1s3d $^3D_2$            | 1s4p $^1P_1^o$ | 6.5793E+00    | 1.389E-03 | 7.134E+10        | 6.5517E+00    | 1.599E-03 | 8.215E+10        | 0.004 |
| 1s3d $^3D_1$            | 1s4p $^1P_1^o$ | 6.5845E+00    | 4.203E-03 | 2.156E+11        | 6.5569E+00    | 4.162E-03 | 2.134E+11        | 0.003 |
| 1s3d $^1D_2$            | 1s4p $^1P_1^o$ | 6.7135E+00    | 5.832E-02 | 2.877E+12        | 6.6851E+00    | 5.917E-02 | 2.918E+12        | 0.003 |
| 1s4s $^3S_1$            | 1s4p $^1P_1^o$ | 2.0225E+02    | 8.298E-02 | 4.510E+09        | 2.0166E+02    | 8.289E-02 | 4.493E+09        | 0.022 |
| 1s4s $^1S_0$            | 1s4p $^1P_1^o$ | 2.3741E+02    | 1.660E-01 | 6.547E+09        | 2.3715E+02    | 1.651E-01 | 6.471E+09        | 0.032 |
| 1s4d $^3D_2$            | 1s4p $^1P_1^o$ | 2.0339E+04    | 1.101E-04 | 5.916E+02        |               |           |                  | 0.306 |
| 1s4d $^3D_1$            | 1s4p $^1P_1^o$ | 2.1218E+06    | 3.210E-06 | 1.585E-03        |               |           |                  | 0.996 |
| 1s2p $^3P_2^o$          | 1s4d $^3D_3$   | 1.7043E+00    | 5.008E-01 | 1.643E+14        | 1.6972E+00    | 5.104E-01 | 1.674E+14        | 0.001 |
| 1s3p $^3P_2^o$          | 1s4d $^3D_3$   | 6.4997E+00    | 2.449E+00 | 5.523E+13        | 6.4725E+00    | 2.491E+00 | 5.619E+13        | 0.001 |
| 1s4p $^3P_2^o$          | 1s4d $^3D_3$   | 6.5884E+02    | 1.960E-01 | 4.302E+08        | 6.5162E+02    | 1.972E-01 | 4.388E+08        | 0.008 |
| 1s3d $^3D_2$            | 1s4f $^3F_3^o$ | 6.5275E+00    | 4.625E+00 | 1.034E+14        | 6.5002E+00    | 4.642E+00 | 1.038E+14        | 0.001 |
| 1s3d $^3D_3$            | 1s4f $^3F_3^o$ | 6.6546E+00    | 3.174E-01 | 6.829E+12        | 6.6265E+00    | 3.157E-01 | 6.793E+12        | 0.001 |
| 1s3d $^1D_2$            | 1s4f $^3F_3^o$ | 6.6595E+00    | 1.909E-02 | 4.102E+11        | 6.6315E+00    | 1.914E-02 | 4.113E+11        | 0.001 |
| 1s4d $^3D_2$            | 1s4f $^3F_3^o$ | 7.9649E+02    | 9.484E-02 | 1.425E+08        | 8.0096E+02    | 9.391E-02 | 1.383E+08        | 0.017 |
| 1s4d $^3D_3$            | 1s4f $^3F_3^o$ | 5.1914E+04    | 9.767E-05 | 3.453E+01        |               |           |                  | 0.674 |
| 1s2s $^3S_1$            | 1s4f $^3F_2^o$ | 1.6017E+00    | 3.265E-09 | 1.698E+06        | 1.5949E+00    | 1.924E-08 | 1.000E+07        | 0.151 |
| 1s3s $^3S_1$            | 1s4f $^3F_2^o$ | 6.0636E+00    | 3.445E-06 | 1.250E+08        |               |           |                  | 0.008 |
| 1s3d $^3D_2$            | 1s4f $^3F_2^o$ | 6.5264E+00    | 3.322E-01 | 1.040E+13        | 6.4991E+00    | 3.338E-01 | 1.045E+13        | 0.000 |
| 1s3d $^3D_1$            | 1s4f $^3F_2^o$ | 6.5315E+00    | 2.975E+00 | 9.304E+13        | 6.5041E+00    | 2.983E+00 | 9.330E+13        | 0.000 |
| 1s3d $^1D_2$            | 1s4f $^3F_2^o$ | 6.6535E+00    | 1.590E-02 | 4.793E+11        | 6.6254E+00    | 1.582E-02 | 4.767E+11        | 0.000 |
| 1s3d $^1D_1$            | 1s4f $^3F_2^o$ | 6.6584E+00    | 2.213E-01 | 6.660E+12        | 6.6303E+00    | 2.198E-01 | 6.613E+12        | 0.001 |
| 1s4s $^3S_1$            | 1s4f $^3F_2^o$ | 1.6191E+02    | 3.320E-07 | 1.689E+04        | 1.6143E+02    | 3.195E-07 | 1.622E+04        | 0.102 |
| 1s4d $^3D_2$            | 1s4f $^3F_2^o$ | 7.8052E+02    | 6.988E-03 | 1.530E+07        | 7.8473E+02    | 6.922E-03 | 1.486E+07        | 0.012 |
| 1s4d $^3D_1$            | 1s4f $^3F_2^o$ | 8.1135E+02    | 5.989E-02 | 1.214E+08        | 8.1580E+02    | 5.930E-02 | 1.178E+08        | 0.014 |
| 1s4d $^3D_3$            | 1s4f $^3F_2^o$ | 2.2242E+04    | 1.126E-05 | 3.037E+01        |               |           |                  | 0.079 |
| 1s2p $^3P_0^o$          | 1s4d $^1D_2$   | 1.6178E+00    | 3.977E-04 | 2.027E+11        | 1.6111E+00    | 4.270E-04 | 2.176E+11        | 0.002 |
| 1s2p $^3P_1^o$          | 1s4d $^1D_2$   | 1.7042E+00    | 3.537E-02 | 1.625E+13        | 1.6970E+00    | 3.597E-02 | 1.652E+13        | 0.001 |
| 1s2p $^1P_1^o$          | 1s4d $^1D_2$   | 1.7124E+00    | 3.214E-01 | 1.462E+14        | 1.7053E+00    | 3.266E-01 | 1.485E+14        | 0.001 |
| 1s3p $^3P_0^o$          | 1s4d $^1D_2$   | 6.1264E+00    | 1.393E-03 | 4.950E+10        | 6.1011E+00    | 1.823E-03 | 6.480E+10        | 0.001 |
| 1s3p $^3P_1^o$          | 1s4d $^1D_2$   | 6.4976E+00    | 1.724E-01 | 5.448E+12        | 6.4704E+00    | 1.755E-01 | 5.545E+12        | 0.001 |
| 1s3p $^1P_1^o$          | 1s4d $^1D_2$   | 6.5315E+00    | 1.593E+00 | 4.980E+13        | 6.5045E+00    | 1.594E+00 | 4.985E+13        | 0.001 |
| 1s4p $^3P_0^o$          | 1s4d $^1D_2$   | 1.8218E+02    | 4.542E-04 | 1.826E+07        | 1.8111E+02    | 4.521E-04 | 1.823E+07        | 0.010 |

(continued on next page)

Table 3 (continued)

| Lower  | Upper  | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|--|--|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|  |  | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4d <sup>1</sup> D <sub>2</sub>              | 6.3767E+02    | 1.428E-02 | 4.685E+07              | 6.3050E+02    | 1.435E-02 | 4.775E+07              | 0.013 |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 4d <sup>1</sup> D <sub>2</sub>              | 8.0810E+02    | 1.027E-01 | 2.098E+08              | 7.9983E+02    | 1.033E-01 | 2.136E+08              | 0.014 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 4d <sup>1</sup> D <sub>2</sub>              | 3.2125E+04    | 1.005E-05 | 1.300E+01              |               |           |                        | 0.305 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 4d <sup>1</sup> D <sub>2</sub>              | 1.8409E+05    | 1.913E-05 | 7.530E-01              |               |           |                        | 0.815 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 6.6276E+00    | 6.440E+00 | 1.087E+14              | 6.5997E+00    | 6.489E+00 | 1.094E+14              | 0.000 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.5856E+03    | 6.582E-02 | 1.940E+07              | 1.6034E+03    | 6.481E-02 | 1.852E+07              | 0.023 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 6.5007E+00    | 1.376E-04 | 3.102E+09              |               |           |                        | 0.001 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 6.6268E+00    | 2.397E-01 | 5.202E+12              | 6.5989E+00    | 2.415E-01 | 5.241E+12              | 0.000 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 6.6317E+00    | 4.771E+00 | 1.034E+14              | 6.6038E+00    | 4.802E+00 | 1.040E+14              | 0.000 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.3023E+02    | 7.960E-06 | 2.698E+04              | 5.3185E+02    | 8.835E-06 | 2.951E+04              | 0.047 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.5391E+03    | 2.525E-03 | 1.016E+06              | 1.5556E+03    | 2.486E-03 | 9.708E+05              | 0.009 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6685E+03    | 4.632E-02 | 1.585E+07              | 1.6908E+03    | 4.551E-02 | 1.504E+07              | 0.015 |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.4605E+00    | 2.662E-03 | 2.774E+12              | 1.4544E+00    | 2.703E-03 | 2.817E+12              | 0.002 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.4615E+00    | 1.303E-03 | 1.356E+12              | 1.4554E+00    | 1.301E-03 | 1.354E+12              | 0.001 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.5306E+00    | 8.845E-03 | 8.395E+12              | 1.5241E+00    | 8.802E-03 | 8.353E+12              | 0.002 |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.5372E+00    | 1.606E-03 | 1.511E+12              | 1.5308E+00    | 1.572E-03 | 1.479E+12              | 0.002 |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 4.3516E+00    | 1.619E-02 | 1.901E+12              | 4.3336E+00    | 1.622E-02 | 1.904E+12              | 0.001 |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 4.3540E+00    | 7.886E-03 | 9.249E+11              | 4.3359E+00    | 7.777E-03 | 9.119E+11              | 0.001 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 4.5356E+00    | 5.271E-02 | 5.697E+12              | 4.5167E+00    | 5.254E-02 | 5.678E+12              | 0.000 |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 4.5521E+00    | 9.615E-03 | 1.032E+12              | 4.5333E+00    | 9.475E-03 | 1.016E+12              | 0.001 |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.3877E+01    | 1.166E-01 | 1.346E+12              | 1.3818E+01    | 1.159E-01 | 1.339E+12              | 0.001 |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.3887E+01    | 5.665E-02 | 6.532E+11              | 1.3827E+01    | 5.525E-02 | 6.371E+11              | 0.002 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.4675E+01    | 3.952E-01 | 4.080E+12              | 1.4612E+01    | 3.932E-01 | 4.060E+12              | 0.001 |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.4747E+01    | 7.255E-02 | 7.417E+11              | 1.4684E+01    | 7.130E-02 | 7.289E+11              | 0.001 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.5020E+01    | 4.244E-08 | 4.183E+05              |               |           |                        | 0.057 |
| 1s 2s <sup>1</sup> S <sub>0</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 3.2030E-01    | 7.183E-03 | 1.556E+14              | 3.1904E-01    | 6.799E-03 | 1.472E+14              | 0.011 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.4466E+00    | 2.787E-02 | 2.961E+13              | 1.4405E+00    | 2.788E-02 | 2.962E+13              | 0.002 |
| 1s 2s <sup>1</sup> S <sub>0</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.4611E+00    | 1.211E-02 | 1.261E+13              | 1.4551E+00    | 1.185E-02 | 1.234E+13              | 0.006 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.3132E+00    | 8.123E-02 | 9.709E+12              | 4.2953E+00    | 8.191E-02 | 9.788E+12              | 0.002 |
| 1s 3s <sup>1</sup> S <sub>0</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.3472E+00    | 3.579E-02 | 4.210E+12              | 4.3296E+00    | 3.517E-02 | 4.136E+12              | 0.002 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.5423E+00    | 1.400E-02 | 1.509E+12              | 4.5233E+00    | 1.405E-02 | 1.514E+12              | 0.001 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.5448E+00    | 3.276E-03 | 3.276E+11              | 4.5258E+00    | 2.992E-03 | 3.221E+11              | 0.004 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.6059E+00    | 1.856E-05 | 1.945E+09              |               |           |                        | 0.012 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.3679E+01    | 3.607E-01 | 4.285E+12              | 1.3623E+01    | 3.658E-01 | 4.346E+12              | 0.002 |
| 1s 4s <sup>1</sup> S <sub>0</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.3818E+01    | 1.618E-01 | 1.884E+12              | 1.3762E+01    | 1.583E-01 | 1.843E+12              | 0.001 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.4661E+01    | 1.771E-01 | 1.832E+12              | 1.4602E+01    | 1.772E-01 | 1.832E+12              | 0.000 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.4671E+01    | 3.825E-02 | 3.951E+11              | 1.4612E+01    | 3.753E-02 | 3.875E+11              | 0.002 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.4943E+01    | 2.115E-04 | 2.106E+09              | 1.4882E+01    | 1.298E-04 | 1.292E+09              | 0.007 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 2.8648E+03    | 3.352E-02 | 9.081E+06              | 2.9004E+03    | 3.303E-02 | 8.656E+06              | 0.158 |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>0</sub>              | 1.4597E+00    | 1.072E-03 | 3.357E+12              | 1.4537E+00    | 1.107E-03 | 3.465E+12              | 0.007 |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>0</sub>              | 1.5363E+00    | 3.681E-03 | 1.040E+13              | 1.5300E+00    | 3.664E-03 | 1.035E+13              | 0.003 |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>0</sub>              | 4.3447E+00    | 6.572E-03 | 2.322E+12              | 4.3266E+00    | 6.732E-03 | 2.378E+12              | 0.001 |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>0</sub>              | 4.5445E+00    | 2.173E-02 | 7.020E+12              | 4.5257E+00    | 2.187E-02 | 7.061E+12              | 0.000 |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>0</sub>              | 1.4807E+01    | 4.696E-02 | 1.643E+12              | 1.3747E+01    | 4.812E-02 | 1.684E+12              | 0.000 |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>0</sub>              | 1.4668E+01    | 1.615E-01 | 5.008E+12              | 1.4605E+01    | 1.637E-01 | 5.077E+12              | 0.000 |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5s <sup>3</sup> S <sub>0</sub>              | 5.6589E+04    | 7.282E-04 | 1.517E+03              | 3.7737E+04    | 1.084E-03 | 5.038E+03              | 0.577 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.4465E+00    | 1.324E-02 | 4.222E+13              | 1.4404E+00    | 1.328E-02 | 4.235E+13              | 0.003 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.3127E+00    | 3.863E-02 | 1.385E+13              | 4.2949E+00    | 3.919E-02 | 1.405E+13              | 0.003 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.5443E+00    | 5.643E-03 | 1.823E+12              | 4.5253E+00    | 5.635E-03 | 1.819E+12              | 0.004 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.3675E+01    | 1.715E-01 | 6.118E+12              | 1.3619E+01    | 1.758E-01 | 6.271E+12              | 0.003 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.4666E+01    | 7.131E-02 | 2.212E+12              | 1.4607E+01    | 7.119E-02 | 2.206E+12              | 0.002 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 2.6711E+03    | 1.723E-02 | 1.611E+07              | 2.7075E+03    | 1.693E-02 | 1.527E+07              | 0.131 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.4424E+00    | 6.070E-02 | 3.892E+13              | 1.4363E+00    | 6.235E-02 | 3.998E+13              | 0.002 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.2763E+00    | 1.651E-01 | 1.205E+13              | 4.2586E+00    | 1.679E-01 | 1.225E+13              | 0.003 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.5014E+00    | 1.723E-03 | 1.135E+11              | 4.4826E+00    | 1.717E-03 | 1.130E+11              | 0.002 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.5039E+00    | 1.857E-04 | 1.222E+10              | 4.4850E+00    | 1.847E-04 | 1.214E+10              | 0.005 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.5615E+00    | 1.853E-02 | 1.188E+12              | 4.5423E+00    | 1.822E-02 | 1.168E+12              | 0.002 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.5638E+00    | 1.318E-03 | 8.443E+10              | 4.5447E+00    | 1.283E-03 | 8.220E+10              | 0.005 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.3315E+01    | 6.598E-01 | 4.965E+12              | 1.3261E+01    | 6.702E-01 | 5.041E+12              | 0.003 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.4243E+01    | 2.163E-02 | 1.422E+11              | 1.4186E+01    | 2.133E-02 | 1.402E+11              | 0.001 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.4253E+01    | 2.338E-03 | 1.535E+10              | 1.4196E+01    | 2.306E-03 | 1.513E+10              | 0.002 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.4499E+01    | 2.318E-01 | 1.471E+12              | 1.4440E+01    | 2.276E-01 | 1.444E+12              | 0.001 |
| 1s 4d <sup>1</sup> D <sub>3</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.4509E+01    | 1.640E-02 | 1.039E+11              | 1.4450E+01    | 1.598E-02 | 1.012E+11              | 0.002 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.2565E+02    | 5.519E-01 | 4.064E+09              | 4.2515E+02    | 5.512E-01 | 4.033E+09              | 0.022 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4552E+00    | 1.097E-01 | 6.914E+13              | 1.4491E+00    | 1.101E-01 | 6.935E+13              | 0.001 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.5247E+00    | 1.907E-02 | 1.094E+13              | 1.5183E+00    | 1.865E-02 | 1.070E+13              | 0.002 |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.5313E+00    | 3.170E-03 | 1.803E+12              | 1.5250E+00    | 3.140E-03 | 1.786E+12              | 0.002 |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.3049E+00    | 3.188E-01 | 2.295E+13              | 4.2870E+00    | 3.199E-01 | 2.302E+13              | 0.001 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.4849E+00    | 6.198E-02 | 4.111E+12              | 4.4661E+00    | 6.194E-02 | 4.107E+12              | 0.001 |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.5010E+00    | 1.016E-02 | 6.693E+11              | 4.4823E+00    | 9.871E-03 | 6.499E+11              | 0.002 |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.3413E+01    | 1.225E+00 | 9.083E+12              | 1.3354E+01    | 1.230E+00 | 9.125E+12              | 0.000 |

(continued on next page)



Table 3 (continued)

| Lower           | Upper          | GRASP2K       |           |                  | FAC           |           |                  | dT    |
|-----------------|----------------|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|                 |                | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) |       |
| 1s4p $^3P_2^0$  | 1s5d $^3D_2$   | 1.4158E+01    | 2.724E-01 | 1.813E+12        | 1.4095E+01    | 2.756E-01 | 1.835E+12        | 0.001 |
| 1s4p $^1P_1^0$  | 1s5d $^3D_2$   | 1.4224E+01    | 4.478E-02 | 2.952E+11        | 1.4162E+01    | 4.221E-02 | 2.784E+11        | 0.001 |
| 1s4f $^3F_3^0$  | 1s5d $^3D_2$   | 1.4473E+01    | 6.876E-02 | 4.380E+11        | 1.4409E+01    | 6.894E-02 | 4.392E+11        | 0.001 |
| 1s4f $^3F_2^0$  | 1s5d $^3D_2$   | 1.4478E+01    | 5.008E-03 | 3.187E+10        | 1.4414E+01    | 5.000E-03 | 3.183E+10        | 0.000 |
| 1s4f $^1F_3^0$  | 1s5d $^3D_2$   | 1.4606E+01    | 5.098E-06 | 3.188E+07        |               |           |                  | 0.008 |
| 1s5p $^3P_0^0$  | 1s5d $^3D_2$   | 4.6651E+02    | 4.431E-01 | 2.716E+09        | 4.6168E+02    | 4.458E-01 | 2.766E+09        | 0.001 |
| 1s5p $^3P_2^0$  | 1s5d $^3D_2$   | 6.9791E+03    | 5.402E-03 | 1.480E+05        |               |           |                  | 0.074 |
| 1s $^2$ $^1S_0$ | 1s5p $^1P_1^0$ | 3.2010E-01    | 1.758E-02 | 3.812E+14        | 3.1882E-01    | 1.876E-02 | 4.069E+14        | 0.030 |
| 1s2s $^3S_1$    | 1s5p $^1P_1^0$ | 1.4421E+00    | 1.083E-02 | 1.158E+13        | 1.4360E+00    | 1.116E-02 | 1.193E+13        | 0.002 |
| 1s2s $^1S_0$    | 1s5p $^1P_1^0$ | 1.4565E+00    | 2.585E-02 | 2.709E+13        | 1.4505E+00    | 2.600E-02 | 2.724E+13        | 0.003 |
| 1s3s $^3S_1$    | 1s5p $^1P_1^0$ | 4.2732E+00    | 2.926E-02 | 3.563E+12        | 4.2555E+00    | 2.990E-02 | 3.640E+12        | 0.003 |
| 1s3s $^1S_0$    | 1s5p $^1P_1^0$ | 4.3066E+00    | 7.083E-02 | 8.491E+12        | 4.2891E+00    | 7.040E-02 | 8.437E+12        | 0.001 |
| 1s3d $^3D_2$    | 1s5p $^1P_1^0$ | 4.4980E+00    | 2.798E-04 | 3.075E+10        | 4.4792E+00    | 3.159E-04 | 3.471E+10        | 0.006 |
| 1s3d $^3D_1$    | 1s5p $^1P_1^0$ | 4.5005E+00    | 8.523E-04 | 9.356E+10        | 4.4816E+00    | 8.478E-04 | 9.306E+10        | 0.006 |
| 1s3d $^1D_2$    | 1s5p $^1P_1^0$ | 4.5603E+00    | 1.161E-02 | 1.241E+12        | 4.5411E+00    | 1.171E-02 | 1.251E+12        | 0.006 |
| 1s4s $^3S_1$    | 1s5p $^1P_1^0$ | 1.3285E+01    | 1.158E-01 | 1.458E+12        | 1.3231E+01    | 1.184E-01 | 1.491E+12        | 0.003 |
| 1s4s $^1S_0$    | 1s5p $^1P_1^0$ | 1.3416E+01    | 2.856E-01 | 3.528E+12        | 1.3362E+01    | 2.818E-01 | 3.479E+12        | 0.000 |
| 1s4d $^3D_2$    | 1s5p $^1P_1^0$ | 1.4209E+01    | 3.407E-03 | 3.752E+10        | 1.4152E+01    | 3.849E-03 | 4.237E+10        | 0.003 |
| 1s4d $^3D_1$    | 1s5p $^1P_1^0$ | 1.4219E+01    | 1.055E-02 | 1.160E+11        | 1.4162E+01    | 1.040E-02 | 1.144E+11        | 0.003 |
| 1s4d $^1D_2$    | 1s5p $^1P_1^0$ | 1.4474E+01    | 1.448E-01 | 1.537E+12        | 1.4415E+01    | 1.466E-01 | 1.555E+12        | 0.003 |
| 1s5s $^3S_1$    | 1s5p $^1P_1^0$ | 3.9729E+02    | 1.063E-01 | 1.497E+09        | 3.9647E+02    | 1.060E-01 | 1.487E+09        | 0.020 |
| 1s5s $^1S_0$    | 1s5p $^1P_1^0$ | 4.6505E+02    | 2.128E-01 | 2.188E+09        | 4.6491E+02    | 2.116E-01 | 2.159E+09        | 0.040 |
| 1s5d $^3D_2$    | 1s5p $^1P_1^0$ | 4.1006E+04    | 1.481E-04 | 1.958E+02        |               |           |                  | 0.294 |
| 1s2p $^3P_0^0$  | 1s5d $^3D_1$   | 1.4551E+00    | 2.353E-02 | 2.470E+13        | 1.4491E+00    | 2.355E-02 | 2.472E+13        | 0.001 |
| 1s2p $^3P_1^0$  | 1s5d $^3D_1$   | 1.4562E+00    | 4.450E-02 | 4.666E+13        | 1.4501E+00    | 4.454E-02 | 4.669E+13        | 0.001 |
| 1s2p $^3P_2^0$  | 1s5d $^3D_1$   | 1.5247E+00    | 2.091E-03 | 2.000E+12        | 1.5182E+00    | 2.036E-03 | 1.947E+12        | 0.002 |
| 1s2p $^1P_1^0$  | 1s5d $^3D_1$   | 1.5313E+00    | 9.303E-03 | 8.822E+12        | 1.5249E+00    | 9.050E-03 | 8.580E+12        | 0.002 |
| 1s3p $^3P_0^0$  | 1s5d $^3D_1$   | 4.3044E+00    | 6.792E-02 | 8.151E+12        | 4.2865E+00    | 6.846E-02 | 8.213E+12        | 0.001 |
| 1s3p $^3P_1^0$  | 1s5d $^3D_1$   | 4.3068E+00    | 1.290E-01 | 1.546E+13        | 4.2888E+00    | 1.293E-01 | 1.550E+13        | 0.001 |
| 1s3p $^3P_2^0$  | 1s5d $^3D_1$   | 4.4844E+00    | 6.769E-03 | 7.484E+11        | 4.4656E+00    | 6.748E-03 | 7.460E+11        | 0.002 |
| 1s3p $^1P_1^0$  | 1s5d $^3D_1$   | 4.5005E+00    | 3.073E-02 | 3.374E+12        | 4.4818E+00    | 3.056E-02 | 3.354E+12        | 0.002 |
| 1s4p $^3P_0^0$  | 1s5d $^3D_1$   | 1.3409E+01    | 2.602E-01 | 3.218E+12        | 1.3350E+01    | 2.644E-01 | 3.271E+12        | 0.001 |
| 1s4p $^3P_1^0$  | 1s5d $^3D_1$   | 1.3418E+01    | 4.953E-01 | 6.116E+12        | 1.3359E+01    | 4.977E-01 | 6.148E+12        | 0.001 |
| 1s4p $^3P_2^0$  | 1s5d $^3D_1$   | 1.4153E+01    | 2.966E-02 | 3.292E+11        | 1.4090E+01    | 2.999E-02 | 3.330E+11        | 0.001 |
| 1s4p $^1P_1^0$  | 1s5d $^3D_1$   | 1.4219E+01    | 1.367E-01 | 1.504E+12        | 1.4157E+01    | 1.374E-01 | 1.512E+12        | 0.001 |
| 1s4f $^3F_3^0$  | 1s5d $^3D_1$   | 1.4473E+01    | 4.410E-02 | 4.681E+11        | 1.4409E+01    | 4.432E-02 | 4.706E+11        | 0.000 |
| 1s5p $^3P_0^0$  | 1s5d $^3D_1$   | 4.6125E+02    | 9.567E-02 | 9.998E+08        | 4.5655E+02    | 9.626E-02 | 1.018E+09        | 0.006 |
| 1s5p $^3P_1^0$  | 1s5d $^3D_1$   | 4.6670E+02    | 1.788E-01 | 1.825E+09        | 4.6173E+02    | 1.798E-01 | 1.860E+09        | 0.005 |
| 1s5p $^3P_2^0$  | 1s5d $^3D_1$   | 5.9615E+03    | 6.837E-04 | 4.277E+04        |               |           |                  | 0.014 |
| 1s5p $^1P_1^0$  | 1s5d $^3D_1$   | 1.4006E+07    | 1.340E-06 | 1.521E-05        |               |           |                  | 0.999 |
| 1s2p $^3P_2^0$  | 1s5d $^3D_3$   | 1.5233E+00    | 1.832E-01 | 7.522E+13        | 1.5168E+00    | 1.864E-01 | 7.654E+13        | 0.000 |
| 1s3p $^3P_2^0$  | 1s5d $^3D_3$   | 4.4722E+00    | 5.674E-01 | 2.703E+13        | 4.4535E+00    | 5.745E-01 | 2.737E+13        | 0.001 |
| 1s4p $^3P_2^0$  | 1s5d $^3D_3$   | 1.4032E+01    | 2.380E+00 | 1.152E+13        | 1.3970E+01    | 2.417E+00 | 1.170E+13        | 0.000 |
| 1s4f $^3F_3^0$  | 1s5d $^3D_3$   | 1.4341E+01    | 3.955E-03 | 1.833E+10        | 1.4279E+01    | 3.981E-03 | 1.844E+10        | 0.001 |
| 1s4f $^3F_2^0$  | 1s5d $^3D_3$   | 1.4347E+01    | 1.850E-04 | 8.566E+08        |               |           |                  | 0.000 |
| 1s4f $^3F_4^0$  | 1s5d $^3D_3$   | 1.4468E+01    | 8.764E-02 | 3.990E+11        | 1.4405E+01    | 8.760E-02 | 3.988E+11        | 0.001 |
| 1s4f $^1F_3^0$  | 1s5d $^3D_3$   | 1.4472E+01    | 3.270E-03 | 1.488E+10        | 1.4409E+01    | 3.258E-03 | 1.482E+10        | 0.000 |
| 1s5p $^3P_2^0$  | 1s5d $^3D_3$   | 1.2888E+03    | 2.743E-01 | 1.574E+08        | 1.2633E+03    | 2.786E-01 | 1.649E+08        | 0.012 |
| 1s3d $^3D_2$    | 1s5f $^3F_3^0$ | 4.4855E+00    | 7.286E-01 | 3.451E+13        | 4.4667E+00    | 7.301E-01 | 3.457E+13        | 0.001 |
| 1s3d $^3D_3$    | 1s5f $^3F_3^0$ | 4.5452E+00    | 4.817E-02 | 2.222E+12        | 4.5260E+00    | 4.762E-02 | 2.196E+12        | 0.001 |
| 1s3d $^1D_2$    | 1s5f $^3F_3^0$ | 4.5475E+00    | 2.879E-03 | 1.327E+11        | 4.5283E+00    | 2.884E-03 | 1.329E+11        | 0.001 |
| 1s4d $^3D_2$    | 1s5f $^3F_3^0$ | 1.4085E+01    | 3.989E+00 | 1.916E+13        | 1.4028E+01    | 3.999E+00 | 1.920E+13        | 0.000 |
| 1s4d $^3D_3$    | 1s5f $^3F_3^0$ | 1.4335E+01    | 2.801E-01 | 1.299E+12        | 1.4276E+01    | 2.797E-01 | 1.296E+12        | 0.001 |
| 1s4d $^1D_2$    | 1s5f $^3F_3^0$ | 1.4345E+01    | 1.780E-02 | 8.244E+10        | 1.4286E+01    | 1.789E-02 | 8.283E+10        | 0.001 |
| 1s5d $^3D_2$    | 1s5f $^3F_3^0$ | 1.5543E+03    | 1.737E-01 | 6.852E+07        | 1.5716E+03    | 1.710E-01 | 6.544E+07        | 0.010 |
| 1s5d $^3D_3$    | 1s5f $^3F_3^0$ | 9.3195E+04    | 1.950E-04 | 2.140E+01        |               |           |                  | 0.340 |
| 1s2s $^3S_1$    | 1s5f $^3F_2^0$ | 1.4408E+00    | 3.299E-09 | 2.120E+06        | 1.4347E+00    | 1.307E-08 | 8.404E+06        | 0.290 |
| 1s3s $^3S_1$    | 1s5f $^3F_2^0$ | 4.2617E+00    | 5.278E-07 | 3.876E+07        |               |           |                  | 0.035 |
| 1s3d $^3D_2$    | 1s5f $^3F_2^0$ | 4.4853E+00    | 5.238E-02 | 3.474E+12        | 4.4664E+00    | 5.249E-02 | 3.480E+12        | 0.000 |
| 1s3d $^3D_1$    | 1s5f $^3F_2^0$ | 4.4877E+00    | 4.685E-01 | 3.103E+13        | 4.4688E+00    | 4.693E-01 | 3.108E+13        | 0.000 |
| 1s3d $^3D_3$    | 1s5f $^3F_2^0$ | 4.5449E+00    | 2.415E-03 | 1.560E+11        | 4.5257E+00    | 2.384E-03 | 1.539E+11        | 0.001 |
| 1s3d $^1D_2$    | 1s5f $^3F_2^0$ | 4.5472E+00    | 3.357E-02 | 2.166E+12        | 4.5280E+00    | 3.314E-02 | 2.138E+12        | 0.001 |
| 1s4s $^3S_1$    | 1s5f $^3F_2^0$ | 1.3175E+01    | 3.531E-06 | 2.714E+07        |               |           |                  | 0.018 |
| 1s4d $^3D_2$    | 1s5f $^3F_2^0$ | 1.4083E+01    | 2.874E-01 | 1.933E+12        | 1.4025E+01    | 2.887E-01 | 1.941E+12        | 0.000 |
| 1s4d $^3D_1$    | 1s5f $^3F_2^0$ | 1.4092E+01    | 2.568E+00 | 1.725E+13        | 1.4035E+01    | 2.571E+00 | 1.726E+13        | 0.000 |
| 1s4d $^3D_3$    | 1s5f $^3F_2^0$ | 1.4332E+01    | 1.400E-02 | 9.090E+10        | 1.4273E+01    | 1.398E-02 | 9.080E+10        | 0.000 |
| 1s4d $^1D_2$    | 1s5f $^3F_2^0$ | 1.4343E+01    | 1.944E-01 | 1.261E+12        | 1.4284E+01    | 1.937E-01 | 1.256E+12        | 0.000 |
| 1s5s $^3S_1$    | 1s5f $^3F_2^0$ | 3.1755E+02    | 6.658E-07 | 8.808E+03        | 3.1643E+02    | 6.490E-07 | 8.574E+03        | 0.156 |
| 1s5d $^3D_2$    | 1s5f $^3F_2^0$ | 1.5232E+03    | 1.282E-02 | 7.370E+06        | 1.5396E+03    | 1.263E-02 | 7.049E+06        | 0.006 |
| 1s5d $^3D_1$    | 1s5f $^3F_2^0$ | 1.5821E+03    | 1.098E-01 | 5.852E+07        | 1.5996E+03    | 1.081E-01 | 5.590E+07        | 0.005 |
| 1s5d $^3D_3$    | 1s5f $^3F_2^0$ | 4.1865E+04    | 2.141E-05 | 1.630E+01        |               |           |                  | 0.064 |

(continued on next page)

Table 3 (continued)

| Lower  | Upper  | GRASP2K       |           |                  | FAC           |           |                  | dT    |
|--|--|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|  |  | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) |       |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4538E+00    | 1.438E-04 | 9.078E+10        | 1.4478E+00    | 1.474E-04 | 9.306E+10        | 0.001 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.5232E+00    | 1.293E-02 | 7.432E+12        | 1.5168E+00    | 1.311E-02 | 7.537E+12        | 0.000 |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.5298E+00    | 1.173E-01 | 6.689E+13        | 1.5234E+00    | 1.193E-01 | 6.803E+13        | 0.000 |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 4.2927E+00    | 3.366E-04 | 2.437E+10        | 4.2749E+00    | 3.884E-04 | 2.811E+10        | 0.001 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 4.4717E+00    | 3.994E-02 | 2.665E+12        | 4.4529E+00    | 4.038E-02 | 2.694E+12        | 0.001 |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 4.4877E+00    | 3.668E-01 | 2.429E+13        | 4.4691E+00    | 3.683E-01 | 2.439E+13        | 0.001 |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.3295E+01    | 1.171E-03 | 8.835E+09        | 1.3238E+01    | 1.596E-03 | 1.204E+10        | 0.001 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4027E+01    | 1.671E-01 | 1.133E+12        | 1.3965E+01    | 1.698E-01 | 1.152E+12        | 0.001 |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4092E+01    | 1.553E+00 | 1.043E+13        | 1.4031E+01    | 1.548E+00 | 1.040E+13        | 0.001 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4336E+01    | 2.568E-04 | 1.667E+09        | 1.4273E+01    | 2.695E-04 | 1.750E+09        | 0.000 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4341E+01    | 2.746E-03 | 1.781E+10        | 1.4279E+01    | 2.764E-03 | 1.793E+10        | 0.001 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4467E+01    | 6.463E-02 | 4.120E+11        | 1.4403E+01    | 6.487E-02 | 4.136E+11        | 0.000 |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 3.5679E+02    | 5.880E-04 | 6.162E+06        | 3.5385E+02    | 5.862E-04 | 6.193E+06        | 0.019 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.2461E+03    | 1.996E-02 | 1.715E+07        | 1.2214E+03    | 2.024E-02 | 1.794E+07        | 0.011 |
| 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.5753E+03    | 1.443E-01 | 7.759E+07        | 1.5418E+03    | 1.468E-01 | 8.171E+07        | 0.014 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 6.3169E+04    | 1.871E-05 | 6.254E+00        |               |           |                  | 0.202 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 3.7392E+05    | 3.369E-05 | 3.214E-01        |               |           |                  | 0.434 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.5387E+00    | 9.978E-01 | 3.590E+13        | 4.5196E+00    | 1.005E+00 | 3.616E+13        | 0.001 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.4271E+01    | 5.607E+00 | 2.040E+13        | 1.4212E+01    | 5.633E+00 | 2.049E+13        | 0.000 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 3.0834E+03    | 1.209E-01 | 9.428E+06        | 3.1501E+03    | 1.178E-01 | 8.729E+06        | 0.017 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 1.4275E+01    | 8.976E+00 | 3.265E+13        | 1.4214E+01    | 8.998E+00 | 3.272E+13        | 0.000 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 1.4400E+01    | 3.232E-01 | 1.155E+12        | 1.4339E+01    | 3.220E-01 | 1.150E+12        | 0.000 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 1.4404E+01    | 9.104E-03 | 3.252E+10        | 1.4343E+01    | 9.083E-03 | 3.244E+10        | 0.000 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 3.1830E+03    | 6.601E-02 | 4.829E+06        | 3.1753E+03    | 6.588E-02 | 4.802E+06        | 0.007 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 1.7265E+06    | 4.338E-06 | 1.079E-03        |               |           |                  | 0.584 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>3</sub>              | 1.5225E+00    | 1.816E-10 | 7.464E+04        | 1.5161E+00    | 8.545E-11 | 3.512E+04        | 0.372 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>3</sub>              | 4.4656E+00    | 2.805E-11 | 1.340E+03        | 4.4470E+00    | 2.636E-10 | 1.259E+04        | 0.160 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>3</sub>              | 1.3967E+01    | 7.568E-07 | 3.697E+06        |               |           |                  | 0.002 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>3</sub>              | 1.4273E+01    | 3.312E-01 | 1.549E+12        | 1.4213E+01    | 3.319E-01 | 1.552E+12        | 0.000 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>3</sub>              | 1.4278E+01    | 6.649E+00 | 3.108E+13        | 1.4218E+01    | 6.662E+00 | 3.113E+13        | 0.000 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>3</sub>              | 1.4399E+01    | 9.264E-03 | 4.258E+10        | 1.4338E+01    | 9.232E-03 | 4.243E+10        | 0.001 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>3</sub>              | 1.4403E+01    | 2.515E-01 | 1.155E+12        | 1.4341E+01    | 2.504E-01 | 1.150E+12        | 0.000 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>3</sub>              | 9.0225E+02    | 3.193E-08 | 3.737E+01        |               |           |                  | 0.058 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>3</sub>              | 3.1085E+03    | 2.495E-03 | 2.460E+05        | 3.1008E+03    | 2.490E-03 | 2.446E+05        | 0.029 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>3</sub>              | 3.2410E+03    | 4.801E-02 | 4.356E+06        | 3.2333E+03    | 4.792E-02 | 4.331E+06        | 0.023 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>3</sub>              | 1.2333E+05    | 1.738E-06 | 1.089E-01        |               |           |                  | 0.822 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.4790E+00    | 2.109E-05 | 1.002E+09        |               |           |                  | 0.005 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.5385E+00    | 3.715E-02 | 1.719E+12        | 4.5194E+00    | 3.740E-02 | 1.730E+12        | 0.000 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.5408E+00    | 7.388E-01 | 3.414E+13        | 4.5217E+00    | 7.440E-01 | 3.438E+13        | 0.000 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4022E+01    | 2.073E-04 | 1.005E+09        |               |           |                  | 0.003 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4269E+01    | 2.086E-01 | 9.761E+11        | 1.4210E+01    | 2.096E-01 | 9.810E+11        | 0.000 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4279E+01    | 4.156E+00 | 1.943E+13        | 1.4221E+01    | 4.169E+00 | 1.948E+13        | 0.000 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.0343E+03    | 1.740E-05 | 1.550E+04        | 1.0413E+03    | 1.923E-05 | 1.675E+04        | 0.068 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.9925E+03    | 4.638E-03 | 4.936E+05        | 3.0547E+03    | 4.522E-03 | 4.579E+05        | 0.007 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.2509E+03    | 8.494E-02 | 7.658E+06        | 3.3306E+03    | 8.255E-02 | 7.031E+06        | 0.005 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.0795E+05    | 1.971E-06 | 1.612E-01        |               |           |                  | 0.573 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.7657E+05    | 1.010E-05 | 2.896E-02        |               |           |                  | 0.888 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>5</sub>              | 1.4362E+01    | 1.142E+01 | 3.356E+13        | 1.4301E+01    | 1.146E+01 | 3.369E+13        | 0.000 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>5</sub>              | 5.3388E+03    | 4.992E-02 | 1.062E+06        | 5.3203E+03    | 4.988E-02 | 1.059E+06        | 0.007 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>1</sup> G <sub>4</sub>              | 1.4236E+01    | 8.057E-07 | 2.947E+06        |               |           |                  | 0.006 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5g <sup>1</sup> G <sub>4</sub>              | 1.4361E+01    | 2.606E-01 | 9.364E+11        | 1.4299E+01    | 2.616E-01 | 9.402E+11        | 0.000 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>1</sup> G <sub>4</sub>              | 1.4364E+01    | 9.081E+00 | 3.262E+13        | 1.4303E+01    | 9.114E+00 | 3.273E+13        | 0.000 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>1</sup> G <sub>4</sub>              | 1.9730E+03    | 2.721E-09 | 5.180E-01        |               |           |                  | 0.788 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5g <sup>1</sup> G <sub>4</sub>              | 5.1744E+03    | 1.176E-03 | 3.255E+04        | 5.1563E+03    | 1.174E-03 | 3.246E+04        | 0.043 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>1</sup> G <sub>4</sub>              | 5.4521E+03    | 3.888E-02 | 9.694E+05        | 5.4339E+03    | 3.884E-02 | 9.667E+05        | 0.028 |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 1.3813E+00    | 1.347E-03 | 1.569E+12        | 1.3756E+00    | 1.386E-03 | 1.615E+12        | 0.002 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 1.3823E+00    | 6.594E-04 | 7.674E+11        | 1.3765E+00    | 6.489E-04 | 7.550E+11        | 0.002 |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 1.4438E+00    | 4.439E-03 | 4.734E+12        | 1.4378E+00    | 4.423E-03 | 4.716E+12        | 0.004 |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 1.4497E+00    | 8.068E-04 | 8.535E+11        | 1.4438E+00    | 7.972E-04 | 8.432E+11        | 0.002 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 3.7169E+00    | 6.581E-03 | 1.059E+12        | 3.7018E+00    | 6.645E-03 | 1.069E+12        | 0.001 |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 3.7187E+00    | 3.203E-03 | 5.150E+11        | 3.7035E+00    | 3.126E-03 | 5.024E+11        | 0.002 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 3.8504E+00    | 2.103E-02 | 3.154E+12        | 3.8346E+00    | 2.093E-02 | 3.139E+12        | 0.000 |
| 1s 3p <sup>1</sup> P <sub>2</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 3.8623E+00    | 3.830E-03 | 5.708E+11        | 3.8466E+00    | 3.799E-03 | 5.660E+11        | 0.001 |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 8.9847E+00    | 2.684E-02 | 7.392E+11        | 8.9484E+00    | 2.691E-02 | 7.410E+11        | 0.001 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 8.9888E+00    | 1.303E-02 | 3.586E+11        | 8.9523E+00    | 1.267E-02 | 3.487E+11        | 0.002 |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 9.3128E+00    | 8.539E-02 | 2.189E+12        | 9.2750E+00    | 8.504E-02 | 2.179E+12        | 0.001 |
| 1s 4p <sup>1</sup> P <sub>2</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 9.3416E+00    | 1.559E-02 | 3.972E+11        | 9.3040E+00    | 1.546E-02 | 3.938E+11        | 0.001 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 9.4503E+00    | 5.582E-09 | 1.390E+05        |               |           |                  | 0.099 |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 2.5714E+01    | 1.642E-01 | 5.522E+11        | 2.5617E+01    | 1.636E-01 | 5.499E+11        | 0.001 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 2.5731E+01    | 7.964E-02 | 2.675E+11        | 2.5633E+01    | 7.696E-02 | 2.582E+11        | 0.002 |
| 1s 5p <sup>1</sup> P <sub>2</sub> <sup>o</sup> | 1s 6s <sup>3</sup> S <sub>1</sub>              | 2.7109E+01    | 5.492E-01 | 1.662E+12        | 2.7006E+01    | 5.457E-01 | 1.649E+12        | 0.002 |

(continued on next page)

Table 3 (continued)

| Lower           | Upper           | GRASP2K       |            |                  | FAC           |           |                  | dT    |
|-----------------|-----------------|---------------|------------|------------------|---------------|-----------|------------------|-------|
|                 |                 | $\lambda$ (Å) | gf         | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) |       |
| 1s 5p $^1P_1^o$ | 1s 6s $^3S_1$   | 2.7232E+01    | 1.009E-01  | 3.024E+11        | 2.7131E+01    | 9.952E-02 | 2.980E+11        | 0.002 |
| 1s 5f $^3F_2^o$ | 1s 6s $^3S_1$   | 2.7709E+01    | 1.281E-07  | 3.709E+05        |               |           |                  | 0.078 |
| 1s $^2S_0$      | 1s 6p $^3P_1^o$ | 3.1640E-01    | 3.992E-03  | 8.865E+13        | 3.1509E-01    | 3.640E-03 | 8.082E+13        | 0.009 |
| 1s 2s $^3S_1$   | 1s 6p $^3P_0^o$ | 1.3692E+00    | 1.433E-02  | 1.699E+13        | 1.3634E+00    | 1.449E-02 | 1.718E+13        | 0.002 |
| 1s 2s $^1S_0$   | 1s 6p $^3P_1^o$ | 1.3822E+00    | 6.212E-03  | 7.230E+12        | 1.3765E+00    | 5.890E-03 | 6.853E+12        | 0.006 |
| 1s 3s $^3S_1$   | 1s 6p $^3P_1^o$ | 3.6909E+00    | 3.452E-02  | 5.634E+12        | 3.6756E+00    | 3.517E-02 | 5.739E+12        | 0.002 |
| 1s 3s $^1S_0$   | 1s 6p $^3P_1^o$ | 3.7158E+00    | 1.517E-02  | 2.443E+12        | 3.7007E+00    | 1.445E-02 | 2.326E+12        | 0.000 |
| 1s 3d $^3D_2$   | 1s 6p $^3P_0^o$ | 3.8574E+00    | 5.268E-03  | 7.872E+11        | 3.8413E+00    | 5.279E-03 | 7.887E+11        | 0.003 |
| 1s 3d $^3D_1$   | 1s 6p $^3P_1^o$ | 3.8592E+00    | 1.151E-03  | 1.719E+11        | 3.8431E+00    | 1.141E-03 | 1.704E+11        | 0.008 |
| 1s 3d $^1D_2$   | 1s 6p $^3P_0^o$ | 3.9032E+00    | 6.779E-06  | 9.894E+08        | 3.8868E+00    | 6.128E-06 | 1.186E+09        | 0.029 |
| 1s 4s $^3S_1$   | 1s 6p $^3P_1^o$ | 8.9132E+00    | 9.266E-02  | 2.593E+12        | 8.8765E+00    | 9.472E-02 | 2.650E+12        | 0.003 |
| 1s 4s $^1S_0$   | 1s 6p $^3P_0^o$ | 8.9717E+00    | 4.111E-02  | 1.136E+12        | 8.9354E+00    | 3.919E-02 | 1.082E+12        | 0.003 |
| 1s 4d $^3D_2$   | 1s 6p $^3P_1^o$ | 9.3198E+00    | 9.3198E-02 | 9.005E+11        | 9.2819E+00    | 3.513E-02 | 8.989E+11        | 0.001 |
| 1s 4d $^3D_1$   | 1s 6p $^3P_0^o$ | 9.3241E+00    | 7.616E-03  | 1.948E+11        | 9.2861E+00    | 7.573E-03 | 1.936E+11        | 0.004 |
| 1s 4d $^1D_2$   | 1s 6p $^3P_0^o$ | 9.4329E+00    | 4.037E-05  | 1.009E+09        | 9.3943E+00    | 4.947E-05 | 1.235E+09        | 0.020 |
| 1s 5s $^3S_1$   | 1s 6p $^3P_1^o$ | 2.5356E+01    | 4.018E-01  | 1.390E+12        | 2.5254E+01    | 4.122E-01 | 1.425E+12        | 0.003 |
| 1s 5s $^1S_0$   | 1s 6p $^3P_0^o$ | 2.5594E+01    | 1.810E-01  | 6.145E+11        | 2.5493E+01    | 1.720E-01 | 5.836E+11        | 0.002 |
| 1s 5d $^3D_2$   | 1s 6p $^3P_1^o$ | 2.7067E+01    | 2.978E-01  | 9.037E+11        | 2.6964E+01    | 2.966E-01 | 8.996E+11        | 0.001 |
| 1s 5d $^3D_1$   | 1s 6p $^3P_0^o$ | 2.7084E+01    | 6.418E-02  | 1.945E+11        | 2.6981E+01    | 6.366E-02 | 1.927E+11        | 0.002 |
| 1s 5d $^1D_2$   | 1s 6p $^3P_0^o$ | 2.7558E+01    | 3.306E-04  | 9.680E+08        | 2.7452E+01    | 3.795E-04 | 1.110E+09        | 0.010 |
| 1s 6s $^3S_1$   | 1s 6p $^3P_1^o$ | 4.9854E+03    | 4.082E-02  | 3.652E+06        | 4.6146E+03    | 4.469E-02 | 4.627E+06        | 0.127 |
| 1s 2p $^3P_1^o$ | 1s 6s $^1S_0$   | 1.3809E+00    | 5.496E-04  | 1.922E+12        | 1.3753E+00    | 5.629E-04 | 1.968E+12        | 0.010 |
| 1s 2p $^1P_1^o$ | 1s 6s $^1S_0$   | 1.4493E+00    | 1.870E-03  | 5.937E+12        | 1.4434E+00    | 1.844E-03 | 5.856E+12        | 0.004 |
| 1s 3p $^3P_1^o$ | 1s 6s $^1S_0$   | 3.7140E+00    | 2.696E-03  | 1.304E+12        | 3.6994E+00    | 2.744E-03 | 1.326E+12        | 0.003 |
| 1s 3p $^1P_1^o$ | 1s 6s $^1S_0$   | 3.8591E+00    | 8.737E-03  | 3.913E+12        | 3.8440E+00    | 8.725E-03 | 3.905E+12        | 0.000 |
| 1s 4p $^3P_1^o$ | 1s 6s $^1S_0$   | 8.9678E+00    | 1.099E-02  | 9.117E+11        | 8.9340E+00    | 1.117E-02 | 9.258E+11        | 0.001 |
| 1s 4p $^1P_1^o$ | 1s 6s $^1S_0$   | 9.3233E+00    | 3.529E-02  | 2.708E+12        | 9.2885E+00    | 3.544E-02 | 2.716E+12        | 0.002 |
| 1s 5p $^3P_1^o$ | 1s 6s $^1S_0$   | 2.5576E+01    | 6.646E-02  | 6.777E+11        | 2.5500E+01    | 6.781E-02 | 6.879E+11        | 0.002 |
| 1s 5p $^1P_1^o$ | 1s 6s $^1S_0$   | 2.7078E+01    | 2.249E-01  | 2.046E+12        | 2.6999E+01    | 2.273E-01 | 2.063E+12        | 0.002 |
| 1s 6p $^3P_1^o$ | 1s 6s $^1S_0$   | 1.0994E+05    | 7.948E-04  | 4.387E+02        |               |           |                  | 0.884 |
| 1s 2s $^3S_1$   | 1s 6p $^3P_0^o$ | 1.3691E+00    | 6.808E-03  | 2.423E+13        | 1.3635E+00    | 6.812E-03 | 2.423E+13        | 0.003 |
| 1s 3s $^3S_1$   | 1s 6p $^3P_0^o$ | 3.6907E+00    | 1.641E-02  | 8.037E+12        | 3.6761E+00    | 1.659E-02 | 8.122E+12        | 0.004 |
| 1s 3d $^3D_1$   | 1s 6p $^3P_0^o$ | 3.8590E+00    | 2.133E-03  | 9.554E+11        | 3.8436E+00    | 2.122E-03 | 9.501E+11        | 0.008 |
| 1s 4s $^3S_1$   | 1s 6p $^3P_0^o$ | 8.9120E+00    | 4.409E-02  | 3.703E+12        | 8.8795E+00    | 4.483E-02 | 3.760E+12        | 0.004 |
| 1s 4d $^3D_1$   | 1s 6p $^3P_0^o$ | 9.3228E+00    | 1.419E-02  | 1.089E+12        | 9.2894E+00    | 1.414E-02 | 1.084E+12        | 0.004 |
| 1s 5s $^3S_1$   | 1s 6p $^3P_0^o$ | 2.5347E+01    | 1.912E-01  | 1.986E+12        | 2.5278E+01    | 1.959E-01 | 2.028E+12        | 0.004 |
| 1s 5d $^3D_1$   | 1s 6p $^3P_0^o$ | 2.7074E+01    | 1.200E-01  | 1.092E+12        | 2.7009E+01    | 1.194E-01 | 1.083E+12        | 0.002 |
| 1s 6s $^3S_1$   | 1s 6p $^3P_0^o$ | 4.6513E+03    | 2.098E-02  | 6.469E+06        | 5.5898E+03    | 1.731E-02 | 3.664E+06        | 0.099 |
| 1s 2s $^3S_1$   | 1s 6p $^3P_2^o$ | 1.3670E+00    | 3.166E-02  | 2.260E+13        | 1.3612E+00    | 3.251E-02 | 2.320E+13        | 0.002 |
| 1s 3s $^3S_1$   | 1s 6p $^3P_2^o$ | 3.6753E+00    | 7.231E-02  | 7.141E+12        | 3.6601E+00    | 7.353E-02 | 7.261E+12        | 0.003 |
| 1s 3d $^3D_2$   | 1s 6p $^3P_2^o$ | 3.8403E+00    | 6.550E-04  | 5.925E+10        | 3.8243E+00    | 6.596E-04 | 5.965E+10        | 0.005 |
| 1s 3d $^3D_1$   | 1s 6p $^3P_2^o$ | 3.8421E+00    | 7.089E-05  | 6.406E+09        | 3.8260E+00    | 6.699E-05 | 6.053E+09        | 0.009 |
| 1s 3d $^3D_3$   | 1s 6p $^3P_2^o$ | 3.8840E+00    | 7.016E-03  | 6.205E+11        | 3.8677E+00    | 6.917E-03 | 6.116E+11        | 0.006 |
| 1s 3d $^1D_2$   | 1s 6p $^3P_2^o$ | 3.8856E+00    | 5.021E-04  | 4.437E+10        | 3.8694E+00    | 4.897E-04 | 4.326E+10        | 0.008 |
| 1s 4s $^3S_1$   | 1s 6p $^3P_2^o$ | 8.8224E+00    | 1.843E-01  | 3.158E+12        | 8.7863E+00    | 1.868E-01 | 3.201E+12        | 0.004 |
| 1s 4d $^3D_2$   | 1s 6p $^3P_2^o$ | 9.2206E+00    | 4.521E-03  | 7.093E+10        | 9.1833E+00    | 4.502E-03 | 7.061E+10        | 0.003 |
| 1s 4d $^3D_1$   | 1s 6p $^3P_2^o$ | 9.2248E+00    | 4.885E-04  | 7.658E+09        | 9.1874E+00    | 4.667E-04 | 7.314E+09        | 0.004 |
| 1s 4d $^3D_3$   | 1s 6p $^3P_2^o$ | 9.3270E+00    | 4.766E-02  | 7.308E+11        | 9.2888E+00    | 4.696E-02 | 7.199E+11        | 0.003 |
| 1s 4d $^1D_2$   | 1s 6p $^3P_2^o$ | 9.3314E+00    | 3.377E-03  | 5.174E+10        | 9.2933E+00    | 3.309E-03 | 5.068E+10        | 0.004 |
| 1s 5s $^3S_1$   | 1s 6p $^3P_2^o$ | 2.4635E+01    | 7.249E-01  | 1.594E+12        | 2.4537E+01    | 7.351E-01 | 1.615E+12        | 0.003 |
| 1s 5d $^3D_2$   | 1s 6p $^3P_2^o$ | 2.6247E+01    | 3.725E-02  | 7.213E+10        | 2.6148E+01    | 3.678E-02 | 7.116E+10        | 0.001 |
| 1s 5d $^3D_1$   | 1s 6p $^3P_2^o$ | 2.6264E+01    | 4.030E-03  | 7.794E+09        | 2.6164E+01    | 3.868E-03 | 7.475E+09        | 0.002 |
| 1s 5d $^3D_3$   | 1s 6p $^3P_2^o$ | 2.6690E+01    | 3.948E-01  | 7.394E+11        | 2.6588E+01    | 3.879E-01 | 7.258E+11        | 0.001 |
| 1s 5d $^1D_2$   | 1s 6p $^3P_2^o$ | 2.6709E+01    | 2.789E-02  | 5.215E+10        | 2.6607E+01    | 2.727E-02 | 5.096E+10        | 0.002 |
| 1s 5g $^3G_3$   | 1s 6p $^3P_2^o$ | 2.6929E+01    | 1.344E-08  | 2.472E+04        |               |           |                  | 0.016 |
| 1s 6s $^3S_1$   | 1s 6p $^3P_2^o$ | 7.3822E+02    | 6.713E-01  | 1.643E+09        | 7.2782E+02    | 6.786E-01 | 1.694E+09        | 0.015 |
| 1s 2p $^3P_0^o$ | 1s 6d $^3D_2$   | 1.3786E+00    | 5.406E-02  | 3.795E+13        | 1.3729E+00    | 5.423E-02 | 3.806E+13        | 0.001 |
| 1s 2p $^3P_2^o$ | 1s 6d $^3D_2$   | 1.4409E+00    | 9.245E-03  | 5.941E+12        | 1.4348E+00    | 9.097E-03 | 5.845E+12        | 0.003 |
| 1s 2p $^1P_1^o$ | 1s 6d $^3D_2$   | 1.4467E+00    | 1.528E-03  | 9.741E+11        | 1.4407E+00    | 1.426E-03 | 9.093E+11        | 0.001 |
| 1s 3p $^3P_1^o$ | 1s 6d $^3D_2$   | 3.6972E+00    | 1.326E-01  | 1.294E+13        | 3.6817E+00    | 1.329E-01 | 1.297E+13        | 0.000 |
| 1s 3p $^3P_2^o$ | 1s 6d $^3D_2$   | 3.8292E+00    | 2.492E-02  | 2.268E+12        | 3.8130E+00    | 2.499E-02 | 2.274E+12        | 0.001 |
| 1s 3p $^1P_1^o$ | 1s 6d $^3D_2$   | 3.8409E+00    | 4.051E-03  | 3.663E+11        | 3.8249E+00    | 3.732E-03 | 3.374E+11        | 0.002 |
| 1s 4p $^3P_1^o$ | 1s 6d $^3D_2$   | 8.8702E+00    | 3.276E-01  | 5.555E+12        | 8.8316E+00    | 3.287E-01 | 5.575E+12        | 0.000 |
| 1s 4p $^3P_2^o$ | 1s 6d $^3D_2$   | 9.1898E+00    | 6.652E-02  | 1.051E+12        | 9.1496E+00    | 6.733E-02 | 1.063E+12        | 0.000 |
| 1s 4p $^1P_1^o$ | 1s 6d $^3D_2$   | 9.2178E+00    | 1.079E-02  | 1.693E+11        | 9.1778E+00    | 9.804E-03 | 1.539E+11        | 0.001 |
| 1s 4f $^3F_2^o$ | 1s 6d $^3D_2$   | 9.3215E+00    | 1.216E-02  | 1.867E+11        | 9.2809E+00    | 1.219E-02 | 1.871E+11        | 0.001 |
| 1s 4f $^3F_3^o$ | 1s 6d $^3D_2$   | 9.3237E+00    | 8.868E-04  | 1.361E+10        | 9.2831E+00    | 8.928E-04 | 1.370E+10        | 0.000 |
| 1s 4f $^1F_3^o$ | 1s 6d $^3D_2$   | 9.3766E+00    | 9.857E-07  | 1.496E+07        |               |           |                  | 0.011 |
| 1s 5p $^3P_1^o$ | 1s 6d $^3D_2$   | 2.4798E+01    | 1.222E+00  | 2.651E+12        | 2.4683E+01    | 1.227E+00 | 2.664E+12        | 0.000 |
| 1s 5p $^3P_2^o$ | 1s 6d $^3D_2$   | 2.6092E+01    | 2.792E-01  | 5.472E+11        | 2.5970E+01    | 2.851E-01 | 5.591E+11        | 0.000 |
| 1s 5p $^1P_1^o$ | 1s 6d $^3D_2$   | 2.6207E+01    | 4.553E-02  | 8.843E+10        | 2.6085E+01    | 4.028E-02 | 7.831E+10        | 0.001 |

(continued on next page)

Table 3 (continued)

| Lower  | Upper  | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|--|--|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|  |  | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 2.6639E+01    | 1.774E-01 | 3.335E+11              | 2.6517E+01    | 1.775E-01 | 3.339E+11              | 0.001 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 2.6648E+01    | 1.291E-02 | 2.426E+10              | 2.6526E+01    | 1.297E-02 | 2.439E+10              | 0.000 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 2.6870E+01    | 1.399E-05 | 2.585E+07              |               |           |                        | 0.010 |
| 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 8.0869E+02    | 5.619E-01 | 1.146E+09              | 7.9302E+02    | 5.686E-01 | 1.196E+09              | 0.003 |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 1.2110E-01    | 6.859E-03 | 6.234E+04              | 9.6399E+03    | 8.661E-03 | 1.232E+05              | 0.102 |
| 1s <sup>2</sup> S <sub>0</sub>                 | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 3.1620E-01    | 9.840E-03 | 2.187E+14              | 3.1497E-01    | 1.063E-02 | 2.362E+14              | 0.031 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.3668E+00    | 5.663E-03 | 6.739E+12              | 1.3611E+00    | 5.637E-03 | 6.708E+12              | 0.001 |
| 1s 2s <sup>1</sup> S <sub>0</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.3798E+00    | 1.346E-02 | 1.572E+13              | 1.3742E+00    | 1.374E-02 | 1.604E+13              | 0.003 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 3.6740E+00    | 1.286E-02 | 2.118E+12              | 3.6589E+00    | 1.267E-02 | 2.087E+12              | 0.003 |
| 1s 3s <sup>1</sup> S <sub>0</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 3.6986E+00    | 3.101E-02 | 5.041E+12              | 3.6837E+00    | 3.125E-02 | 5.077E+12              | 0.002 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 3.8389E+00    | 1.069E-04 | 1.613E+10              | 3.8230E+00    | 1.372E-04 | 2.069E+10              | 0.011 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 3.8407E+00    | 3.272E-04 | 4.932E+10              | 3.8248E+00    | 3.122E-04 | 4.705E+10              | 0.011 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 3.8842E+00    | 4.432E-03 | 6.532E+11              | 3.8681E+00    | 4.442E-03 | 6.545E+11              | 0.010 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 8.8149E+00    | 3.260E-02 | 9.327E+11              | 8.7796E+00    | 3.204E-02 | 9.164E+11              | 0.003 |
| 1s 4s <sup>1</sup> S <sub>0</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 8.8722E+00    | 7.942E-02 | 2.243E+12              | 8.8372E+00    | 7.964E-02 | 2.248E+12              | 0.004 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 9.2125E+00    | 7.164E-04 | 1.877E+10              | 9.1760E+00    | 9.080E-04 | 2.377E+10              | 0.007 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 9.2166E+00    | 2.227E-03 | 5.828E+10              | 9.1801E+00    | 2.117E-03 | 5.539E+10              | 0.006 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 9.3230E+00    | 2.999E-02 | 7.671E+11              | 9.2858E+00    | 3.019E-02 | 7.720E+11              | 0.005 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 2.4577E+01    | 1.271E-01 | 4.677E+11              | 2.4485E+01    | 1.249E-01 | 4.593E+11              | 0.003 |
| 1s 5s <sup>1</sup> S <sub>0</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 2.4800E+01    | 3.145E-01 | 1.137E+12              | 2.4710E+01    | 3.143E-01 | 1.134E+12              | 0.004 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 2.6180E+01    | 5.800E-03 | 1.881E+10              | 2.6089E+01    | 7.458E-03 | 2.415E+10              | 0.003 |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 2.6197E+01    | 1.815E-02 | 5.882E+10              | 2.6105E+01    | 1.715E-02 | 5.550E+10              | 0.003 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 2.6640E+01    | 2.473E-01 | 7.746E+11              | 2.6546E+01    | 2.497E-01 | 7.814E+11              | 0.003 |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 6.8918E+02    | 1.292E-01 | 6.050E+08              | 6.8482E+02    | 1.256E-01 | 5.907E+08              | 0.015 |
| 1s 6s <sup>1</sup> S <sub>0</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 8.0559E+02    | 2.588E-01 | 8.867E+08              | 7.8073E+02    | 2.693E-01 | 9.741E+08              | 0.057 |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 7.2196E+04    | 1.839E-04 | 7.843E+01              |               |           |                        | 0.369 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 1.3786E+00    | 1.160E-02 | 1.357E+13              | 1.3729E+00    | 1.157E-02 | 1.354E+13              | 0.001 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 1.3795E+00    | 2.193E-02 | 2.563E+13              | 1.3737E+00    | 2.194E-02 | 2.563E+13              | 0.001 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 1.4408E+00    | 1.013E-03 | 1.085E+12              | 1.4348E+00    | 9.908E-04 | 1.061E+12              | 0.004 |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 1.4467E+00    | 4.506E-03 | 4.787E+12              | 1.4407E+00    | 4.362E-03 | 4.633E+12              | 0.003 |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 3.6970E+00    | 2.828E-02 | 4.600E+12              | 3.6817E+00    | 2.835E-02 | 4.611E+12              | 0.001 |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 3.6987E+00    | 5.368E-02 | 8.725E+12              | 3.6834E+00    | 5.377E-02 | 8.738E+12              | 0.001 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 3.8290E+00    | 2.722E-03 | 4.128E+11              | 3.8131E+00    | 2.724E-03 | 4.131E+11              | 0.002 |
| 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 3.8407E+00    | 1.233E-02 | 1.858E+12              | 3.8249E+00    | 1.218E-02 | 1.836E+12              | 0.002 |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 8.8691E+00    | 6.971E-02 | 1.970E+12              | 8.8318E+00    | 7.019E-02 | 1.983E+12              | 0.001 |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 8.8731E+00    | 1.325E-01 | 3.743E+12              | 8.8357E+00    | 1.329E-01 | 3.755E+12              | 0.001 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 9.1886E+00    | 7.247E-03 | 1.908E+11              | 9.1499E+00    | 7.347E-03 | 1.934E+11              | 0.001 |
| 1s 4p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 9.2166E+00    | 3.316E-02 | 8.679E+11              | 9.1781E+00    | 3.306E-02 | 8.654E+11              | 0.001 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 9.3225E+00    | 7.803E-03 | 1.996E+11              | 9.2834E+00    | 7.840E-03 | 2.005E+11              | 0.000 |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.4789E+01    | 2.595E-01 | 9.388E+11              | 2.4685E+01    | 2.631E-01 | 9.519E+11              | 0.001 |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.4805E+01    | 4.939E-01 | 1.785E+12              | 2.4700E+01    | 4.967E-01 | 1.794E+12              | 0.001 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6083E+01    | 3.034E-02 | 9.915E+10              | 2.5972E+01    | 3.115E-02 | 1.018E+11              | 0.001 |
| 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6197E+01    | 1.405E-01 | 4.553E+11              | 2.6087E+01    | 1.410E-01 | 4.568E+11              | 0.001 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6638E+01    | 1.138E-01 | 3.567E+11              | 2.6529E+01    | 1.142E-01 | 3.577E+11              | 0.000 |
| 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 7.9964E+02    | 1.213E-01 | 4.217E+08              | 7.9517E+02    | 1.225E-01 | 4.272E+08              | 0.006 |
| 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 8.0896E+02    | 2.267E-01 | 7.701E+08              | 7.7196E+02    | 2.370E-01 | 8.770E+08              | 0.005 |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 1.0358E+04    | 8.674E-04 | 1.798E+04              |               |           |                        | 0.007 |
| 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 6.7159E+06    | 6.153E-06 | 3.033E-04              |               |           |                        | 0.995 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 1.4401E+00    | 8.934E-02 | 4.105E+13              | 1.4340E+00    | 9.091E-02 | 4.176E+13              | 0.000 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 3.8238E+00    | 2.308E-01 | 1.504E+13              | 3.8077E+00    | 2.333E-01 | 1.520E+13              | 0.000 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.1590E+00    | 5.989E-01 | 6.802E+12              | 9.1192E+00    | 6.053E-01 | 6.877E+12              | 0.000 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.2898E+00    | 7.076E-04 | 7.813E+09              | 9.2496E+00    | 7.143E-04 | 7.889E+09              | 0.001 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.2920E+00    | 3.269E-05 | 3.608E+08              |               |           |                        | 0.001 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.3429E+00    | 1.559E-02 | 1.702E+11              | 9.3023E+00    | 1.557E-02 | 1.700E+11              | 0.001 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.3445E+00    | 5.815E-04 | 6.346E+09              | 9.3039E+00    | 5.794E-04 | 6.324E+09              | 0.000 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.5845E+01    | 2.417E+00 | 3.448E+12              | 2.5726E+01    | 2.453E+00 | 3.503E+12              | 0.000 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.6382E+01    | 1.034E-02 | 1.416E+10              | 2.6263E+01    | 1.037E-02 | 1.421E+10              | 0.001 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.6391E+01    | 4.907E-04 | 6.713E+08              | 2.6272E+01    | 4.885E-04 | 6.687E+08              | 0.000 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.6602E+01    | 2.275E-01 | 3.063E+11              | 2.6482E+01    | 2.272E-01 | 3.062E+11              | 0.001 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.6609E+01    | 8.482E-03 | 1.142E+10              | 2.6489E+01    | 8.453E-03 | 1.138E+10              | 0.000 |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.2306E+03    | 3.482E-01 | 6.669E+07              | 2.1370E+03    | 3.618E-01 | 7.486E+07              | 0.018 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.8336E+00    | 2.524E-01 | 1.637E+13              | 3.8174E+00    | 2.527E-01 | 1.638E+13              | 0.001 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.8771E+00    | 1.644E-02 | 1.042E+12              | 3.8607E+00    | 1.627E-02 | 1.031E+12              | 0.002 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.8788E+00    | 9.798E-04 | 6.205E+10              | 3.8624E+00    | 9.022E-04 | 5.714E+10              | 0.001 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 9.1821E+00    | 8.572E-01 | 9.689E+12              | 9.1440E+00    | 8.586E-01 | 9.702E+12              | 0.001 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 9.2876E+00    | 5.814E-02 | 6.423E+11              | 9.2486E+00    | 5.812E-02 | 6.419E+11              | 0.001 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 9.2919E+00    | 3.683E-03 | 4.065E+10              | 9.2530E+00    | 3.427E-03 | 3.782E+10              | 0.000 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.5937E+01    | 3.743E+00 | 5.302E+12              | 2.5831E+01    | 3.751E+00 | 5.311E+12              | 0.000 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.6370E+01    | 2.663E-01 | 3.649E+11              | 2.6261E+01    | 2.675E-01 | 3.665E+11              | 0.001 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.6388E+01    | 1.732E-02 | 2.370E+10              | 2.6279E+01    | 1.612E-02 | 2.205E+10              | 0.000 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.6598E+01    | 7.014E-02 | 9.448E+10              | 2.6482E+01    | 7.027E-02 | 9.468E+10              | 0.001 |

(continued on next page)

Table 3 (continued)

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |           |                  | dT    |
|-----------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|                 |                 | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) |       |
| 1s 5g $^3G_3$   | 1s 6f $^3F_3^0$ | 2.6603E+01    | 2.597E-03 | 3.497E+09        | 2.6487E+01    | 2.606E-03 | 3.509E+09        | 0.002 |
| 1s 5g $^1G_4$   | 1s 6f $^3F_3^0$ | 2.6735E+01    | 2.453E-10 | 3.270E+02        |               |           |                  | 0.683 |
| 1s 6d $^3D_2$   | 1s 6f $^3F_3^0$ | 2.6863E+03    | 2.445E-01 | 3.228E+07        | 2.7429E+03    | 2.382E-01 | 2.991E+07        | 0.009 |
| 1s 6d $^3D_3$   | 1s 6f $^3F_3^0$ | 1.5394E+05    | 2.876E-04 | 1.156E+01        |               |           |                  | 0.292 |
| 1s 2s $^3S_1$   | 1s 6f $^3F_2^0$ | 1.3662E+00    | 2.099E-09 | 1.500E+06        |               |           |                  | 0.160 |
| 1s 3s $^3S_1$   | 1s 6f $^3F_2^0$ | 3.6690E+00    | 1.653E-07 | 1.638E+07        |               |           |                  | 0.106 |
| 1s 3d $^3D_2$   | 1s 6f $^3F_2^0$ | 3.8335E+00    | 1.815E-02 | 1.648E+12        | 3.8174E+00    | 1.816E-02 | 1.648E+12        | 0.000 |
| 1s 3d $^3D_1$   | 1s 6f $^3F_2^0$ | 3.8353E+00    | 1.623E-01 | 1.472E+13        | 3.8192E+00    | 1.624E-01 | 1.473E+13        | 0.000 |
| 1s 3d $^3D_3$   | 1s 6f $^3F_2^0$ | 3.8770E+00    | 8.259E-04 | 7.330E+10        | 3.8607E+00    | 8.130E-04 | 7.215E+10        | 0.004 |
| 1s 3d $^1D_2$   | 1s 6f $^3F_2^0$ | 3.8787E+00    | 1.146E-02 | 1.016E+12        | 3.8624E+00    | 1.127E-02 | 9.996E+11        | 0.001 |
| 1s 4s $^3S_1$   | 1s 6f $^3F_2^0$ | 8.7866E+00    | 7.760E-07 | 1.341E+07        |               |           |                  | 0.060 |
| 1s 4d $^3D_2$   | 1s 6f $^3F_2^0$ | 9.1815E+00    | 6.181E-02 | 9.781E+11        | 9.1440E+00    | 6.194E-02 | 9.799E+11        | 0.000 |
| 1s 4d $^3D_1$   | 1s 6f $^3F_2^0$ | 9.1856E+00    | 5.516E-01 | 8.722E+12        | 9.1480E+00    | 5.521E-01 | 8.727E+12        | 0.000 |
| 1s 4d $^3D_3$   | 1s 6f $^3F_2^0$ | 9.2869E+00    | 2.907E-03 | 4.496E+10        | 9.2486E+00    | 2.903E-03 | 4.489E+10        | 0.000 |
| 1s 4d $^1D_2$   | 1s 6f $^3F_2^0$ | 9.2913E+00    | 4.034E-02 | 6.234E+11        | 9.2530E+00    | 4.006E-02 | 6.189E+11        | 0.001 |
| 1s 5s $^3S_1$   | 1s 6f $^3F_2^0$ | 2.4358E+01    | 3.345E-06 | 7.522E+06        |               |           |                  | 0.037 |
| 1s 5d $^3D_2$   | 1s 6f $^3F_2^0$ | 2.5932E+01    | 2.700E-01 | 5.357E+11        | 2.5831E+01    | 2.711E-01 | 5.374E+11        | 0.000 |
| 1s 5d $^3D_1$   | 1s 6f $^3F_2^0$ | 2.5948E+01    | 2.411E+00 | 4.776E+12        | 2.5848E+01    | 2.411E+00 | 4.775E+12        | 0.000 |
| 1s 5d $^3D_3$   | 1s 6f $^3F_2^0$ | 2.6365E+01    | 1.328E-02 | 2.549E+10        | 2.6261E+01    | 1.336E-02 | 2.563E+10        | 0.000 |
| 1s 5d $^1D_2$   | 1s 6f $^3F_2^0$ | 2.6383E+01    | 1.846E-01 | 3.537E+11        | 2.6280E+01    | 1.840E-01 | 3.525E+11        | 0.000 |
| 1s 5g $^3G_3$   | 1s 6f $^3F_2^0$ | 2.6598E+01    | 5.191E-02 | 9.789E+10        | 2.6488E+01    | 5.205E-02 | 9.813E+10        | 0.002 |
| 1s 6s $^3S_1$   | 1s 6f $^3F_2^0$ | 5.5035E+02    | 9.794E-07 | 4.314E+03        |               |           |                  | 0.252 |
| 1s 6d $^3D_2$   | 1s 6f $^3F_2^0$ | 2.6325E+03    | 1.805E-02 | 3.475E+06        | 2.7436E+03    | 1.736E-02 | 3.051E+06        | 0.007 |
| 1s 6d $^3D_1$   | 1s 6f $^3F_2^0$ | 2.7332E+03    | 1.546E-01 | 2.760E+07        | 2.7182E+03    | 1.547E-01 | 2.770E+07        | 0.001 |
| 1s 6d $^3D_3$   | 1s 6f $^3F_2^0$ | 7.0900E+04    | 3.077E-05 | 8.167E+00        |               |           |                  | 0.051 |
| 1s 2p $^3P_0^0$ | 1s 6d $^1D_2$   | 1.3779E+00    | 6.889E-05 | 4.840E+10        | 1.3722E+00    | 5.228E-05 | 3.673E+10        | 0.008 |
| 1s 2p $^3P_2^0$ | 1s 6d $^1D_2$   | 1.4401E+00    | 6.303E-03 | 4.055E+12        | 1.4340E+00    | 6.314E-03 | 4.061E+12        | 0.000 |
| 1s 2p $^1P_1^0$ | 1s 6d $^1D_2$   | 1.4459E+00    | 5.724E-02 | 3.652E+13        | 1.4399E+00    | 5.833E-02 | 3.721E+13        | 0.000 |
| 1s 3p $^3P_0^0$ | 1s 6d $^1D_2$   | 3.6920E+00    | 1.380E-04 | 1.350E+10        | 3.6767E+00    | 1.115E-04 | 1.091E+10        | 0.003 |
| 1s 3p $^3P_2^0$ | 1s 6d $^1D_2$   | 3.8236E+00    | 1.625E-02 | 1.483E+12        | 3.8077E+00    | 1.618E-02 | 1.476E+12        | 0.001 |
| 1s 3p $^1P_1^0$ | 1s 6d $^1D_2$   | 3.8353E+00    | 1.489E-01 | 1.351E+13        | 3.8195E+00    | 1.498E-01 | 1.359E+13        | 0.001 |
| 1s 4p $^3P_0^0$ | 1s 6d $^1D_2$   | 8.8403E+00    | 3.141E-04 | 5.361E+09        | 8.8028E+00    | 2.765E-04 | 4.721E+09        | 0.003 |
| 1s 4p $^3P_2^0$ | 1s 6d $^1D_2$   | 9.1577E+00    | 4.208E-02 | 6.694E+11        | 9.1187E+00    | 4.197E-02 | 6.676E+11        | 0.001 |
| 1s 4p $^1P_1^0$ | 1s 6d $^1D_2$   | 9.1855E+00    | 3.883E-01 | 6.139E+12        | 9.1467E+00    | 3.889E-01 | 6.149E+12        | 0.001 |
| 1s 4f $^3F_3^0$ | 1s 6d $^1D_2$   | 9.2884E+00    | 4.663E-05 | 7.211E+08        | 9.2491E+00    | 5.670E-05 | 8.767E+08        | 0.000 |
| 1s 4f $^3F_2^0$ | 1s 6d $^1D_2$   | 9.2907E+00    | 4.915E-04 | 7.596E+09        | 9.2513E+00    | 4.896E-04 | 7.566E+09        | 0.000 |
| 1s 4f $^1F_3^0$ | 1s 6d $^1D_2$   | 9.3432E+00    | 1.150E-02 | 1.758E+11        | 9.3035E+00    | 1.152E-02 | 1.761E+11        | 0.000 |
| 1s 5p $^3P_0^0$ | 1s 6d $^1D_2$   | 2.4566E+01    | 1.099E-03 | 2.430E+09        | 2.4460E+01    | 1.147E-03 | 2.538E+09        | 0.003 |
| 1s 5p $^3P_2^0$ | 1s 6d $^1D_2$   | 2.5835E+01    | 1.695E-01 | 3.387E+11        | 2.5723E+01    | 1.700E-01 | 3.399E+11        | 0.001 |
| 1s 5p $^1P_1^0$ | 1s 6d $^1D_2$   | 2.5947E+01    | 1.579E+00 | 3.130E+12        | 2.5836E+01    | 1.574E+00 | 3.121E+12        | 0.001 |
| 1s 5f $^3F_3^0$ | 1s 6d $^1D_2$   | 2.6371E+01    | 6.778E-04 | 1.300E+09        | 2.6259E+01    | 8.212E-04 | 1.575E+09        | 0.001 |
| 1s 5f $^3F_2^0$ | 1s 6d $^1D_2$   | 2.6380E+01    | 7.165E-03 | 1.373E+10        | 2.6269E+01    | 7.091E-03 | 1.359E+10        | 0.000 |
| 1s 5f $^1F_3^0$ | 1s 6d $^1D_2$   | 2.6598E+01    | 1.678E-01 | 3.164E+11        | 2.6485E+01    | 1.682E-01 | 3.173E+11        | 0.000 |
| 1s 6p $^3P_0^0$ | 1s 6d $^1D_2$   | 6.1807E+02    | 7.142E-04 | 2.494E+06        | 6.1320E+02    | 1.025E-03 | 3.607E+06        | 0.033 |
| 1s 6p $^3P_2^0$ | 1s 6d $^1D_2$   | 2.1556E+03    | 2.532E-02 | 7.269E+06        | 2.1118E+03    | 2.540E-02 | 7.534E+06        | 0.009 |
| 1s 6p $^1P_1^0$ | 1s 6d $^1D_2$   | 2.7210E+03    | 1.836E-01 | 3.308E+07        | 2.5822E+03    | 1.928E-01 | 3.826E+07        | 0.017 |
| 1s 6f $^3F_3^0$ | 1s 6d $^1D_2$   | 1.0989E+05    | 2.647E-05 | 2.924E+00        |               |           |                  | 0.645 |
| 1s 6f $^3F_2^0$ | 1s 6d $^1D_2$   | 6.7056E+05    | 4.571E-05 | 1.356E-01        |               |           |                  | 0.206 |
| 1s 3d $^3D_3$   | 1s 6f $^3F_4^0$ | 3.8744E+00    | 3.435E-01 | 1.696E+13        | 3.8580E+00    | 3.460E-01 | 1.708E+13        | 0.001 |
| 1s 4d $^3D_3$   | 1s 6f $^3F_4^0$ | 9.2719E+00    | 1.185E+00 | 1.022E+13        | 9.2331E+00    | 1.190E+00 | 1.026E+13        | 0.001 |
| 1s 5d $^3D_3$   | 1s 6f $^3F_4^0$ | 2.6244E+01    | 5.292E+00 | 5.695E+12        | 2.6136E+01    | 5.311E+00 | 5.713E+12        | 0.000 |
| 1s 5g $^3G_4$   | 1s 6f $^3F_4^0$ | 2.6470E+01    | 2.307E-03 | 2.440E+09        | 2.6356E+01    | 2.319E-03 | 2.453E+09        | 0.000 |
| 1s 5g $^3G_3$   | 1s 6f $^3F_4^0$ | 2.6475E+01    | 6.552E-05 | 6.928E+07        |               |           |                  | 0.002 |
| 1s 5g $^3G_5$   | 1s 6f $^3F_4^0$ | 2.6601E+01    | 8.595E-02 | 9.002E+10        | 2.6486E+01    | 8.606E-02 | 9.015E+10        | 0.000 |
| 1s 5g $^1G_4$   | 1s 6f $^3F_4^0$ | 2.6606E+01    | 1.966E-03 | 2.059E+09        | 2.6491E+01    | 1.963E-03 | 2.056E+09        | 0.002 |
| 1s 6d $^3D_3$   | 1s 6f $^3F_4^0$ | 5.3175E+03    | 1.705E-01 | 4.469E+06        | 5.5117E+03    | 1.637E-01 | 3.962E+06        | 0.017 |
| 1s 4f $^3F_3^0$ | 1s 6g $^3G_4$   | 9.2736E+00    | 1.229E+00 | 1.060E+13        | 9.2341E+00    | 1.231E+00 | 1.061E+13        | 0.000 |
| 1s 4f $^3F_4^0$ | 1s 6g $^3G_4$   | 9.3264E+00    | 4.335E-02 | 3.694E+11        | 9.2866E+00    | 4.316E-02 | 3.678E+11        | 0.000 |
| 1s 4f $^1F_3^0$ | 1s 6g $^3G_4$   | 9.3281E+00    | 1.220E-03 | 1.039E+10        | 9.2883E+00    | 1.070E-03 | 9.114E+09        | 0.000 |
| 1s 5f $^3F_3^0$ | 1s 6g $^3G_4$   | 2.6251E+01    | 7.866E+00 | 8.460E+12        | 2.6139E+01    | 7.880E+00 | 8.475E+12        | 0.000 |
| 1s 5f $^3F_4^0$ | 1s 6g $^3G_4$   | 2.6469E+01    | 2.860E-01 | 3.026E+11        | 2.6355E+01    | 2.865E-01 | 3.031E+11        | 0.000 |
| 1s 5f $^1F_3^0$ | 1s 6g $^3G_4$   | 2.6476E+01    | 8.129E-03 | 8.594E+09        | 2.6362E+01    | 7.195E-03 | 7.608E+09        | 0.000 |
| 1s 6f $^3F_3^0$ | 1s 6g $^3G_4$   | 5.4970E+03    | 1.224E-01 | 3.001E+06        | 5.5303E+03    | 1.210E-01 | 2.909E+06        | 0.000 |
| 1s 6f $^3F_4^0$ | 1s 6g $^3G_4$   | 2.7996E+06    | 8.576E-06 | 8.111E-04        |               |           |                  | 0.475 |
| 1s 2p $^3P_2^0$ | 1s 6g $^3G_3$   | 1.4397E+00    | 2.240E-10 | 1.030E+05        |               |           |                  | 0.229 |
| 1s 3p $^3P_0^0$ | 1s 6g $^3G_3$   | 3.8210E+00    | 1.594E-12 | 1.041E+02        |               |           |                  | 0.345 |
| 1s 4p $^3P_2^0$ | 1s 6g $^3G_3$   | 9.1429E+00    | 1.067E-07 | 1.217E+06        |               |           |                  | 0.002 |
| 1s 4f $^3F_3^0$ | 1s 6g $^3G_3$   | 9.2732E+00    | 4.539E-02 | 5.029E+11        | 9.2341E+00    | 4.543E-02 | 5.033E+11        | 0.000 |
| 1s 4f $^3F_2^0$ | 1s 6g $^3G_3$   | 9.2754E+00    | 9.106E-01 | 1.009E+13        | 9.2363E+00    | 9.117E-01 | 1.009E+13        | 0.000 |
| 1s 4f $^3F_4^0$ | 1s 6g $^3G_3$   | 9.3261E+00    | 1.232E-03 | 1.362E+10        | 9.2866E+00    | 1.233E-03 | 1.351E+10        | 0.001 |
| 1s 4f $^1F_3^0$ | 1s 6g $^3G_3$   | 9.3277E+00    | 3.373E-02 | 3.694E+11        | 9.2883E+00    | 3.346E-02 | 3.664E+11        | 0.001 |

(continued on next page)

Table 3 (continued)

| Lower  | Upper  | GRASP2K       |           |                      | FAC           |           |                      | dT    |
|--|--|---------------|-----------|----------------------|---------------|-----------|----------------------|-------|
|  |  | $\lambda$ (Å) | gf        | A (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | A (s <sup>-1</sup> ) |       |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.5717E+01    | 1.070E-06 | 1.542E+06            |               |           |                      | 0.001 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.6248E+01    | 2.902E-01 | 4.014E+11            | 2.6139E+01    | 2.908E-01 | 4.021E+11            | 0.000 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.6257E+01    | 5.828E+00 | 8.055E+12            | 2.6148E+01    | 5.834E+00 | 8.062E+12            | 0.000 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.6466E+01    | 8.195E-03 | 1.115E+10            | 2.6355E+01    | 8.187E-03 | 1.113E+10            | 0.001 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.6473E+01    | 2.225E-01 | 3.025E+11            | 2.6362E+01    | 2.220E-01 | 3.018E+11            | 0.000 |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>3</sub>              | 1.5598E+03    | 7.276E-08 | 2.849E+01            |               |           |                      | 0.044 |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>3</sub>              | 5.3682E+03    | 4.626E-03 | 1.530E+05            | 5.5303E+03    | 4.489E-03 | 1.386E+05            | 0.028 |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>3</sub>              | 5.5968E+03    | 8.901E-02 | 2.708E+06            | 5.5277E+03    | 8.974E-02 | 2.774E+06            | 0.024 |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.1175E+05    | 3.244E-06 | 6.894E-02            |               |           |                      | 0.774 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.8309E+00    | 7.118E-06 | 4.622E+08            |               |           |                      | 0.014 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.8743E+00    | 1.279E-02 | 8.119E+11            | 3.8580E+00    | 1.279E-02 | 8.125E+11            | 0.000 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.8760E+00    | 2.543E-01 | 1.613E+13            | 3.8597E+00    | 2.562E-01 | 1.625E+13            | 0.000 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 9.1664E+00    | 4.419E-05 | 5.012E+08            |               |           |                      | 0.009 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 9.2714E+00    | 4.411E-02 | 4.890E+11            | 9.2331E+00    | 4.404E-02 | 4.880E+11            | 0.000 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 9.2758E+00    | 8.782E-01 | 9.726E+12            | 9.2375E+00    | 8.816E-01 | 9.761E+12            | 0.000 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.5812E+01    | 2.352E-04 | 3.364E+08            |               |           |                      | 0.006 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.6240E+01    | 1.968E-01 | 2.723E+11            | 2.6136E+01    | 1.964E-01 | 2.716E+11            | 0.000 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.6259E+01    | 3.925E+00 | 5.424E+12            | 2.6155E+01    | 3.931E+00 | 5.429E+12            | 0.000 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.6466E+01    | 6.562E-05 | 8.927E+07            |               |           |                      | 0.004 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.6471E+01    | 1.795E-03 | 2.440E+09            | 2.6361E+01    | 1.792E-03 | 2.437E+09            | 0.002 |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.6601E+01    | 6.833E-02 | 9.201E+10            | 2.6490E+01    | 6.844E-02 | 9.214E+10            | 0.001 |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.7871E+03    | 2.665E-05 | 7.950E+03            | 1.8323E+03    | 4.615E-05 | 1.298E+04            | 0.111 |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.1604E+03    | 6.538E-03 | 2.340E+05            | 5.5079E+03    | 6.062E-03 | 1.888E+05            | 0.009 |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.6121E+03    | 1.196E-01 | 3.619E+06            | 5.6823E+03    | 1.176E-01 | 3.443E+06            | 0.002 |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.8628E+05    | 3.680E-06 | 1.011E-01            |               |           |                      | 0.917 |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 9.9701E+05    | 1.872E-05 | 1.795E-02            |               |           |                      | 0.869 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>5</sub>              | 9.3170E+00    | 1.552E+00 | 1.084E+13            | 9.2773E+00    | 1.558E+00 | 1.088E+13            | 0.000 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>5</sub>              | 2.6394E+01    | 1.003E+01 | 8.734E+12            | 2.6281E+01    | 1.006E+01 | 8.758E+12            | 0.000 |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>5</sub>              | 9.2152E+03    | 9.257E-02 | 6.610E+05            | 9.2775E+03    | 9.155E-02 | 6.395E+05            | 0.002 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 2.6394E+01    | 1.465E+01 | 1.275E+13            | 2.6281E+01    | 1.467E+01 | 1.277E+13            | 0.000 |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 2.6525E+01    | 3.263E-01 | 2.812E+11            | 2.6411E+01    | 3.264E-01 | 2.813E+11            | 0.000 |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 2.6529E+01    | 5.862E-03 | 5.051E+09            | 2.6415E+01    | 4.968E-03 | 4.281E+09            | 0.001 |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 9.2359E+03    | 5.084E-02 | 3.614E+05            | 9.2564E+03    | 5.050E-02 | 3.544E+05            | 0.018 |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 8.7873E+06    | 1.183E-06 | 9.290E-06            |               |           |                      | 0.948 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 3.8727E+00    | 3.209E-12 | 1.586E+02            |               |           |                      | 0.851 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 9.2624E+00    | 6.140E-11 | 5.305E+02            |               |           |                      | 0.185 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 2.6168E+01    | 4.788E-09 | 5.183E+03            |               |           |                      | 0.002 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 2.6392E+01    | 3.318E-01 | 3.530E+11            | 2.6281E+01    | 3.323E-01 | 3.536E+11            | 0.000 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 2.6397E+01    | 1.165E+01 | 1.239E+13            | 2.6286E+01    | 1.166E+01 | 1.241E+13            | 0.000 |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 2.6523E+01    | 6.061E-03 | 6.385E+09            | 2.6411E+01    | 6.044E-03 | 6.367E+09            | 0.001 |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 2.6527E+01    | 2.678E-01 | 2.820E+11            | 2.6415E+01    | 2.670E-01 | 2.812E+11            | 0.000 |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 3.3388E+03    | 1.016E-10 | 6.754E-03            |               |           |                      | 0.436 |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 9.0013E+03    | 1.182E-03 | 1.081E+04            | 9.2564E+03    | 1.147E-03 | 9.845E+03            | 0.004 |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 9.3695E+03    | 3.986E-02 | 3.365E+05            | 9.2564E+03    | 4.017E-02 | 3.445E+05            | 0.012 |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 3.4069E+05    | 5.670E-07 | 3.620E-03            |               |           |                      | 0.752 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>4</sub>              | 9.2640E+00    | 1.114E-07 | 9.625E+05            |               |           |                      | 0.014 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>4</sub>              | 9.3167E+00    | 3.545E-02 | 3.027E+11            | 9.2773E+00    | 3.542E-02 | 3.024E+11            | 0.000 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>4</sub>              | 9.3184E+00    | 1.235E+00 | 1.054E+13            | 9.2790E+00    | 1.239E+00 | 1.057E+13            | 0.000 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>4</sub>              | 2.6175E+01    | 1.994E-07 | 2.157E+05            |               |           |                      | 0.031 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>4</sub>              | 2.6391E+01    | 2.290E-01 | 2.437E+11            | 2.6281E+01    | 2.286E-01 | 2.432E+11            | 0.000 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>4</sub>              | 2.6398E+01    | 7.983E+00 | 8.490E+12            | 2.6287E+01    | 8.001E+00 | 8.508E+12            | 0.000 |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>4</sub>              | 3.4068E+03    | 1.222E-09 | 7.804E-02            |               |           |                      | 0.960 |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>4</sub>              | 8.9311E+03    | 2.180E-03 | 2.026E+04            | 9.2773E+03    | 2.080E-03 | 1.776E+04            | 0.042 |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>4</sub>              | 9.4124E+03    | 7.208E-02 | 6.030E+05            | 9.2882E+03    | 7.274E-02 | 6.196E+05            | 0.031 |
| 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>4</sub>              | 2.9962E+05    | 6.236E-07 | 5.149E-03            |               |           |                      | 0.526 |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 6g <sup>3</sup> G <sub>4</sub>              | 1.9372E+06    | 4.406E-06 | 8.701E-04            |               |           |                      | 0.711 |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 2.6474E+01    | 1.773E+01 | 1.298E+13            | 2.6361E+01    | 1.777E+01 | 1.301E+13            | 0.000 |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1.3897E+04    | 4.086E-02 | 1.085E+05            | 1.3933E+04    | 4.057E-02 | 1.063E+05            | 0.026 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.6342E+01    | 1.711E-06 | 1.496E+06            |               |           |                      | 0.001 |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.6473E+01    | 2.737E-01 | 2.369E+11            | 2.6361E+01    | 2.735E-01 | 2.366E+11            | 0.000 |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.6477E+01    | 1.473E+01 | 1.274E+13            | 2.6365E+01    | 1.476E+01 | 1.277E+13            | 0.000 |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 5.4809E+03    | 9.930E-09 | 2.004E-01            |               |           |                      | 0.195 |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.3461E+04    | 6.513E-04 | 2.180E+03            | 1.3933E+04    | 6.242E-04 | 1.933E+03            | 0.002 |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.4116E+04    | 3.341E-02 | 1.017E+05            | 1.3934E+04    | 3.370E-02 | 1.043E+05            | 0.019 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7s <sup>3</sup> S <sub>1</sub>              | 1.3378E+00    | 7.720E-04 | 9.590E+11            | 1.3323E+00    | 8.087E-04 | 1.004E+12            | 0.015 |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7s <sup>3</sup> S <sub>1</sub>              | 1.3387E+00    | 3.810E-04 | 4.727E+11            | 1.3331E+00    | 3.785E-04 | 4.696E+11            | 0.001 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7s <sup>3</sup> S <sub>1</sub>              | 1.3964E+00    | 2.525E-03 | 2.879E+12            | 1.3905E+00    | 2.566E-03 | 2.926E+12            | 0.019 |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7s <sup>3</sup> S <sub>1</sub>              | 1.4019E+00    | 4.638E-04 | 5.247E+11            | 1.3961E+00    | 4.626E-04 | 5.232E+11            | 0.004 |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7s <sup>3</sup> S <sub>1</sub>              | 3.4180E+00    | 3.432E-03 | 6.531E+11            | 3.4039E+00    | 3.453E-03 | 6.570E+11            | 0.006 |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7s <sup>3</sup> S <sub>1</sub>              | 3.4195E+00    | 1.667E-03 | 3.171E+11            | 3.4054E+00    | 1.625E-03 | 3.089E+11            | 0.006 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7s <sup>3</sup> S <sub>1</sub>              | 3.5305E+00    | 1.085E-02 | 1.935E+12            | 3.5159E+00    | 1.077E-02 | 1.922E+12            | 0.004 |

(continued on next page)

Table 3 (continued)

| Lower           | Upper             | GRASP2K       |           |                  | FAC           |           |                  | dT    |
|-----------------|-------------------|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|                 |                   | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) |       |
| 1s 3p $^1P_0^o$ | 1s 7s $^3S_1$     | 3.5405E+00    | 1.974E-03 | 3.501E+11        | 3.5260E+00    | 1.955E-03 | 3.467E+11        | 0.005 |
| 1s 4p $^3P_1^o$ | 1s 7s $^3S_1$     | 7.4166E+00    | 1.104E-02 | 4.464E+11        | 7.3859E+00    | 1.108E-02 | 4.478E+11        | 0.004 |
| 1s 4p $^3P_0^o$ | 1s 7s $^3S_1$     | 7.4194E+00    | 5.355E-03 | 2.163E+11        | 7.3886E+00    | 5.225E-03 | 2.110E+11        | 0.004 |
| 1s 4p $^3P_2^o$ | 1s 7s $^3S_1$     | 7.6388E+00    | 3.445E-02 | 1.313E+12        | 7.6070E+00    | 3.431E-02 | 1.307E+12        | 0.004 |
| 1s 4p $^1P_1^o$ | 1s 7s $^3S_1$     | 7.6581E+00    | 6.277E-03 | 2.380E+11        | 7.6265E+00    | 6.235E-03 | 2.363E+11        | 0.004 |
| 1s 4f $^3F_2^o$ | 1s 7s $^3S_1$     | 7.7310E+00    | 1.468E-09 | 5.461E+04        |               |           |                  | 0.174 |
| 1s 5p $^3P_1^o$ | 1s 7s $^3S_1$     | 1.6020E+01    | 3.789E-02 | 3.283E+11        | 1.5955E+01    | 3.806E-02 | 3.296E+11        | 0.001 |
| 1s 5p $^3P_0^o$ | 1s 7s $^3S_1$     | 1.6027E+01    | 1.835E-02 | 1.589E+11        | 1.5961E+01    | 1.794E-02 | 1.553E+11        | 0.001 |
| 1s 5p $^3P_2^o$ | 1s 7s $^3S_1$     | 1.6551E+01    | 1.189E-01 | 9.653E+11        | 1.6483E+01    | 1.187E-01 | 9.639E+11        | 0.001 |
| 1s 5p $^1P_1^o$ | 1s 7s $^3S_1$     | 1.6597E+01    | 2.172E-02 | 1.753E+11        | 1.6529E+01    | 2.161E-02 | 1.744E+11        | 0.000 |
| 1s 5f $^3F_2^o$ | 1s 7s $^3S_1$     | 1.6773E+01    | 1.742E-08 | 1.377E+05        |               |           |                  | 0.145 |
| 1s 6p $^3P_1^o$ | 1s 7s $^3S_1$     | 4.2860E+01    | 2.134E-01 | 2.582E+11        | 4.2690E+01    | 2.157E-01 | 2.610E+11        | 0.005 |
| 1s 6p $^3P_0^o$ | 1s 7s $^3S_1$     | 4.2887E+01    | 1.033E-01 | 1.249E+11        | 4.2622E+01    | 1.000E-01 | 1.214E+11        | 0.006 |
| 1s 6p $^3P_2^o$ | 1s 7s $^3S_1$     | 4.5091E+01    | 7.068E-01 | 7.730E+11        | 4.4909E+01    | 7.019E-01 | 7.672E+11        | 0.005 |
| 1s 6p $^1P_1^o$ | 1s 7s $^3S_1$     | 4.5287E+01    | 1.298E-01 | 1.408E+11        | 4.5084E+01    | 1.247E-01 | 1.352E+11        | 0.004 |
| 1s 6f $^3F_2^o$ | 1s 7s $^3S_1$     | 4.6051E+01    | 2.376E-07 | 2.491E+05        |               |           |                  | 0.119 |
| 1s $^2^1S_0$    | 1s 7p $^3P_0^o$ 8 | 3.1400E-01    | 2.473E-03 | 5.575E+13        | 3.1277E-01    | 2.233E-03 | 5.033E+13        | 0.014 |
| 1s 2s $^3S_1$   | 1s 7p $^3P_1^o$   | 1.3266E+00    | 8.485E-03 | 1.072E+13        | 1.3210E+00    | 8.499E-03 | 1.073E+13        | 0.001 |
| 1s 2s $^1S_0$   | 1s 7p $^3P_0^o$   | 1.3387E+00    | 3.675E-03 | 4.559E+12        | 1.3333E+00    | 3.455E-03 | 4.285E+12        | 0.005 |
| 1s 3s $^3S_1$   | 1s 7p $^3P_1^o$   | 3.3968E+00    | 1.851E-02 | 3.568E+12        | 3.3827E+00    | 1.869E-02 | 3.601E+12        | 0.003 |
| 1s 3s $^1S_0$   | 1s 7p $^3P_0^o$   | 3.4178E+00    | 8.150E-03 | 1.551E+12        | 3.4039E+00    | 7.676E-03 | 1.460E+12        | 0.004 |
| 1s 3d $^3D_2$   | 1s 7p $^3P_1^o$   | 3.5373E+00    | 2.636E-03 | 4.685E+11        | 3.5225E+00    | 2.629E-03 | 4.672E+11        | 0.007 |
| 1s 3d $^3D_1$   | 1s 7p $^3P_1^o$   | 3.5388E+00    | 5.820E-04 | 1.033E+11        | 3.5240E+00    | 5.690E-04 | 1.010E+11        | 0.014 |
| 1s 3d $^1D_2$   | 1s 7p $^3P_0^o$   | 3.5757E+00    | 3.300E-06 | 5.739E+08        | 3.5607E+00    | 4.032E-06 | 7.011E+08        | 0.058 |
| 1s 4s $^3S_1$   | 1s 7p $^3P_1^o$   | 7.3716E+00    | 4.040E-02 | 1.653E+12        | 7.3412E+00    | 4.095E-02 | 1.675E+12        | 0.005 |
| 1s 4s $^1S_0$   | 1s 7p $^3P_0^o$   | 7.4116E+00    | 1.804E-02 | 7.300E+11        | 7.3814E+00    | 1.691E-02 | 6.845E+11        | 0.013 |
| 1s 4d $^3D_2$   | 1s 7p $^3P_1^o$   | 7.6476E+00    | 1.361E-02 | 5.173E+11        | 7.6163E+00    | 1.350E-02 | 5.132E+11        | 0.004 |
| 1s 4d $^3D_1$   | 1s 7p $^3P_1^o$   | 7.6504E+00    | 2.969E-03 | 1.128E+11        | 7.6191E+00    | 2.915E-03 | 1.106E+11        | 0.011 |
| 1s 4d $^1D_2$   | 1s 7p $^3P_0^o$   | 7.7236E+00    | 1.514E-05 | 5.643E+08        | 7.6918E+00    | 1.914E-05 | 7.134E+08        | 0.050 |
| 1s 5s $^3S_1$   | 1s 7p $^3P_0^o$   | 1.5898E+01    | 1.045E-01 | 9.197E+11        | 1.5833E+01    | 1.061E-01 | 9.332E+11        | 0.005 |
| 1s 5s $^1S_0$   | 1s 7p $^3P_1^o$   | 1.5991E+01    | 4.695E-02 | 4.082E+11        | 1.5927E+01    | 4.406E-02 | 3.829E+11        | 0.014 |
| 1s 5d $^3D_2$   | 1s 7p $^3P_1^o$   | 1.6554E+01    | 6.096E-02 | 4.946E+11        | 1.6489E+01    | 6.030E-02 | 4.890E+11        | 0.002 |
| 1s 5d $^3D_1$   | 1s 7p $^3P_1^o$   | 1.6561E+01    | 1.320E-02 | 1.070E+11        | 1.6495E+01    | 1.298E-02 | 1.052E+11        | 0.007 |
| 1s 5d $^1D_2$   | 1s 7p $^3P_0^o$   | 1.6737E+01    | 6.527E-05 | 5.181E+08        | 1.6670E+01    | 8.178E-05 | 6.487E+08        | 0.033 |
| 1s 6s $^3S_1$   | 1s 7p $^3P_1^o$   | 4.2260E+01    | 4.475E-01 | 5.571E+11        | 4.2057E+01    | 4.571E-01 | 5.697E+11        | 0.006 |
| 1s 6s $^1S_0$   | 1s 7p $^3P_0^o$   | 4.2638E+01    | 2.029E-01 | 2.482E+11        | 4.2377E+01    | 1.912E-01 | 2.347E+11        | 0.009 |
| 1s 6d $^3D_2$   | 1s 7p $^3P_1^o$   | 4.4993E+01    | 4.312E-01 | 4.736E+11        | 4.4844E+01    | 4.266E-01 | 4.677E+11        | 0.002 |
| 1s 6d $^3D_1$   | 1s 7p $^3P_1^o$   | 4.5021E+01    | 9.291E-02 | 1.019E+11        | 4.4837E+01    | 9.088E-02 | 9.966E+10        | 0.002 |
| 1s 6d $^1D_2$   | 1s 7p $^3P_0^o$   | 4.5778E+01    | 4.619E-04 | 4.901E+08        | 4.5600E+01    | 3.977E-04 | 4.217E+08        | 0.019 |
| 1s 7s $^3S_1$   | 1s 7p $^3P_1^o$   | 7.6504E+03    | 4.971E-02 | 1.888E+06        | 7.3461E+03    | 5.274E-02 | 2.154E+06        | 0.473 |
| 1s 2p $^3P_1^o$ | 1s 7s $^1S_0$     | 1.3376E+00    | 3.292E-04 | 1.227E+12        | 1.3321E+00    | 3.285E-04 | 1.224E+12        | 0.026 |
| 1s 2p $^1P_1^o$ | 1s 7s $^1S_0$     | 1.4017E+00    | 1.114E-03 | 3.782E+12        | 1.3959E+00    | 1.070E-03 | 3.634E+12        | 0.019 |
| 1s 3p $^3P_1^o$ | 1s 7s $^1S_0$     | 3.4164E+00    | 1.425E-03 | 8.144E+11        | 3.4026E+00    | 1.427E-03 | 8.155E+11        | 0.006 |
| 1s 3p $^1P_1^o$ | 1s 7s $^1S_0$     | 3.5388E+00    | 4.562E-03 | 2.430E+12        | 3.5246E+00    | 4.493E-03 | 2.392E+12        | 0.001 |
| 1s 4p $^3P_1^o$ | 1s 7s $^1S_0$     | 7.4094E+00    | 4.589E-03 | 5.575E+11        | 7.3798E+00    | 4.609E-03 | 5.597E+11        | 0.001 |
| 1s 4p $^1P_1^o$ | 1s 7s $^1S_0$     | 7.6504E+00    | 1.442E-02 | 1.643E+12        | 7.6200E+00    | 1.430E-02 | 1.629E+12        | 0.002 |
| 1s 5p $^3P_1^o$ | 1s 7s $^1S_0$     | 1.5987E+01    | 1.568E-02 | 4.091E+11        | 1.5926E+01    | 1.585E-02 | 4.135E+11        | 0.008 |
| 1s 5p $^1P_1^o$ | 1s 7s $^1S_0$     | 1.6561E+01    | 4.949E-02 | 1.204E+12        | 1.6498E+01    | 4.952E-02 | 1.203E+12        | 0.007 |
| 1s 6p $^3P_1^o$ | 1s 7s $^1S_0$     | 4.2620E+01    | 8.694E-02 | 3.193E+11        | 4.2488E+01    | 8.468E-02 | 3.102E+11        | 0.004 |
| 1s 6p $^1P_1^o$ | 1s 7s $^1S_0$     | 4.5020E+01    | 2.908E-01 | 9.571E+11        | 4.4858E+01    | 2.959E-01 | 9.728E+11        | 0.004 |
| 1s 7p $^3P_1^o$ | 1s 7s $^1S_0$     | 1.5939E+06    | 1.021E-04 | 2.681E-01        |               |           |                  | 0.803 |
| 1s 2s $^3S_1$   | 1s 7p $^3P_0^o$   | 1.3265E+00    | 4.036E-03 | 1.530E+13        | 1.3210E+00    | 3.995E-03 | 1.514E+13        | 0.003 |
| 1s 3s $^3S_1$   | 1s 7p $^3P_0^o$   | 3.3967E+00    | 8.794E-03 | 5.084E+12        | 3.3830E+00    | 8.817E-03 | 5.095E+12        | 0.006 |
| 1s 3d $^3D_1$   | 1s 7p $^3P_0^o$   | 3.5387E+00    | 1.077E-03 | 5.739E+11        | 3.5243E+00    | 1.057E-03 | 5.628E+11        | 0.014 |
| 1s 4s $^3S_1$   | 1s 7p $^3P_0^o$   | 7.3711E+00    | 1.921E-02 | 2.358E+12        | 7.3425E+00    | 1.936E-02 | 2.376E+12        | 0.007 |
| 1s 4d $^3D_1$   | 1s 7p $^3P_0^o$   | 7.6499E+00    | 5.527E-03 | 6.300E+11        | 7.6205E+00    | 5.438E-03 | 6.193E+11        | 0.010 |
| 1s 5s $^3S_1$   | 1s 7p $^3P_0^o$   | 1.5896E+01    | 4.976E-02 | 1.314E+12        | 1.5839E+01    | 5.030E-02 | 1.326E+12        | 0.007 |
| 1s 5d $^3D_1$   | 1s 7p $^3P_0^o$   | 1.6558E+01    | 2.465E-02 | 5.997E+11        | 1.6502E+01    | 2.430E-02 | 5.902E+11        | 0.006 |
| 1s 6s $^3S_1$   | 1s 7p $^3P_0^o$   | 4.2244E+01    | 2.130E-01 | 7.963E+11        | 4.2099E+01    | 2.165E-01 | 8.080E+11        | 0.007 |
| 1s 6d $^3D_1$   | 1s 7p $^3P_0^o$   | 4.5003E+01    | 1.739E-01 | 5.729E+11        | 4.4885E+01    | 1.725E-01 | 5.665E+11        | 0.001 |
| 1s 7s $^3S_1$   | 1s 7p $^3P_0^o$   | 7.1550E+03    | 2.549E-02 | 3.321E+06        | 8.8861E+03    | 2.046E-02 | 1.714E+06        | 0.480 |
| 1s 2s $^3S_1$   | 1s 7p $^3P_2^o$   | 1.3253E+00    | 1.891E-02 | 1.437E+13        | 1.3197E+00    | 1.925E-02 | 1.462E+13        | 0.001 |
| 1s 3s $^3S_1$   | 1s 7p $^3P_2^o$   | 3.3884E+00    | 3.934E-02 | 4.571E+12        | 3.3744E+00    | 3.973E-02 | 4.615E+12        | 0.005 |
| 1s 3d $^3D_2$   | 1s 7p $^3P_2^o$   | 3.5282E+00    | 3.283E-04 | 3.518E+10        | 3.5135E+00    | 3.304E-04 | 3.541E+10        | 0.010 |
| 1s 3d $^3D_1$   | 1s 7p $^3P_2^o$   | 3.5297E+00    | 3.595E-05 | 3.849E+09        | 3.5150E+00    | 3.345E-05 | 3.581E+09        | 0.017 |
| 1s 3d $^3D_3$   | 1s 7p $^3P_2^o$   | 3.5650E+00    | 3.513E-03 | 3.687E+11        | 3.5501E+00    | 3.455E-03 | 3.626E+11        | 0.013 |
| 1s 3d $^1D_2$   | 1s 7p $^3P_2^o$   | 3.5665E+00    | 2.544E-04 | 2.668E+10        | 3.5515E+00    | 2.446E-04 | 2.565E+10        | 0.013 |
| 1s 4s $^3S_1$   | 1s 7p $^3P_2^o$   | 7.3324E+00    | 8.272E-02 | 2.052E+12        | 7.3023E+00    | 8.341E-02 | 2.069E+12        | 0.007 |
| 1s 4d $^3D_2$   | 1s 7p $^3P_2^o$   | 7.6054E+00    | 1.768E-03 | 4.077E+10        | 7.5744E+00    | 1.757E-03 | 4.050E+10        | 0.006 |
| 1s 4d $^3D_1$   | 1s 7p $^3P_2^o$   | 7.6082E+00    | 1.921E-04 | 4.428E+09        | 7.5772E+00    | 1.813E-04 | 4.178E+09        | 0.008 |
| 1s 4d $^3D_3$   | 1s 7p $^3P_2^o$   | 7.6776E+00    | 1.856E-02 | 4.201E+11        | 7.6461E+00    | 1.822E-02 | 4.122E+11        | 0.008 |

(continued on next page)

Table 3 (continued)

| Lower                             | Upper  | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|-----------------------------------|--|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|                                   |  | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s 4d <sup>1</sup> D <sub>2</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.6806E+00    | 1.326E-03 | 2.999E+10              | 7.6491E+00    | 1.284E-03 | 2.903E+10              | 0.009 |
| 1s 5s <sup>3</sup> S <sub>1</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.5717E+01    | 2.047E-01 | 1.106E+12              | 1.5653E+01    | 2.060E-01 | 1.112E+12              | 0.007 |
| 1s 5d <sup>3</sup> D <sub>2</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6358E+01    | 8.043E-03 | 4.010E+10              | 1.6293E+01    | 7.930E-03 | 3.951E+10              | 0.003 |
| 1s 5d <sup>3</sup> D <sub>1</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6364E+01    | 8.712E-04 | 4.340E+09              | 1.6300E+01    | 8.288E-04 | 4.126E+09              | 0.004 |
| 1s 5d <sup>3</sup> D <sub>3</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6529E+01    | 8.380E-02 | 4.092E+11              | 1.6463E+01    | 8.203E-02 | 4.003E+11              | 0.004 |
| 1s 5d <sup>1</sup> D <sub>2</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6536E+01    | 5.940E-03 | 2.898E+10              | 1.6471E+01    | 5.769E-03 | 2.812E+10              | 0.005 |
| 1s 5g <sup>3</sup> G <sub>3</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6620E+01    | 2.424E-09 | 1.171E+04              |               |           |                        | 0.041 |
| 1s 6s <sup>3</sup> S <sub>1</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.1005E+01    | 7.989E-01 | 6.339E+11              | 4.0810E+01    | 8.054E-01 | 6.397E+11              | 0.007 |
| 1s 6d <sup>3</sup> D <sub>2</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.3572E+01    | 5.481E-02 | 3.851E+10              | 4.3429E+01    | 5.418E-02 | 3.800E+10              | 0.003 |
| 1s 6d <sup>3</sup> D <sub>1</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.3599E+01    | 5.937E-03 | 4.167E+09              | 4.3422E+01    | 5.899E-03 | 4.138E+09              | 0.000 |
| 1s 6d <sup>3</sup> D <sub>3</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4278E+01    | 5.768E-01 | 3.925E+11              | 4.4127E+01    | 5.633E-01 | 3.826E+11              | 0.003 |
| 1s 6d <sup>1</sup> D <sub>2</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4308E+01    | 4.074E-02 | 2.768E+10              | 4.4138E+01    | 3.914E-02 | 2.657E+10              | 0.001 |
| 1s 6g <sup>3</sup> G <sub>3</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4659E+01    | 4.072E-08 | 2.724E+04              |               |           |                        | 0.013 |
| 1s 7s <sup>3</sup> S <sub>1</sub> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.1691E+03    | 7.901E-01 | 7.712E+08              | 1.1590E+03    | 7.980E-01 | 7.858E+08              | 0.072 |
| 1s 2p <sup>3</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.3362E+00    | 3.096E-02 | 2.313E+13              | 1.3307E+00    | 3.108E-02 | 2.321E+13              | 0.001 |
| 1s 2p <sup>3</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.3946E+00    | 5.230E-03 | 3.587E+12              | 1.3888E+00    | 5.160E-03 | 3.539E+12              | 0.008 |
| 1s 2p <sup>1</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.4001E+00    | 8.791E-04 | 5.983E+11              | 1.3943E+00    | 8.081E-04 | 5.498E+11              | 0.013 |
| 1s 3p <sup>3</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 3.4075E+00    | 6.964E-02 | 8.001E+12              | 3.3932E+00    | 6.971E-02 | 8.008E+12              | 0.001 |
| 1s 3p <sup>3</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 3.5193E+00    | 1.286E-02 | 1.385E+12              | 3.5045E+00    | 1.286E-02 | 1.385E+12              | 0.001 |
| 1s 3p <sup>1</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 3.5292E+00    | 2.078E-03 | 2.225E+11              | 3.5145E+00    | 1.921E-03 | 2.057E+11              | 0.003 |
| 1s 4p <sup>3</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.3673E+00    | 1.429E-01 | 3.511E+12              | 7.3356E+00    | 1.431E-01 | 3.519E+12              | 0.001 |
| 1s 4p <sup>3</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.5864E+00    | 2.803E-02 | 6.498E+11              | 7.5537E+00    | 2.826E-02 | 6.552E+11              | 0.001 |
| 1s 4p <sup>1</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.6055E+00    | 4.508E-03 | 1.040E+11              | 7.5729E+00    | 4.133E-03 | 9.533E+10              | 0.003 |
| 1s 4f <sup>3</sup> F <sub>3</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.6759E+00    | 4.363E-03 | 9.879E+10              | 7.6429E+00    | 4.349E-03 | 9.848E+10              | 0.006 |
| 1s 4f <sup>3</sup> F <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.6774E+00    | 3.185E-04 | 7.208E+09              | 7.6444E+00    | 3.188E-04 | 7.218E+09              | 0.006 |
| 1s 4f <sup>1</sup> F <sub>3</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.7133E+00    | 3.659E-07 | 8.205E+06              |               |           |                        | 0.014 |
| 1s 5p <sup>3</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.5792E+01    | 3.371E-01 | 1.803E+12              | 1.5722E+01    | 3.385E-01 | 1.811E+12              | 0.001 |
| 1s 5p <sup>3</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.6307E+01    | 7.040E-02 | 3.532E+11              | 1.6234E+01    | 7.148E-02 | 3.587E+11              | 0.001 |
| 1s 5p <sup>1</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.6352E+01    | 1.134E-02 | 5.658E+10              | 1.6279E+01    | 1.027E-02 | 5.130E+10              | 0.004 |
| 1s 5f <sup>3</sup> F <sub>3</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.6519E+01    | 3.339E-02 | 1.633E+11              | 1.6446E+01    | 3.340E-02 | 1.633E+11              | 0.001 |
| 1s 5f <sup>3</sup> F <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.6522E+01    | 2.432E-03 | 1.189E+10              | 1.6450E+01    | 2.444E-03 | 1.195E+10              | 0.001 |
| 1s 5f <sup>1</sup> F <sub>3</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.6607E+01    | 2.729E-06 | 1.320E+07              |               |           |                        | 0.014 |
| 1s 6p <sup>3</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.1263E+01    | 1.251E+00 | 9.802E+11              | 4.1063E+01    | 1.250E+00 | 9.806E+11              | 0.001 |
| 1s 6p <sup>3</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.3326E+01    | 2.912E-01 | 2.069E+11              | 4.3112E+01    | 2.974E-01 | 2.116E+11              | 0.001 |
| 1s 6p <sup>1</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.3508E+01    | 4.727E-02 | 3.331E+10              | 4.3273E+01    | 4.648E-02 | 3.283E+10              | 0.001 |
| 1s 6f <sup>3</sup> F <sub>3</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.4197E+01    | 3.118E-01 | 2.129E+11              | 4.4000E+01    | 3.118E-01 | 2.130E+11              | 0.000 |
| 1s 6f <sup>3</sup> F <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.4212E+01    | 2.269E-02 | 1.548E+10              | 4.4000E+01    | 2.271E-02 | 1.552E+10              | 0.000 |
| 1s 6f <sup>1</sup> F <sub>3</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.4566E+01    | 2.533E-05 | 1.702E+07              |               |           |                        | 0.015 |
| 1s 7p <sup>3</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.2946E+03    | 6.694E-01 | 5.328E+08              | 1.2624E+03    | 6.847E-01 | 5.683E+08              | 0.085 |
| 1s 7p <sup>3</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 2.0924E+04    | 7.595E-03 | 2.314E+04              | 1.5290E+04    | 1.048E-02 | 5.933E+04              | 0.623 |
| 1s 2p <sup>3</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.3362E+00    | 6.637E-03 | 8.265E+12              | 1.3307E+00    | 6.631E-03 | 8.256E+12              | 0.004 |
| 1s 2p <sup>3</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.3371E+00    | 1.257E-02 | 1.564E+13              | 1.3315E+00    | 1.257E-02 | 1.563E+13              | 0.002 |
| 1s 2p <sup>1</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.3946E+00    | 5.723E-04 | 6.542E+11              | 1.3888E+00    | 5.618E-04 | 6.421E+11              | 0.010 |
| 1s 2p <sup>1</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.4001E+00    | 2.555E-03 | 2.898E+12              | 1.3943E+00    | 2.472E-03 | 2.803E+12              | 0.006 |
| 1s 3p <sup>3</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 3.4074E+00    | 1.488E-02 | 2.849E+12              | 3.3932E+00    | 1.485E-02 | 2.844E+12              | 0.000 |
| 1s 3p <sup>3</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 3.4088E+00    | 2.822E-02 | 5.400E+12              | 3.3947E+00    | 2.819E-02 | 5.393E+12              | 0.000 |
| 1s 3p <sup>1</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 3.5192E+00    | 1.406E-03 | 2.523E+11              | 3.5045E+00    | 1.401E-03 | 2.515E+11              | 0.000 |
| 1s 3p <sup>1</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 3.5291E+00    | 6.358E-03 | 1.135E+12              | 3.5145E+00    | 6.259E-03 | 1.117E+12              | 0.000 |
| 1s 4p <sup>3</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 7.3668E+00    | 3.045E-02 | 1.248E+12              | 7.3357E+00    | 3.052E-02 | 1.250E+12              | 0.000 |
| 1s 4p <sup>3</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 7.3695E+00    | 5.785E-02 | 2.368E+12              | 7.3384E+00    | 5.791E-02 | 2.370E+12              | 0.000 |
| 1s 4p <sup>1</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 7.5859E+00    | 3.056E-03 | 1.181E+11              | 7.5538E+00    | 3.082E-03 | 1.190E+11              | 0.000 |
| 1s 4p <sup>1</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 7.6050E+00    | 1.395E-02 | 5.361E+11              | 7.5730E+00    | 1.384E-02 | 5.323E+11              | 0.000 |
| 1s 4f <sup>3</sup> F <sub>3</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 7.6769E+00    | 2.803E-03 | 1.058E+11              | 7.6445E+00    | 2.797E-03 | 1.055E+11              | 0.006 |
| 1s 5p <sup>3</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.5790E+01    | 7.173E-02 | 6.397E+11              | 1.5722E+01    | 7.230E-02 | 6.448E+11              | 0.002 |
| 1s 5p <sup>3</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.5796E+01    | 1.364E-01 | 1.215E+12              | 1.5728E+01    | 1.369E-01 | 1.220E+12              | 0.002 |
| 1s 5p <sup>1</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.6305E+01    | 7.659E-03 | 6.406E+10              | 1.6235E+01    | 7.804E-03 | 6.528E+10              | 0.001 |
| 1s 5p <sup>1</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.6349E+01    | 3.522E-02 | 2.929E+11              | 1.6280E+01    | 3.519E-02 | 2.927E+11              | 0.002 |
| 1s 5f <sup>3</sup> F <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.6520E+01    | 2.145E-02 | 1.748E+11              | 1.6451E+01    | 2.148E-02 | 1.750E+11              | 0.001 |
| 1s 6p <sup>3</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 4.1248E+01    | 2.657E-01 | 3.472E+11              | 4.1067E+01    | 2.734E-01 | 3.574E+11              | 0.000 |
| 1s 6p <sup>3</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 4.1273E+01    | 5.057E-01 | 6.601E+11              | 4.1003E+01    | 5.090E-01 | 6.675E+11              | 0.000 |
| 1s 6p <sup>1</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 4.3310E+01    | 3.160E-02 | 3.746E+10              | 4.3116E+01    | 3.243E-02 | 3.846E+10              | 0.000 |
| 1s 6p <sup>1</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 4.3491E+01    | 1.469E-01 | 1.726E+11              | 4.3277E+01    | 1.432E-01 | 1.686E+11              | 0.000 |
| 1s 6f <sup>3</sup> F <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 4.4195E+01    | 2.002E-01 | 2.279E+11              | 4.4004E+01    | 2.007E-01 | 2.285E+11              | 0.000 |
| 1s 7p <sup>3</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.2801E+03    | 1.445E-01 | 1.960E+08              | 1.2659E+03    | 1.475E-01 | 2.029E+08              | 0.069 |
| 1s 7p <sup>3</sup> P <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.2951E+03    | 2.699E-01 | 3.578E+08              | 1.2292E+03    | 2.853E-01 | 4.163E+08              | 0.073 |
| 1s 7p <sup>1</sup> P <sub>0</sub> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.7684E+04    | 9.719E-04 | 6.910E+03              |               |           |                        | 0.539 |
| 1s 2 <sup>1</sup> S <sub>0</sub>  | 1s 7p <sup>1</sup> P <sub>0</sub>              | 3.1400E-01    | 6.133E-03 | 1.383E+14              | 3.1269E-01    | 6.558E-03 | 1.478E+14              | 0.034 |
| 1s 2s <sup>3</sup> S <sub>1</sub> | 1s 7p <sup>1</sup> P <sub>0</sub>              | 1.3252E+00    | 3.384E-03 | 4.284E+12              | 1.3196E+00    | 3.343E-03 | 4.232E+12              | 0.001 |
| 1s 2s <sup>1</sup> S <sub>0</sub> | 1s 7p <sup>1</sup> P <sub>0</sub>              | 1.3373E+00    | 8.044E-03 | 1.000E+13              | 1.3319E+00    | 8.135E-03 | 1.011E+13              | 0.002 |
| 1s 3s <sup>3</sup> S <sub>1</sub> | 1s 7p <sup>1</sup> P <sub>0</sub>              | 3.3877E+00    | 7.007E-03 | 1.358E+12              | 3.3738E+00    | 6.862E-03 | 1.329E+12              | 0.004 |
| 1s 3s <sup>1</sup> S <sub>0</sub> | 1s 7p <sup>1</sup> P <sub>0</sub>              | 3.4087E+00    | 1.698E-02 | 3.249E+12              | 3.3948E+00    | 1.687E-02 | 3.228E+12              | 0.007 |

(continued on next page)



Table 3 (continued)

| Lower  | Upper  | GRASP2K       |           |                  | FAC           |           |                  | dT    |
|--|--|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|  |  | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) |       |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.5275E+00    | 5.455E-05 | 9.748E+09        | 3.5128E+00    | 6.841E-05 | 1.222E+10        | 0.020 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.5290E+00    | 1.667E-04 | 2.975E+10        | 3.5143E+00    | 1.567E-04 | 2.797E+10        | 0.023 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.5657E+00    | 2.254E-03 | 3.941E+11        | 3.5508E+00    | 2.218E-03 | 3.879E+11        | 0.018 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.3292E+00    | 1.467E-02 | 6.074E+11        | 7.2994E+00    | 1.435E-02 | 5.938E+11        | 0.006 |
| 1s 4s <sup>1</sup> S <sub>0</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.3687E+00    | 3.615E-02 | 1.480E+12        | 7.3391E+00    | 3.552E-02 | 1.453E+12        | 0.018 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.6019E+00    | 2.848E-04 | 1.096E+10        | 7.5713E+00    | 3.513E-04 | 1.351E+10        | 0.015 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.6047E+00    | 8.821E-04 | 3.391E+10        | 7.5741E+00    | 8.289E-04 | 3.185E+10        | 0.015 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.6770E+00    | 1.182E-02 | 4.460E+11        | 7.6459E+00    | 1.171E-02 | 4.416E+11        | 0.012 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.5702E+01    | 3.615E-02 | 3.260E+11        | 1.5640E+01    | 3.530E-02 | 3.181E+11        | 0.006 |
| 1s 5s <sup>1</sup> S <sub>0</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.5793E+01    | 8.962E-02 | 7.989E+11        | 1.5731E+01    | 8.793E-02 | 7.833E+11        | 0.020 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.6342E+01    | 1.272E-03 | 1.059E+10        | 1.6279E+01    | 1.567E-03 | 1.303E+10        | 0.010 |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.6348E+01    | 3.965E-03 | 3.299E+10        | 1.6286E+01    | 3.728E-03 | 3.099E+10        | 0.009 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.6520E+01    | 5.302E-02 | 4.320E+11        | 1.6456E+01    | 5.276E-02 | 4.295E+11        | 0.008 |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.0902E+01    | 1.398E-01 | 1.858E+11        | 4.0720E+01    | 1.370E-01 | 1.821E+11        | 0.007 |
| 1s 6s <sup>1</sup> S <sub>0</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.1256E+01    | 3.498E-01 | 4.569E+11        | 4.1020E+01    | 3.451E-01 | 4.522E+11        | 0.014 |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.3457E+01    | 8.540E-03 | 1.005E+10        | 4.3327E+01    | 1.016E-02 | 1.193E+10        | 0.003 |
| 1s 6d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.3483E+01    | 2.672E-02 | 3.142E+10        | 4.3321E+01    | 2.490E-02 | 2.926E+10        | 0.003 |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.4189E+01    | 3.623E-01 | 4.126E+11        | 4.4032E+01    | 3.636E-01 | 4.134E+11        | 0.002 |
| 1s 7s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.0915E+03    | 1.520E-01 | 2.837E+08        | 1.0907E+03    | 1.478E-01 | 2.739E+08        | 0.066 |
| 1s 7s <sup>1</sup> S <sub>0</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.2741E+03    | 3.038E-01 | 4.162E+08        | 1.2422E+03    | 3.169E-01 | 4.528E+08        | 0.028 |
| 1s 7d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.6625E+04    | 7.302E-04 | 1.250E+02        | 7.6625E+04    | 7.302E-04 | 1.250E+02        | 0.321 |
| 1s 7d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.3287E+05    | 3.390E-04 | 1.390E+01        | 2.3287E+05    | 3.390E-04 | 1.390E+01        | 0.942 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.3942E+00    | 5.071E-02 | 2.486E+13        | 1.3883E+00    | 5.182E-02 | 2.540E+13        | 0.003 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 3.5164E+00    | 1.199E-01 | 9.238E+12        | 3.5016E+00    | 1.209E-01 | 9.318E+12        | 0.001 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 7.5732E+00    | 2.553E-01 | 4.241E+12        | 7.5406E+00    | 2.573E-01 | 4.276E+12        | 0.001 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 7.6624E+00    | 2.543E-04 | 4.128E+09        | 7.6295E+00    | 2.555E-04 | 4.148E+09        | 0.002 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 7.6639E+00    | 1.167E-05 | 1.894E+08        | 7.6639E+00    | 1.167E-05 | 1.894E+08        | 0.001 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 7.6985E+00    | 5.558E-03 | 8.936E+10        | 7.6654E+00    | 5.556E-03 | 8.934E+10        | 0.000 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 7.6996E+00    | 2.073E-04 | 3.331E+09        | 7.6665E+00    | 2.067E-04 | 3.323E+09        | 0.001 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.6246E+01    | 6.275E-01 | 2.266E+12        | 1.6174E+01    | 6.344E-01 | 2.291E+12        | 0.001 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.6456E+01    | 1.973E-03 | 6.943E+09        | 1.6385E+01    | 1.981E-03 | 6.974E+09        | 0.002 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.6460E+01    | 9.278E-05 | 3.263E+08        | 1.6388E+01    | 9.234E-05 | 3.248E+08        | 0.001 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.6542E+01    | 4.307E-02 | 1.500E+11        | 1.6469E+01    | 4.303E-02 | 1.498E+11        | 0.001 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.6544E+01    | 1.605E-03 | 5.589E+09        | 1.6472E+01    | 1.600E-03 | 5.573E+09        | 0.000 |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.2898E+01    | 2.505E+00 | 1.297E+12        | 4.2690E+01    | 2.541E+00 | 1.317E+12        | 0.001 |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.3752E+01    | 1.834E-02 | 9.130E+09        | 4.3561E+01    | 1.845E-02 | 9.187E+09        | 0.001 |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.3767E+01    | 8.773E-04 | 4.364E+08        | 4.3561E+01    | 9.216E-04 | 4.589E+08        | 0.000 |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.4102E+01    | 4.014E-01 | 1.966E+11        | 4.3907E+01    | 4.009E-01 | 1.965E+11        | 0.001 |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.4114E+01    | 1.496E-02 | 7.327E+09        | 4.3908E+01    | 1.483E-02 | 7.268E+09        | 0.000 |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.4320E+01    | 7.374E-11 | 3.577E+01        | 4.4320E+01    | 7.374E-11 | 3.577E+01        | 0.055 |
| 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 3.5985E+03    | 4.118E-01 | 3.031E+07        | 3.3938E+03    | 4.365E-01 | 3.581E+07        | 0.194 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.5247E+00    | 1.202E-01 | 9.218E+12        | 3.5099E+00    | 1.203E-01 | 9.226E+12        | 0.001 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.5615E+00    | 7.764E-03 | 5.832E+11        | 3.5464E+00    | 7.675E-03 | 5.766E+11        | 0.002 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.5629E+00    | 4.626E-04 | 3.472E+10        | 3.5478E+00    | 4.247E-04 | 3.188E+10        | 0.001 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 7.5891E+00    | 3.358E-01 | 5.555E+12        | 7.5575E+00    | 3.361E-01 | 5.561E+12        | 0.001 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 7.6610E+00    | 2.246E-02 | 3.646E+11        | 7.6289E+00    | 2.240E-02 | 3.637E+11        | 0.002 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 7.6640E+00    | 1.423E-03 | 2.309E+10        | 7.6319E+00    | 1.320E-03 | 2.142E+10        | 0.002 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6283E+01    | 8.980E-01 | 3.228E+12        | 1.6216E+01    | 8.992E-01 | 3.231E+12        | 0.001 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6452E+01    | 6.182E-02 | 2.176E+11        | 1.6384E+01    | 6.195E-02 | 2.180E+11        | 0.001 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6459E+01    | 4.017E-03 | 1.413E+10        | 1.6391E+01    | 3.740E-03 | 1.315E+10        | 0.002 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6541E+01    | 1.113E-02 | 3.876E+10        | 1.6470E+01    | 1.117E-02 | 3.890E+10        | 0.003 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6543E+01    | 4.140E-04 | 1.442E+09        | 1.6472E+01    | 4.143E-04 | 1.442E+09        | 0.005 |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6593E+01    | 1.212E-10 | 4.195E+02        | 1.6593E+01    | 1.212E-10 | 4.195E+02        | 0.342 |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.3043E+01    | 3.664E+00 | 1.885E+12        | 4.2880E+01    | 3.666E+00 | 1.884E+12        | 0.000 |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.3731E+01    | 2.630E-01 | 1.310E+11        | 4.3560E+01    | 2.642E-01 | 1.315E+11        | 0.001 |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.3761E+01    | 1.732E-02 | 8.618E+09        | 4.3571E+01    | 1.851E-02 | 9.214E+09        | 0.002 |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4095E+01    | 1.866E-01 | 9.147E+10        | 4.3907E+01    | 1.868E-01 | 9.159E+10        | 0.001 |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4103E+01    | 6.915E-03 | 3.388E+09        | 4.3907E+01    | 6.929E-03 | 3.396E+09        | 0.002 |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4313E+01    | 1.954E-11 | 9.481E+00        | 4.4313E+01    | 1.954E-11 | 9.481E+00        | 0.976 |
| 1s 7d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.2661E+03    | 3.105E-01 | 1.626E+07        | 4.3591E+03    | 3.024E-01 | 1.504E+07        | 0.021 |
| 1s 7d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.3237E+05    | 3.848E-04 | 6.791E+00        | 2.3237E+05    | 3.848E-04 | 6.791E+00        | 0.802 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3248E+00    | 4.328E-14 | 3.290E+01        | 1.3248E+00    | 4.328E-14 | 3.290E+01        | 1.000 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.3851E+00    | 6.587E-08 | 7.668E+06        | 3.3851E+00    | 6.587E-08 | 7.668E+06        | 0.230 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.5247E+00    | 8.645E-03 | 9.283E+11        | 3.5099E+00    | 8.646E-03 | 9.283E+11        | 0.001 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.5262E+00    | 7.731E-02 | 8.295E+12        | 3.5113E+00    | 7.733E-02 | 8.296E+12        | 0.000 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.5614E+00    | 3.920E-04 | 4.123E+10        | 3.5464E+00    | 3.833E-04 | 4.031E+10        | 0.009 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.5628E+00    | 5.413E-03 | 5.689E+11        | 3.5478E+00    | 5.315E-03 | 5.586E+11        | 0.001 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.3170E+00    | 2.637E-07 | 6.571E+06        | 7.3170E+00    | 2.637E-07 | 6.571E+06        | 0.196 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.5889E+00    | 2.421E-02 | 5.609E+11        | 7.5575E+00    | 2.425E-02 | 5.616E+11        | 0.001 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.5917E+00    | 2.162E-01 | 5.004E+12        | 7.5603E+00    | 2.161E-01 | 5.003E+12        | 0.000 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.6607E+00    | 1.123E-03 | 2.554E+10        | 7.6289E+00    | 1.119E-03 | 2.543E+10        | 0.001 |

(continued on next page)

Table 3 (continued)

| Lower  | Upper  | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|--|--|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|  |  | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.6637E+00    | 1.559E-02 | 3.541E+11              | 7.6319E+00    | 1.544E-02 | 3.507E+11              | 0.000 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.5646E+01    | 7.887E-07 | 4.298E+06              |               |           |                        | 0.141 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6281E+01    | 6.482E-02 | 3.262E+11              | 1.6216E+01    | 6.497E-02 | 3.268E+11              | 0.001 |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6288E+01    | 5.783E-01 | 2.908E+12              | 1.6222E+01    | 5.783E-01 | 2.906E+12              | 0.000 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6451E+01    | 3.084E-03 | 1.520E+10              | 1.6384E+01    | 3.094E-03 | 1.524E+10              | 0.001 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6458E+01    | 4.283E-02 | 2.110E+11              | 1.6391E+01    | 4.261E-02 | 2.098E+11              | 0.000 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6541E+01    | 8.275E-03 | 4.035E+10              | 1.6472E+01    | 8.273E-03 | 4.033E+10              | 0.005 |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.0528E+01    | 3.074E-06 | 2.497E+06              |               |           |                        | 0.094 |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3034E+01    | 2.645E-01 | 1.905E+11              | 4.2880E+01    | 2.675E-01 | 1.924E+11              | 0.000 |
| 1s 6d <sup>3</sup> D <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3060E+01    | 2.361E+00 | 1.698E+12              | 4.2874E+01    | 2.361E+00 | 1.699E+12              | 0.000 |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3722E+01    | 1.309E-02 | 9.135E+09              | 4.3560E+01    | 1.319E-02 | 9.200E+09              | 0.000 |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3752E+01    | 1.821E-01 | 1.269E+11              | 4.3571E+01    | 1.795E-01 | 1.251E+11              | 0.000 |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4094E+01    | 1.383E-01 | 9.486E+10              | 4.3907E+01    | 1.384E-01 | 9.499E+10              | 0.002 |
| 1s 7s <sup>3</sup> S <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 8.7540E+02    | 1.283E-06 | 2.234E+03              |               |           |                        | 0.488 |
| 1s 7d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.1806E+03    | 2.294E-02 | 1.751E+06              | 4.3602E+03    | 2.205E-02 | 1.534E+06              | 0.022 |
| 1s 7d <sup>3</sup> D <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3395E+03    | 1.964E-01 | 1.391E+07              | 4.3189E+03    | 1.965E-01 | 1.393E+07              | 0.003 |
| 1s 7d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.0992E+05    | 4.006E-05 | 4.423E+00              |               |           |                        | 0.425 |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.3358E+00    | 3.593E-05 | 2.686E+10              | 1.3303E+00    | 2.913E-05 | 2.177E+10              | 0.084 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.3942E+00    | 3.581E-03 | 2.458E+12              | 1.3883E+00    | 3.597E-03 | 2.468E+12              | 0.003 |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.3997E+00    | 3.271E-02 | 2.227E+13              | 1.3939E+00    | 3.326E-02 | 2.264E+13              | 0.003 |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.4047E+00    | 7.199E-05 | 8.285E+09              | 3.3905E+00    | 5.619E-05 | 6.465E+09              | 0.008 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.5163E+00    | 8.443E-03 | 9.110E+11              | 3.5016E+00    | 8.386E-03 | 9.046E+11              | 0.000 |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.5262E+00    | 7.729E-02 | 8.293E+12              | 3.5116E+00    | 7.772E-02 | 8.336E+12              | 0.000 |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.3543E+00    | 1.374E-04 | 3.390E+09              | 7.3231E+00    | 1.131E-04 | 2.791E+09              | 0.017 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.5726E+00    | 1.795E-02 | 4.176E+11              | 7.5404E+00    | 1.783E-02 | 4.149E+11              | 0.000 |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.5916E+00    | 1.652E-01 | 3.823E+12              | 7.5595E+00    | 1.654E-01 | 3.829E+12              | 0.001 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.6618E+00    | 1.695E-05 | 3.852E+08              | 7.6293E+00    | 2.044E-05 | 4.644E+08              | 0.001 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.6633E+00    | 1.769E-04 | 4.018E+09              | 7.6308E+00    | 1.751E-04 | 3.978E+09              | 0.001 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.6990E+00    | 4.105E-03 | 9.239E+10              | 7.6663E+00    | 4.113E-03 | 9.258E+10              | 0.001 |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.5732E+01    | 3.089E-04 | 1.665E+09              | 1.5665E+01    | 2.767E-04 | 1.492E+09              | 0.013 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6243E+01    | 4.406E-02 | 2.228E+11              | 1.6173E+01    | 4.394E-02 | 2.222E+11              | 0.002 |
| 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6288E+01    | 4.077E-01 | 2.050E+12              | 1.6218E+01    | 4.078E-01 | 2.051E+12              | 0.002 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6454E+01    | 1.308E-04 | 6.446E+08              | 1.6384E+01    | 1.575E-04 | 7.764E+08              | 0.001 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6457E+01    | 1.369E-03 | 6.741E+09              | 1.6387E+01    | 1.355E-03 | 6.674E+09              | 0.001 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6542E+01    | 3.181E-02 | 1.551E+11              | 1.6471E+01    | 3.185E-02 | 1.553E+11              | 0.000 |
| 1s 6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.0858E+01    | 1.084E-03 | 8.665E+08              | 4.0674E+01    | 2.276E-03 | 1.819E+09              | 0.010 |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.2880E+01    | 1.755E-01 | 1.273E+11              | 4.2684E+01    | 1.759E-01 | 1.277E+11              | 0.000 |
| 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.3058E+01    | 1.639E+00 | 1.180E+12              | 4.2841E+01    | 1.631E+00 | 1.175E+12              | 0.000 |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.3733E+01    | 1.210E-03 | 8.439E+08              | 4.3554E+01    | 1.357E-03 | 9.465E+08              | 0.002 |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.3748E+01    | 1.269E-02 | 8.846E+09              | 4.3554E+01    | 1.249E-02 | 8.711E+09              | 0.000 |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.4094E+01    | 2.963E-01 | 2.033E+11              | 4.3901E+01    | 2.970E-01 | 2.038E+11              | 0.000 |
| 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 9.8772E+02    | 8.471E-04 | 1.158E+06              | 9.7564E+02    | 1.201E-03 | 1.670E+06              | 0.072 |
| 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.4747E+03    | 2.994E-02 | 3.308E+06              | 3.3529E+03    | 3.063E-02 | 3.604E+06              | 0.158 |
| 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.4062E+03    | 2.162E-01 | 1.486E+07              | 4.0947E+03    | 2.330E-01 | 1.838E+07              | 0.194 |
| 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.7858E+05    | 3.308E-05 | 1.384E+00              |               |           |                        | 0.998 |
| 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.2412E+06    | 4.984E-05 | 4.316E-02              |               |           |                        | 0.703 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 3.5600E+00    | 1.630E-01 | 9.533E+12              | 3.5449E+00    | 1.642E-01 | 9.604E+12              | 0.001 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 7.6543E+00    | 4.614E-01 | 5.836E+12              | 7.6222E+00    | 4.634E-01 | 5.861E+12              | 0.001 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6421E+01    | 1.249E+00 | 3.434E+12              | 1.6353E+01    | 1.253E+00 | 3.444E+12              | 0.001 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6509E+01    | 3.674E-04 | 9.991E+08              | 1.6439E+01    | 3.709E-04 | 1.008E+09              | 0.002 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6511E+01    | 1.046E-05 | 2.843E+07              |               |           |                        | 0.007 |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6560E+01    | 1.366E-02 | 3.691E+10              | 1.6489E+01    | 1.369E-02 | 3.700E+10              | 0.003 |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6562E+01    | 3.137E-04 | 8.476E+08              | 1.6491E+01    | 3.124E-04 | 8.442E+08              | 0.005 |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.3514E+01    | 5.201E+00 | 2.036E+12              | 4.3345E+01    | 5.214E+00 | 2.039E+12              | 0.001 |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.3874E+01    | 6.176E-03 | 2.378E+09              | 4.3688E+01    | 6.221E-03 | 2.395E+09              | 0.001 |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.3882E+01    | 1.758E-04 | 6.767E+07              |               |           |                        | 0.003 |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.4083E+01    | 2.292E-01 | 8.743E+10              | 4.3895E+01    | 2.295E-01 | 8.752E+10              | 0.001 |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.4090E+01    | 5.247E-03 | 2.001E+09              | 4.3895E+01    | 5.215E-03 | 1.989E+09              | 0.002 |
| 1s 7d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 8.4332E+03    | 2.169E-01 | 2.260E+06              | 8.7593E+03    | 2.079E-01 | 1.991E+06              | 0.031 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7g <sup>3</sup> G <sub>4</sub>              | 7.6554E+00    | 3.948E-01 | 4.993E+12              | 7.6229E+00    | 3.951E-01 | 4.997E+12              | 0.000 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7g <sup>3</sup> G <sub>4</sub>              | 7.6914E+00    | 1.379E-02 | 1.728E+11              | 7.6587E+00    | 1.370E-02 | 1.716E+11              | 0.001 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7g <sup>3</sup> G <sub>4</sub>              | 7.6926E+00    | 3.877E-04 | 4.856E+09              | 7.6598E+00    | 3.390E-04 | 4.246E+09              | 0.000 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7g <sup>3</sup> G <sub>4</sub>              | 1.6424E+01    | 1.538E+00 | 4.224E+12              | 1.6354E+01    | 1.539E+00 | 4.229E+12              | 0.000 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7g <sup>3</sup> G <sub>4</sub>              | 1.6509E+01    | 5.485E-02 | 1.492E+11              | 1.6439E+01    | 5.482E-02 | 1.490E+11              | 0.000 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7g <sup>3</sup> G <sub>4</sub>              | 1.6512E+01    | 1.557E-03 | 4.233E+09              | 1.6441E+01    | 1.373E-03 | 3.733E+09              | 0.000 |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.3526E+01    | 7.332E+00 | 2.868E+12              | 4.3346E+01    | 7.341E+00 | 2.871E+12              | 0.000 |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.3873E+01    | 2.683E-01 | 1.033E+11              | 4.3689E+01    | 2.690E-01 | 1.035E+11              | 0.000 |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.3884E+01    | 7.664E-03 | 2.949E+09              | 4.3689E+01    | 7.956E-03 | 3.063E+09              | 0.000 |
| 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.4083E+01    | 7.172E-02 | 2.735E+10              | 4.3896E+01    | 7.180E-02 | 2.738E+10              | 0.001 |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.4088E+01    | 1.627E-03 | 6.203E+08              | 4.3896E+01    | 1.632E-03 | 6.224E+08              | 0.000 |
| 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.4227E+01    | 8.330E-09 | 3.156E+03              |               |           |                        | 0.017 |

(continued on next page)

Table 3 (continued)

| Lower   | Upper   | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|---|---|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|   |   | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>4</sub>              | 8.7347E+03    | 1.730E-01 | 1.681E+06              | 8.7974E+03    | 1.710E-01 | 1.623E+06              | 0.020 |
| 1s7f <sup>3</sup> F <sub>5</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>4</sub>              | 4.7642E+06    | 1.133E-05 | 3.699E-04              |               |           |                        | 0.957 |
| 1s2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.3940E+00    | 7.262E-10 | 3.561E+05              |               |           |                        | 0.771 |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 3.5149E+00    | 7.323E-13 | 5.648E+01              |               |           |                        | 0.981 |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 7.5662E+00    | 3.484E-08 | 5.800E+05              |               |           |                        | 0.013 |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 7.6553E+00    | 1.458E-02 | 2.371E+11              | 7.6229E+00    | 1.457E-02 | 2.370E+11              | 0.000 |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 7.6568E+00    | 2.925E-01 | 4.754E+12              | 7.6244E+00    | 2.926E-01 | 4.755E+12              | 0.000 |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 7.6913E+00    | 3.956E-04 | 6.373E+09              | 7.6587E+00    | 3.914E-04 | 6.305E+09              | 0.001 |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 7.6924E+00    | 1.073E-02 | 1.728E+11              | 7.6598E+00    | 1.062E-02 | 1.710E+11              | 0.001 |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6214E+01    | 2.161E-07 | 7.833E+05              |               |           |                        | 0.004 |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6423E+01    | 5.677E-02 | 2.005E+11              | 1.6354E+01    | 5.681E-02 | 2.006E+11              | 0.000 |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6427E+01    | 1.139E+00 | 4.023E+12              | 1.6358E+01    | 1.139E+00 | 4.025E+12              | 0.000 |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6508E+01    | 1.573E-03 | 5.499E+09              | 1.6439E+01    | 1.566E-03 | 5.476E+09              | 0.001 |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6511E+01    | 4.267E-02 | 1.491E+11              | 1.6441E+01    | 4.248E-02 | 1.484E+11              | 0.001 |
| 1s6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.2676E+01    | 1.217E-06 | 6.370E+05              |               |           |                        | 0.001 |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.3521E+01    | 2.705E-01 | 1.361E+11              | 4.3346E+01    | 2.721E-01 | 1.368E+11              | 0.000 |
| 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.3535E+01    | 5.434E+00 | 2.732E+12              | 4.3346E+01    | 5.438E+00 | 2.734E+12              | 0.000 |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.3867E+01    | 7.685E-03 | 3.806E+09              | 4.3689E+01    | 7.686E-03 | 3.804E+09              | 0.000 |
| 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.3878E+01    | 2.087E-01 | 1.033E+11              | 4.3689E+01    | 2.072E-01 | 1.025E+11              | 0.000 |
| 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.4083E+01    | 5.701E-02 | 2.796E+10              | 4.3896E+01    | 5.711E-02 | 2.800E+10              | 0.000 |
| 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 2.5035E+03    | 1.166E-07 | 1.772E+01              |               |           |                        | 0.002 |
| 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 8.5297E+03    | 6.540E-03 | 8.565E+04              | 8.7975E+03    | 6.341E-03 | 7.740E+04              | 0.028 |
| 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 8.8934E+03    | 1.258E-01 | 1.516E+06              | 8.7928E+03    | 1.267E-01 | 1.548E+06              | 0.024 |
| 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 3.3768E+05    | 4.572E-06 | 3.820E-02              |               |           |                        | 0.857 |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.5233E+00    | 3.298E-06 | 2.531E+08              |               |           |                        | 0.031 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.5600E+00    | 6.068E-03 | 4.563E+11              | 3.5449E+00    | 6.074E-03 | 4.567E+11              | 0.001 |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.5614E+00    | 1.207E-01 | 9.071E+12              | 3.5463E+00    | 1.216E-01 | 9.136E+12              | 0.000 |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.5823E+00    | 1.691E-05 | 2.802E+08              |               |           |                        | 0.029 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.6541E+00    | 1.717E-02 | 2.792E+11              | 7.6222E+00    | 1.713E-02 | 2.787E+11              | 0.001 |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.6570E+00    | 3.420E-01 | 5.558E+12              | 7.6252E+00    | 3.431E-01 | 5.576E+12              | 0.001 |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6251E+01    | 5.598E-05 | 2.020E+08              |               |           |                        | 0.022 |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6420E+01    | 4.647E-02 | 1.642E+11              | 1.6353E+01    | 4.635E-02 | 1.637E+11              | 0.000 |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6427E+01    | 9.263E-01 | 3.271E+12              | 1.6360E+01    | 9.280E-01 | 3.275E+12              | 0.000 |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6508E+01    | 1.041E-05 | 3.639E+07              |               |           |                        | 0.015 |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6510E+01    | 2.872E-04 | 1.004E+09              | 1.6441E+01    | 2.866E-04 | 1.002E+09              | 0.006 |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6561E+01    | 1.090E-02 | 3.787E+10              | 1.6491E+01    | 1.088E-02 | 3.782E+10              | 0.004 |
| 1s6d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.2826E+01    | 2.508E-04 | 1.303E+08              | 4.2671E+01    | 4.916E-04 | 2.551E+08              | 0.014 |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3507E+01    | 1.933E-01 | 9.731E+10              | 4.3345E+01    | 1.928E-01 | 9.698E+10              | 0.000 |
| 1s6d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3537E+01    | 3.859E+00 | 1.940E+12              | 4.3355E+01    | 3.861E+00 | 1.941E+12              | 0.000 |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3867E+01    | 1.761E-04 | 8.718E+07              |               |           |                        | 0.006 |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3875E+01    | 4.808E-03 | 2.380E+09              | 4.3688E+01    | 4.791E-03 | 2.372E+09              | 0.003 |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.4083E+01    | 1.824E-01 | 8.943E+10              | 4.3895E+01    | 1.825E-01 | 8.952E+10              | 0.002 |
| 1s7d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.8385E+03    | 3.561E-05 | 4.211E+03              | 2.9112E+03    | 6.098E-05 | 6.798E+03              | 0.242 |
| 1s7d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 8.1837E+03    | 8.316E-03 | 1.183E+05              | 8.7525E+03    | 7.695E-03 | 9.491E+04              | 0.023 |
| 1s7d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 8.9054E+03    | 1.521E-01 | 1.827E+06              | 9.0373E+03    | 1.492E-01 | 1.726E+06              | 0.011 |
| 1s7g <sup>3</sup> G <sub>4</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.9370E+05    | 5.267E-06 | 5.818E-02              |               |           |                        | 0.814 |
| 1s7g <sup>3</sup> G <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.5307E+06    | 2.742E-05 | 1.115E-02              |               |           |                        | 0.915 |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 7.6874E+00    | 4.969E-01 | 5.098E+12              | 7.6547E+00    | 4.989E-01 | 5.120E+12              | 0.000 |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 1.6491E+01    | 1.948E+00 | 4.343E+12              | 1.6420E+01    | 1.952E+00 | 4.354E+12              | 0.000 |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 4.3742E+01    | 9.373E+00 | 2.970E+12              | 4.3559E+01    | 9.390E+00 | 2.975E+12              | 0.000 |
| 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 4.3951E+01    | 1.512E-03 | 4.745E+08              | 4.3765E+01    | 1.522E-03 | 4.777E+08              | 0.001 |
| 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 4.3956E+01    | 2.810E-05 | 8.818E+06              |               |           |                        | 0.001 |
| 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 4.4090E+01    | 8.517E-02 | 2.657E+10              | 4.3903E+01    | 8.525E-02 | 2.659E+10              | 0.000 |
| 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 4.4094E+01    | 1.316E-03 | 4.106E+08              | 4.3903E+01    | 1.311E-03 | 4.091E+08              | 0.000 |
| 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 1.4632E+04    | 1.310E-01 | 3.709E+05              | 1.4765E+04    | 1.292E-01 | 3.564E+05              | 0.023 |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.6491E+01    | 1.774E+00 | 3.956E+12              | 1.6420E+01    | 1.776E+00 | 3.960E+12              | 0.000 |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.6542E+01    | 3.898E-02 | 8.638E+10              | 1.6471E+01    | 3.887E-02 | 8.615E+10              | 0.001 |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.6543E+01    | 6.999E-04 | 1.551E+09              | 1.6473E+01    | 5.907E-04 | 1.308E+09              | 0.001 |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.3742E+01    | 1.301E+01 | 4.123E+12              | 4.3559E+01    | 1.302E+01 | 4.126E+12              | 0.000 |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.3950E+01    | 2.913E-01 | 9.143E+10              | 4.3765E+01    | 2.917E-01 | 9.156E+10              | 0.000 |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.3957E+01    | 5.234E-03 | 1.643E+09              | 4.3765E+01    | 5.401E-03 | 1.695E+09              | 0.001 |
| 1s7g <sup>3</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.4659E+04    | 9.514E-02 | 2.685E+05              | 1.4689E+04    | 9.453E-02 | 2.634E+05              | 0.021 |
| 1s7g <sup>3</sup> G <sub>5</sub>              | 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.1751E+07    | 2.630E-06 | 1.154E-05              |               |           |                        | 0.964 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 3.5591E+00    | 1.547E-12 | 9.050E+01              |               |           |                        | 0.940 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 7.6502E+00    | 3.959E-11 | 5.014E+02              |               |           |                        | 0.538 |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6402E+01    | 7.418E-10 | 2.043E+03              |               |           |                        | 0.061 |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6490E+01    | 4.020E-02 | 1.096E+11              | 1.6420E+01    | 4.022E-02 | 1.096E+11              | 0.000 |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6492E+01    | 1.411E+00 | 3.845E+12              | 1.6423E+01    | 1.412E+00 | 3.848E+12              | 0.000 |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6541E+01    | 7.259E-04 | 1.966E+09              | 1.6471E+01    | 7.199E-04 | 1.950E+09              | 0.004 |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6543E+01    | 3.199E-02 | 8.663E+10              | 1.6473E+01    | 3.181E-02 | 8.614E+10              | 0.000 |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.3381E+01    | 8.687E-09 | 3.421E+03              |               |           |                        | 0.040 |

(continued on next page)

Table 3 (continued)

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |           |                  | dT    |
|-----------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|                 |                 | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) |       |
| 1s 6g $^3G_4$   | 1s 7h $^3H_4^0$ | 4.3739E+01    | 2.946E-01 | 1.141E+11        | 4.3559E+01    | 2.959E-01 | 1.146E+11        | 0.000 |
| 1s 6g $^3G_3$   | 1s 7h $^3H_4^0$ | 4.3747E+01    | 1.035E+01 | 4.007E+12        | 4.3559E+01    | 1.035E+01 | 4.012E+12        | 0.000 |
| 1s 6g $^3G_5$   | 1s 7h $^3H_4^0$ | 4.3947E+01    | 5.409E-03 | 2.076E+09        | 4.3765E+01    | 5.401E-03 | 2.072E+09        | 0.001 |
| 1s 6g $^1G_4$   | 1s 7h $^3H_4^0$ | 4.3954E+01    | 2.390E-01 | 9.169E+10        | 4.3765E+01    | 2.376E-01 | 9.119E+10        | 0.000 |
| 1s 7d $^3D_3$   | 1s 7h $^3H_4^0$ | 5.2970E+03    | 2.748E-10 | 7.259E-03        |               |           |                  | 0.966 |
| 1s 7g $^3G_4$   | 1s 7h $^3H_4^0$ | 1.4287E+04    | 2.211E-03 | 8.030E+03        | 1.4689E+04    | 2.148E-03 | 7.317E+03        | 0.009 |
| 1s 7g $^3G_3$   | 1s 7h $^3H_4^0$ | 1.4871E+04    | 7.459E-02 | 2.500E+05        | 1.4689E+04    | 7.520E-02 | 2.561E+05        | 0.009 |
| 1s 7g $^3G_5$   | 1s 7h $^3H_4^0$ | 5.3648E+05    | 1.070E-06 | 2.756E-03        |               |           |                  | 0.163 |
| 1s 4f $^3F_3^0$ | 1s 7g $^1G_4$   | 7.6513E+00    | 3.467E-08 | 4.389E+05        |               |           |                  | 0.018 |
| 1s 4f $^3F_4^0$ | 1s 7g $^1G_4$   | 7.6873E+00    | 1.135E-02 | 1.424E+11        | 7.6547E+00    | 1.134E-02 | 1.422E+11        | 0.000 |
| 1s 4f $^1F_3^0$ | 1s 7g $^1G_4$   | 7.6884E+00    | 3.952E-01 | 4.955E+12        | 7.6558E+00    | 3.968E-01 | 4.975E+12        | 0.000 |
| 1s 5f $^3F_3^0$ | 1s 7g $^1G_4$   | 1.6405E+01    | 3.735E-08 | 1.029E+05        |               |           |                  | 0.050 |
| 1s 5f $^3F_4^0$ | 1s 7g $^1G_4$   | 1.6490E+01    | 4.447E-02 | 1.212E+11        | 1.6420E+01    | 4.438E-02 | 1.209E+11        | 0.000 |
| 1s 5f $^1F_3^0$ | 1s 7g $^1G_4$   | 1.6493E+01    | 1.549E+00 | 4.222E+12        | 1.6423E+01    | 1.553E+00 | 4.231E+12        | 0.000 |
| 1s 6f $^3F_3^0$ | 1s 7g $^1G_4$   | 4.3393E+01    | 4.042E-08 | 1.591E+04        |               |           |                  | 0.133 |
| 1s 6f $^3F_4^0$ | 1s 7g $^1G_4$   | 4.3738E+01    | 2.139E-01 | 8.286E+10        | 4.3559E+01    | 2.134E-01 | 8.265E+10        | 0.000 |
| 1s 6f $^1F_3^0$ | 1s 7g $^1G_4$   | 4.3749E+01    | 7.458E+00 | 2.888E+12        | 4.3560E+01    | 7.469E+00 | 2.892E+12        | 0.000 |
| 1s 6h $^3H_5^0$ | 1s 7g $^1G_4$   | 4.3947E+01    | 2.711E-05 | 1.041E+07        |               |           |                  | 0.001 |
| 1s 6h $^3H_4^0$ | 1s 7g $^1G_4$   | 4.3952E+01    | 1.240E-03 | 4.758E+08        | 4.3765E+01    | 1.240E-03 | 4.757E+08        | 0.000 |
| 1s 6h $^1H_5^0$ | 1s 7g $^1G_4$   | 4.4090E+01    | 7.073E-02 | 2.696E+10        | 4.3903E+01    | 7.082E-02 | 2.700E+10        | 0.000 |
| 1s 7f $^3F_3^0$ | 1s 7g $^1G_4$   | 5.4114E+03    | 2.878E-10 | 7.284E-03        |               |           |                  | 0.998 |
| 1s 7f $^3F_4^0$ | 1s 7g $^1G_4$   | 1.4181E+04    | 3.084E-03 | 1.137E+04        | 1.4765E+04    | 2.937E-03 | 9.900E+03        | 0.048 |
| 1s 7f $^1F_3^0$ | 1s 7g $^1G_4$   | 1.4947E+04    | 1.020E-01 | 3.382E+05        | 1.4784E+04    | 1.026E-01 | 3.451E+05        | 0.037 |
| 1s 7h $^3H_5^0$ | 1s 7g $^1G_4$   | 4.7824E+05    | 1.162E-06 | 3.764E-03        |               |           |                  | 0.645 |
| 1s 7h $^3H_4^0$ | 1s 7g $^1G_4$   | 3.2051E+06    | 7.916E-06 | 5.712E-04        |               |           |                  | 0.700 |
| 1s 5g $^3G_5$   | 1s 7h $^3H_6^0$ | 1.6529E+01    | 2.139E+00 | 4.017E+12        | 1.6459E+01    | 2.144E+00 | 4.027E+12        | 0.000 |
| 1s 6g $^3G_5$   | 1s 7h $^3H_6^0$ | 4.3863E+01    | 1.577E+01 | 4.205E+12        | 4.3678E+01    | 1.579E+01 | 4.211E+12        | 0.000 |
| 1s 7g $^3G_5$   | 1s 7h $^3H_6^0$ | 2.2048E+04    | 7.648E-02 | 8.073E+04        | 2.2104E+04    | 7.596E-02 | 7.910E+04        | 0.025 |
| 1s 6h $^3H_6^0$ | 1s 7i $^3I_6$   | 4.3863E+01    | 2.165E+01 | 5.775E+12        | 4.3678E+01    | 2.167E+01 | 5.780E+12        | 0.000 |
| 1s 6h $^3H_5^0$ | 1s 7i $^3I_6$   | 4.4002E+01    | 3.281E-01 | 8.695E+10        | 4.3816E+01    | 3.283E-01 | 8.699E+10        | 0.000 |
| 1s 6h $^1H_6^0$ | 1s 7i $^3I_6$   | 4.4006E+01    | 4.130E-03 | 1.094E+09        | 4.3816E+01    | 4.263E-03 | 1.129E+09        | 0.000 |
| 1s 7h $^3H_6^0$ | 1s 7i $^3I_6$   | 2.2088E+04    | 4.138E-02 | 4.352E+04        | 2.2113E+04    | 4.114E-02 | 4.281E+04        | 0.010 |
| 1s 7h $^3H_5^0$ | 1s 7i $^3I_6$   | 2.7778E+08    | 4.919E-08 | 3.208E-10        |               |           |                  | 1.000 |
| 1s 4f $^3F_4^0$ | 1s 7i $^3I_5$   | 7.6846E+00    | 6.513E-12 | 6.688E+01        |               |           |                  | 0.024 |
| 1s 5f $^3F_4^0$ | 1s 7i $^3I_5$   | 1.6478E+01    | 2.181E-11 | 4.870E+01        |               |           |                  | 0.047 |
| 1s 6f $^3F_4^0$ | 1s 7i $^3I_5$   | 4.3653E+01    | 1.093E-14 | 3.479E-03        |               |           |                  | 0.317 |
| 1s 6h $^3H_5^0$ | 1s 7i $^3I_5$   | 4.3861E+01    | 3.322E-01 | 1.047E+11        | 4.3678E+01    | 3.335E-01 | 1.051E+11        | 0.000 |
| 1s 6h $^3H_4^0$ | 1s 7i $^3I_5$   | 4.3866E+01    | 1.799E+01 | 5.669E+12        | 4.3678E+01    | 1.800E+01 | 5.675E+12        | 0.000 |
| 1s 6h $^3H_6^0$ | 1s 7i $^3I_5$   | 4.4000E+01    | 4.274E-03 | 1.339E+09        | 4.3816E+01    | 4.263E-03 | 1.335E+09        | 0.001 |
| 1s 6h $^1H_6^0$ | 1s 7i $^3I_5$   | 4.4004E+01    | 2.786E-01 | 8.725E+10        | 4.3816E+01    | 2.771E-01 | 8.679E+10        | 0.000 |
| 1s 7f $^3F_4^0$ | 1s 7i $^3I_5$   | 8.6997E+03    | 2.746E-16 | 2.200E-09        |               |           |                  | 1.000 |
| 1s 7h $^3H_6^0$ | 1s 7i $^3I_5$   | 2.1496E+04    | 6.522E-04 | 8.558E+02        | 2.2113E+04    | 6.330E-04 | 7.784E+02        | 0.060 |
| 1s 7h $^3H_4^0$ | 1s 7i $^3I_5$   | 2.2351E+04    | 3.396E-02 | 4.123E+04        | 2.2113E+04    | 3.418E-02 | 4.203E+04        | 0.048 |
| 1s 7h $^3H_5^0$ | 1s 7i $^3I_5$   | 8.0038E+05    | 2.245E-07 | 2.125E-04        |               |           |                  | 0.972 |
| 1s 5g $^3G_4$   | 1s 7h $^1H_5^0$ | 1.6478E+01    | 2.072E-07 | 4.628E+05        |               |           |                  | 0.011 |
| 1s 5g $^3G_5$   | 1s 7h $^1H_5^0$ | 1.6529E+01    | 3.303E-02 | 7.332E+10        | 1.6459E+01    | 3.299E-02 | 7.323E+10        | 0.000 |
| 1s 5g $^1G_4$   | 1s 7h $^1H_5^0$ | 1.6530E+01    | 1.777E+00 | 3.943E+12        | 1.6460E+01    | 1.781E+00 | 3.953E+12        | 0.000 |
| 1s 6g $^3G_4$   | 1s 7h $^1H_5^0$ | 4.3653E+01    | 1.484E-06 | 4.723E+05        |               |           |                  | 0.007 |
| 1s 6g $^3G_5$   | 1s 7h $^1H_5^0$ | 4.3860E+01    | 2.434E-01 | 7.671E+10        | 4.3678E+01    | 2.429E-01 | 7.657E+10        | 0.000 |
| 1s 6g $^1G_4$   | 1s 7h $^1H_5^0$ | 4.3867E+01    | 1.310E+01 | 4.128E+12        | 4.3678E+01    | 1.312E+01 | 4.135E+12        | 0.000 |
| 1s 7g $^3G_4$   | 1s 7h $^1H_5^0$ | 8.6987E+03    | 1.842E-08 | 1.476E-01        |               |           |                  | 0.636 |
| 1s 7g $^3G_5$   | 1s 7h $^1H_5^0$ | 2.1355E+04    | 1.219E-03 | 1.621E+03        | 2.2104E+04    | 1.168E-03 | 1.438E+03        | 0.005 |
| 1s 7g $^1G_4$   | 1s 7h $^1H_5^0$ | 2.2395E+04    | 6.255E-02 | 7.562E+04        | 2.2104E+04    | 6.310E-02 | 7.765E+04        | 0.011 |
| 1s 7i $^3I_6$   | 1s 7h $^1H_5^0$ | 6.8074E+05    | 2.552E-07 | 3.340E-04        |               |           |                  | 0.629 |
| 1s 7i $^3I_5$   | 1s 7h $^1H_5^0$ | 4.4823E+06    | 2.614E-06 | 7.893E-05        |               |           |                  | 0.959 |
| 1s 6h $^3H_6^0$ | 1s 7i $^3I_7$   | 4.3940E+01    | 2.539E+01 | 5.847E+12        | 4.3754E+01    | 2.543E+01 | 5.857E+12        | 0.000 |
| 1s 7h $^3H_6^0$ | 1s 7i $^3I_7$   | 3.1010E+04    | 3.454E-02 | 1.597E+04        | 3.1022E+04    | 3.437E-02 | 1.574E+04        | 0.010 |
| 1s 6h $^3H_5^0$ | 1s 7i $^1I_6$   | 4.3799E+01    | 1.223E-06 | 3.271E+05        |               |           |                  | 0.004 |
| 1s 6h $^3H_6^0$ | 1s 7i $^1I_6$   | 4.3938E+01    | 2.829E-01 | 7.519E+10        | 4.3754E+01    | 2.825E-01 | 7.509E+10        | 0.000 |
| 1s 6h $^1H_5^0$ | 1s 7i $^1I_6$   | 4.3942E+01    | 2.172E+01 | 5.772E+12        | 4.3754E+01    | 2.175E+01 | 5.782E+12        | 0.000 |
| 1s 7h $^3H_6^0$ | 1s 7i $^1I_6$   | 1.2726E+04    | 4.183E-09 | 1.325E-02        |               |           |                  | 0.903 |
| 1s 7h $^3H_5^0$ | 1s 7i $^1I_6$   | 3.0020E+04    | 3.975E-04 | 2.263E+02        | 3.1022E+04    | 3.819E-04 | 2.019E+02        | 0.083 |
| 1s 7h $^1H_5^0$ | 1s 7i $^1I_6$   | 3.1409E+04    | 2.917E-02 | 1.517E+04        | 3.1022E+04    | 2.940E-02 | 1.554E+04        | 0.060 |

**Table 4**  
Electric quadrupole transitions E2 calculated with GRASP2K and FAC for all  $n = 1-7$  configurations. For the GRASP2K calculation, the active set is expanded to  $n = 10$  (GRASP3) and only the length form is considered. A comparison between the wavelengths, weighted oscillator strengths and transition probabilities is given. The relative difference between transition probabilities in the velocity and length gauge is given in the last column by  $dT$ .

| Lower           | Upper          | GRASP2K       |           |                  | FAC           |           |                  | $dT$  |
|-----------------|----------------|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|                 |                | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |       |
| 1s2p $^3P_1^o$  | 1s2p $^3P_2^o$ | 3.1908E+01    | 3.112E-07 | 4.078E+05        | 3.1815E+01    | 3.135E-07 | 4.098E+05        | 0.006 |
| 1s2p $^3P_0^o$  | 1s2p $^3P_2^o$ | 3.2407E+01    | 1.878E-07 | 2.386E+05        | 3.2290E+01    | 1.887E-07 | 2.394E+05        | 0.019 |
| 1s2p $^3P_1^o$  | 1s2p $^1P_1^o$ | 2.9274E+01    | 3.608E-07 | 9.361E+05        | 2.9150E+01    | 3.594E-07 | 9.325E+05        | 0.011 |
| 1s2p $^3P_2^o$  | 1s2p $^1P_1^o$ | 3.5465E+02    | 1.078E-10 | 1.905E+00        |               |           |                  | 0.174 |
| 1s2s $^3S_1$    | 1s3s $^3S_1$   | 2.1766E+00    | 4.067E-09 | 1.909E+06        | 2.1673E+00    | 4.604E-09 | 2.161E+06        | 0.026 |
| 1s2p $^3P_0^o$  | 1s3p $^3P_0^o$ | 2.1983E+00    | 3.696E-06 | 1.700E+09        | 2.1892E+00    | 4.175E-06 | 1.920E+09        | 0.009 |
| 1s2p $^3P_2^o$  | 1s3p $^3P_0^o$ | 2.3610E+00    | 7.133E-04 | 2.845E+11        | 2.3509E+00    | 7.174E-04 | 2.861E+11        | 0.002 |
| 1s2p $^1P_1^o$  | 1s3p $^3P_1^o$ | 2.3768E+00    | 6.407E-04 | 2.522E+11        | 2.3669E+00    | 6.330E-04 | 2.491E+11        | 0.001 |
| 1s2p $^3P_2^o$  | 1s3p $^3P_0^o$ | 2.3603E+00    | 4.510E-04 | 5.400E+11        | 2.3503E+00    | 4.561E-04 | 5.461E+11        | 0.000 |
| 1s2p $^3P_0^o$  | 1s3p $^3P_2^o$ | 2.1541E+00    | 6.263E-04 | 1.800E+11        | 2.1452E+00    | 6.425E-04 | 1.846E+11        | 0.002 |
| 1s2p $^3P_2^o$  | 1s3p $^3P_2^o$ | 2.1564E+00    | 3.953E-04 | 1.134E+11        | 2.1474E+00    | 4.009E-04 | 1.150E+11        | 0.001 |
| 1s2p $^3P_2^o$  | 1s3p $^3P_2^o$ | 2.3101E+00    | 7.422E-04 | 1.855E+11        | 2.3003E+00    | 7.550E-04 | 1.887E+11        | 0.000 |
| 1s2p $^1P_1^o$  | 1s3p $^3P_2^o$ | 2.3252E+00    | 2.840E-04 | 7.006E+10        | 2.3156E+00    | 2.859E-04 | 7.054E+10        | 0.002 |
| 1s3p $^3P_0^o$  | 1s3p $^3P_2^o$ | 1.0725E+02    | 3.088E-07 | 3.581E+04        | 1.0689E+02    | 3.098E-07 | 3.587E+04        | 0.001 |
| 1s3p $^3P_0^o$  | 1s3p $^3P_2^o$ | 1.0873E+02    | 1.880E-07 | 2.121E+04        | 1.0831E+02    | 1.883E-07 | 2.123E+04        | 0.002 |
| 1s $^2$ 1S $_0$ | 1s3d $^3D_2$   | 3.4460E-01    | 8.826E-04 | 9.910E+12        | 3.4325E-01    | 9.055E-04 | 1.016E+13        | 0.003 |
| 1s2s $^3S_1$    | 1s3d $^3D_2$   | 2.1226E+00    | 2.875E-03 | 8.513E+11        | 2.1136E+00    | 2.919E-03 | 8.644E+11        | 0.003 |
| 1s2s $^1S_0$    | 1s3d $^3D_2$   | 2.1539E+00    | 1.869E-03 | 5.374E+11        | 2.1452E+00    | 1.833E-03 | 5.270E+11        | 0.003 |
| 1s3s $^3S_1$    | 1s3d $^3D_2$   | 8.5509E+01    | 3.819E-07 | 6.968E+04        | 8.5230E+01    | 3.815E-07 | 6.947E+04        | 0.030 |
| 1s3s $^1S_0$    | 1s3d $^3D_2$   | 1.0120E+02    | 1.521E-07 | 1.982E+04        | 1.0108E+02    | 1.504E-07 | 1.947E+04        | 0.037 |
| 1s2s $^3S_1$    | 1s3d $^3D_1$   | 2.1220E+00    | 2.860E-03 | 1.412E+12        | 2.1130E+00    | 2.904E-03 | 1.434E+12        | 0.002 |
| 1s3s $^3S_1$    | 1s3d $^3D_1$   | 8.4639E+01    | 3.934E-07 | 1.221E+05        | 8.4368E+01    | 3.922E-07 | 1.214E+05        | 0.027 |
| 1s3d $^3D_2$    | 1s3d $^3D_1$   | 8.3264E+03    | 1.645E-13 | 5.276E-06        |               |           |                  | 0.531 |
| 1s2p $^3P_0^o$  | 1s3p $^1P_1^o$ | 2.1504E+00    | 5.523E-04 | 2.655E+11        | 2.1415E+00    | 5.632E-04 | 2.707E+11        | 0.000 |
| 1s2p $^3P_2^o$  | 1s3p $^1P_1^o$ | 2.3058E+00    | 2.829E-04 | 1.183E+11        | 2.2961E+00    | 2.891E-04 | 1.209E+11        | 0.002 |
| 1s2p $^1P_1^o$  | 1s3p $^1P_1^o$ | 2.3209E+00    | 3.899E-04 | 1.610E+11        | 2.3113E+00    | 3.893E-04 | 1.606E+11        | 0.000 |
| 1s3p $^3P_0^o$  | 1s3p $^1P_1^o$ | 9.8786E+01    | 3.556E-07 | 8.103E+04        | 9.8358E+01    | 3.546E-07 | 8.082E+04        | 0.005 |
| 1s3p $^3P_2^o$  | 1s3p $^1P_1^o$ | 1.2519E+03    | 8.846E-11 | 1.255E-01        |               |           |                  | 0.052 |
| 1s2s $^3S_1$    | 1s3d $^3D_3$   | 2.1095E+00    | 6.734E-03 | 1.442E+12        | 2.1005E+00    | 6.967E-03 | 1.492E+12        | 0.003 |
| 1s3s $^3S_1$    | 1s3d $^3D_3$   | 6.8392E+01    | 1.793E-06 | 3.652E+05        | 6.8186E+01    | 1.790E-06 | 3.637E+05        | 0.024 |
| 1s3d $^3D_2$    | 1s3d $^3D_3$   | 3.4166E+02    | 2.752E-09 | 2.246E+01        |               |           |                  | 0.004 |
| 1s3d $^3D_1$    | 1s3d $^3D_3$   | 3.5628E+02    | 3.967E-10 | 2.978E+00        |               |           |                  | 0.044 |
| 1s $^2$ 1S $_0$ | 1s3d $^1D_2$   | 3.4430E-01    | 1.235E-03 | 1.389E+13        | 3.4289E-01    | 1.431E-03 | 1.610E+13        | 0.003 |
| 1s2s $^3S_1$    | 1s3d $^1D_2$   | 2.1090E+00    | 1.910E-03 | 5.729E+11        | 2.1000E+00    | 1.974E-03 | 5.922E+11        | 0.002 |
| 1s2s $^1S_0$    | 1s3d $^1D_2$   | 2.1399E+00    | 2.871E-03 | 8.364E+11        | 2.1313E+00    | 2.875E-03 | 8.373E+11        | 0.002 |
| 1s3s $^3S_1$    | 1s3d $^1D_2$   | 6.7876E+01    | 5.194E-07 | 1.504E+05        | 6.7664E+01    | 5.176E-07 | 1.495E+05        | 0.021 |
| 1s3s $^1S_0$    | 1s3d $^1D_2$   | 7.7401E+01    | 5.347E-07 | 1.191E+05        | 7.7288E+01    | 5.296E-07 | 1.172E+05        | 0.025 |
| 1s3d $^3D_2$    | 1s3d $^1D_2$   | 3.2917E+02    | 7.638E-10 | 9.405E+00        |               |           |                  | 0.034 |
| 1s3d $^3D_1$    | 1s3d $^1D_2$   | 3.4272E+02    | 1.578E-09 | 1.792E+01        |               |           |                  | 0.011 |
| 1s3d $^3D_3$    | 1s3d $^1D_2$   | 8.9990E+03    | 1.023E-13 | 1.685E-06        |               |           |                  | 0.644 |
| 1s2s $^3S_1$    | 1s4s $^3S_1$   | 1.6177E+00    | 1.741E-10 | 1.480E+05        | 1.6108E+00    | 4.748E-10 | 4.034E+05        | 0.331 |
| 1s3s $^3S_1$    | 1s4s $^3S_1$   | 6.2995E+00    | 5.359E-09 | 3.003E+05        |               |           |                  | 0.020 |
| 1s3d $^3D_2$    | 1s4s $^3S_1$   | 6.8005E+00    | 1.094E-04 | 5.261E+09        | 6.7717E+00    | 1.086E-04 | 5.221E+09        | 0.001 |
| 1s3d $^3D_1$    | 1s4s $^3S_1$   | 6.8061E+00    | 1.100E-04 | 5.277E+09        | 6.7772E+00    | 1.084E-04 | 5.207E+09        | 0.002 |
| 1s3d $^3D_3$    | 1s4s $^3S_1$   | 6.9386E+00    | 2.664E-04 | 1.230E+10        | 6.9089E+00    | 2.627E-04 | 1.213E+10        | 0.001 |
| 1s3d $^1D_2$    | 1s4s $^3S_1$   | 6.9440E+00    | 7.527E-05 | 3.471E+09        | 6.9143E+00    | 7.389E-05 | 3.407E+09        | 0.001 |
| 1s2p $^3P_0^o$  | 1s4p $^3P_0^o$ | 1.6323E+00    | 8.176E-07 | 6.823E+08        | 1.6255E+00    | 9.043E-07 | 7.545E+08        | 0.004 |
| 1s2p $^3P_2^o$  | 1s4p $^3P_0^o$ | 1.7203E+00    | 1.481E-04 | 1.113E+11        | 1.7131E+00    | 1.462E-04 | 1.099E+11        | 0.004 |
| 1s2p $^1P_1^o$  | 1s4p $^3P_0^o$ | 1.7287E+00    | 1.320E-04 | 9.819E+10        | 1.7215E+00    | 1.289E-04 | 9.594E+10        | 0.002 |
| 1s3p $^3P_1^o$  | 1s4p $^3P_0^o$ | 6.3396E+00    | 2.991E-06 | 1.655E+08        | 6.3138E+00    | 3.265E-06 | 1.806E+08        | 0.000 |
| 1s3p $^3P_2^o$  | 1s4p $^3P_0^o$ | 6.7379E+00    | 6.333E-04 | 3.101E+10        | 6.7101E+00    | 6.376E-04 | 3.122E+10        | 0.000 |
| 1s3p $^1P_1^o$  | 1s4p $^3P_0^o$ | 6.7743E+00    | 5.713E-04 | 2.768E+10        | 6.7469E+00    | 5.671E-04 | 2.746E+10        | 0.000 |
| 1s3d $^3D_2$    | 1s4s $^1S_0$   | 6.7668E+00    | 7.055E-05 | 1.028E+10        | 6.7378E+00    | 7.263E-05 | 1.058E+10        | 0.001 |
| 1s3d $^1D_2$    | 1s4s $^1S_0$   | 6.9088E+00    | 1.123E-04 | 1.569E+10        | 6.8790E+00    | 1.145E-04 | 1.601E+10        | 0.001 |
| 1s2p $^3P_2^o$  | 1s4p $^3P_0^o$ | 1.7201E+00    | 9.380E-05 | 2.115E+11        | 1.7129E+00    | 9.268E-05 | 2.089E+11        | 0.000 |
| 1s3p $^3P_2^o$  | 1s4p $^3P_0^o$ | 6.7356E+00    | 4.014E-04 | 5.902E+10        | 6.7079E+00    | 4.061E-04 | 5.970E+10        | 0.000 |
| 1s2p $^3P_0^o$  | 1s4p $^3P_2^o$ | 1.6219E+00    | 1.580E-04 | 8.014E+10        | 1.6152E+00    | 1.612E-04 | 8.177E+10        | 0.002 |
| 1s2p $^3P_0^o$  | 1s4p $^3P_2^o$ | 1.6232E+00    | 9.919E-05 | 5.022E+10        | 1.6164E+00    | 1.007E-04 | 5.101E+10        | 0.001 |
| 1s2p $^3P_2^o$  | 1s4p $^3P_2^o$ | 1.7088E+00    | 1.710E-04 | 7.811E+10        | 1.7016E+00    | 1.722E-04 | 7.870E+10        | 0.001 |
| 1s2p $^1P_1^o$  | 1s4p $^3P_2^o$ | 1.7170E+00    | 6.489E-05 | 2.936E+10        | 1.7100E+00    | 6.523E-05 | 2.950E+10        | 0.004 |
| 1s3p $^3P_1^o$  | 1s4p $^3P_2^o$ | 6.1858E+00    | 5.474E-04 | 1.909E+10        | 6.1607E+00    | 5.538E-04 | 1.930E+10        | 0.000 |
| 1s3p $^3P_0^o$  | 1s4p $^3P_2^o$ | 6.1907E+00    | 3.483E-04 | 1.212E+10        | 6.1653E+00    | 3.485E-04 | 1.212E+10        | 0.000 |
| 1s3p $^3P_2^o$  | 1s4p $^3P_2^o$ | 6.5644E+00    | 6.573E-04 | 2.035E+10        | 6.5375E+00    | 6.633E-04 | 2.052E+10        | 0.000 |
| 1s3p $^1P_1^o$  | 1s4p $^3P_2^o$ | 6.5991E+00    | 2.535E-04 | 7.766E+09        | 6.5723E+00    | 2.534E-04 | 7.759E+09        | 0.000 |
| 1s4p $^3P_1^o$  | 1s4p $^3P_2^o$ | 2.5504E+02    | 2.619E-07 | 5.371E+03        | 2.5410E+02    | 2.626E-07 | 5.380E+03        | 0.002 |
| 1s4p $^3P_0^o$  | 1s4p $^3P_2^o$ | 2.5839E+02    | 6.100E-07 | 3.197E+03        | 2.5732E+02    | 6.203E-07 | 3.202E+03        | 0.001 |
| 1s $^2$ 1S $_0$ | 1s4d $^3D_2$   | 3.2750E-01    | 4.379E-04 | 5.445E+12        | 3.2616E-01    | 4.466E-04 | 5.553E+12        | 0.003 |
| 1s2s $^3S_1$    | 1s4d $^3D_2$   | 1.6050E+00    | 2.179E-04 | 1.128E+11        | 1.5981E+00    | 2.096E-04 | 1.085E+11        | 0.002 |

(continued on next page)

Table 4 (continued)

| Lower                             | Upper                             | GRASP2K       |           |                      | FAC           |           |                      | dT    |
|-----------------------------------|-----------------------------------|---------------|-----------|----------------------|---------------|-----------|----------------------|-------|
|                                   |                                   | $\lambda$ (Å) | gf        | A (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | A (s <sup>-1</sup> ) |       |
| 1s 2s <sup>1</sup> S <sub>0</sub> | 1s 4d <sup>3</sup> D <sub>2</sub> | 1.6228E+00    | 1.321E-04 | 6.689E+10            | 1.6162E+00    | 1.318E-04 | 6.677E+10            | 0.003 |
| 1s 3s <sup>3</sup> S <sub>1</sub> | 1s 4d <sup>3</sup> D <sub>2</sub> | 6.1111E+00    | 1.685E-03 | 6.018E+10            | 6.0854E+00    | 1.711E-03 | 6.113E+10            | 0.002 |
| 1s 3s <sup>1</sup> S <sub>0</sub> | 1s 4d <sup>3</sup> D <sub>2</sub> | 6.1795E+00    | 1.100E-03 | 3.842E+10            | 6.1544E+00    | 1.079E-03 | 3.768E+10            | 0.002 |
| 1s 3d <sup>3</sup> D <sub>2</sub> | 1s 4d <sup>3</sup> D <sub>2</sub> | 6.5814E+00    | 4.239E-04 | 1.306E+10            | 6.5534E+00    | 4.253E-04 | 1.310E+10            | 0.000 |
| 1s 3d <sup>3</sup> D <sub>1</sub> | 1s 4d <sup>3</sup> D <sub>2</sub> | 6.5866E+00    | 1.859E-04 | 5.715E+09            | 6.5585E+00    | 1.860E-04 | 5.720E+09            | 0.000 |
| 1s 3d <sup>3</sup> D <sub>3</sub> | 1s 4d <sup>3</sup> D <sub>2</sub> | 6.7107E+00    | 2.138E-04 | 6.333E+09            | 6.6818E+00    | 2.135E-04 | 6.326E+09            | 0.000 |
| 1s 3d <sup>1</sup> D <sub>2</sub> | 1s 4d <sup>3</sup> D <sub>2</sub> | 6.7157E+00    | 5.225E-05 | 1.545E+09            | 6.6868E+00    | 5.192E-05 | 1.536E+09            | 0.000 |
| 1s 4s <sup>3</sup> S <sub>1</sub> | 1s 4d <sup>3</sup> D <sub>2</sub> | 2.0428E+02    | 4.053E-07 | 1.296E+04            | 2.0324E+02    | 4.072E-07 | 1.304E+04            | 0.029 |
| 1s 4s <sup>1</sup> S <sub>0</sub> | 1s 4d <sup>3</sup> D <sub>2</sub> | 2.4021E+02    | 1.633E-07 | 3.776E+03            | 2.3934E+02    | 1.627E-07 | 3.756E+03            | 0.039 |
| 1s 2s <sup>3</sup> S <sub>1</sub> | 1s 4d <sup>3</sup> D <sub>1</sub> | 1.6048E+00    | 2.169E-04 | 1.872E+11            | 1.5980E+00    | 2.076E-04 | 1.792E+11            | 0.002 |
| 1s 3s <sup>3</sup> S <sub>1</sub> | 1s 4d <sup>3</sup> D <sub>1</sub> | 6.1092E+00    | 1.673E-03 | 9.967E+10            | 6.0836E+00    | 1.700E-03 | 1.013E+11            | 0.002 |
| 1s 3d <sup>3</sup> D <sub>2</sub> | 1s 4d <sup>3</sup> D <sub>1</sub> | 6.5793E+00    | 1.840E-04 | 9.451E+09            | 6.5513E+00    | 1.852E-04 | 9.515E+09            | 0.000 |
| 1s 3d <sup>3</sup> D <sub>1</sub> | 1s 4d <sup>3</sup> D <sub>1</sub> | 6.5845E+00    | 1.810E-04 | 9.280E+09            | 6.5564E+00    | 1.814E-04 | 9.306E+09            | 0.000 |
| 1s 3d <sup>3</sup> D <sub>3</sub> | 1s 4d <sup>3</sup> D <sub>1</sub> | 6.7085E+00    | 3.503E-05 | 1.731E+09            | 6.6796E+00    | 3.499E-05 | 1.729E+09            | 0.001 |
| 1s 3d <sup>1</sup> D <sub>2</sub> | 1s 4d <sup>3</sup> D <sub>1</sub> | 6.7135E+00    | 1.229E-04 | 6.065E+09            | 6.6847E+00    | 1.225E-04 | 6.044E+09            | 0.000 |
| 1s 4s <sup>3</sup> S <sub>1</sub> | 1s 4d <sup>3</sup> D <sub>1</sub> | 2.0227E+02    | 4.160E-07 | 2.261E+04            | 2.0125E+02    | 4.171E-07 | 2.270E+04            | 0.026 |
| 1s 4d <sup>3</sup> D <sub>2</sub> | 1s 4d <sup>3</sup> D <sub>1</sub> | 2.0536E+04    | 1.788E-13 | 9.425E-07            |               |           |                      | 0.337 |
| 1s 2p <sup>3</sup> P <sub>0</sub> | 1s 4p <sup>1</sup> P <sub>0</sub> | 1.6210E+00    | 1.402E-04 | 1.186E+11            | 1.6143E+00    | 1.421E-04 | 1.202E+11            | 0.001 |
| 1s 2p <sup>3</sup> P <sub>2</sub> | 1s 4p <sup>1</sup> P <sub>0</sub> | 1.7078E+00    | 6.574E-05 | 5.012E+10            | 1.7006E+00    | 6.655E-05 | 5.072E+10            | 0.006 |
| 1s 2p <sup>1</sup> P <sub>0</sub> | 1s 4p <sup>1</sup> P <sub>0</sub> | 1.7161E+00    | 8.979E-05 | 6.779E+10            | 1.7090E+00    | 8.874E-05 | 6.699E+10            | 0.000 |
| 1s 3p <sup>3</sup> P <sub>0</sub> | 1s 4p <sup>1</sup> P <sub>0</sub> | 6.1732E+00    | 4.872E-04 | 2.843E+10            | 6.1480E+00    | 4.916E-04 | 2.867E+10            | 0.000 |
| 1s 3p <sup>3</sup> P <sub>2</sub> | 1s 4p <sup>1</sup> P <sub>0</sub> | 6.5502E+00    | 2.512E-04 | 1.302E+10            | 6.5232E+00    | 2.544E-04 | 1.318E+10            | 0.001 |
| 1s 3p <sup>1</sup> P <sub>0</sub> | 1s 4p <sup>1</sup> P <sub>0</sub> | 6.5847E+00    | 3.422E-04 | 1.755E+10            | 6.5579E+00    | 3.415E-04 | 1.750E+10            | 0.000 |
| 1s 4p <sup>3</sup> P <sub>0</sub> | 1s 4p <sup>1</sup> P <sub>0</sub> | 2.3520E+02    | 3.010E-07 | 1.210E+04            | 2.3412E+02    | 3.005E-07 | 1.208E+04            | 0.004 |
| 1s 4p <sup>3</sup> P <sub>2</sub> | 1s 4p <sup>1</sup> P <sub>0</sub> | 3.0236E+03    | 7.051E-11 | 1.715E-02            |               |           |                      | 0.024 |
| 1s 2s <sup>3</sup> S <sub>1</sub> | 1s 4d <sup>3</sup> D <sub>3</sub> | 1.6018E+00    | 5.612E-04 | 2.084E+11            | 1.5950E+00    | 5.556E-04 | 2.063E+11            | 0.002 |
| 1s 3s <sup>3</sup> S <sub>1</sub> | 1s 4d <sup>3</sup> D <sub>3</sub> | 6.0652E+00    | 3.882E-03 | 1.005E+11            | 6.0400E+00    | 3.968E-03 | 1.027E+11            | 0.002 |
| 1s 3d <sup>3</sup> D <sub>2</sub> | 1s 4d <sup>3</sup> D <sub>3</sub> | 6.5283E+00    | 2.062E-04 | 4.610E+09            | 6.5006E+00    | 2.084E-04 | 4.660E+09            | 0.000 |
| 1s 3d <sup>3</sup> D <sub>1</sub> | 1s 4d <sup>3</sup> D <sub>3</sub> | 6.5334E+00    | 3.327E-05 | 7.427E+08            | 6.5057E+00    | 3.358E-05 | 7.497E+08            | 0.001 |
| 1s 3d <sup>3</sup> D <sub>3</sub> | 1s 4d <sup>3</sup> D <sub>3</sub> | 6.6555E+00    | 8.341E-04 | 1.794E+10            | 6.6270E+00    | 8.375E-04 | 1.801E+10            | 0.000 |
| 1s 3d <sup>1</sup> D <sub>2</sub> | 1s 4d <sup>3</sup> D <sub>3</sub> | 6.6604E+00    | 1.380E-04 | 2.964E+09            | 6.6320E+00    | 1.380E-04 | 2.966E+09            | 0.000 |
| 1s 4s <sup>3</sup> S <sub>1</sub> | 1s 4d <sup>3</sup> D <sub>3</sub> | 1.6310E+02    | 1.890E-06 | 6.771E+04            | 1.6240E+02    | 1.893E-06 | 6.783E+04            | 0.022 |
| 1s 4d <sup>3</sup> D <sub>2</sub> | 1s 4d <sup>3</sup> D <sub>3</sub> | 8.0890E+02    | 3.369E-09 | 4.906E+00            |               |           |                      | 0.003 |
| 1s 4d <sup>3</sup> D <sub>1</sub> | 1s 4d <sup>3</sup> D <sub>3</sub> | 8.4207E+02    | 4.858E-10 | 6.529E-01            |               |           |                      | 0.015 |
| 1s 2p <sup>3</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 1.6179E+00    | 2.847E-03 | 1.036E+12            | 1.6112E+00    | 2.908E-03 | 1.058E+12            | 0.001 |
| 1s 2p <sup>3</sup> P <sub>2</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 1.7043E+00    | 7.811E-04 | 2.562E+11            | 1.6971E+00    | 7.937E-04 | 2.603E+11            | 0.001 |
| 1s 2p <sup>1</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 1.7125E+00    | 1.912E-04 | 6.213E+10            | 1.7055E+00    | 1.844E-04 | 5.990E+10            | 0.003 |
| 1s 3p <sup>3</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 6.1276E+00    | 4.973E-03 | 1.262E+11            | 6.1026E+00    | 4.989E-03 | 1.265E+11            | 0.000 |
| 1s 3p <sup>3</sup> P <sub>2</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 6.4989E+00    | 1.148E-03 | 2.591E+10            | 6.4721E+00    | 1.153E-03 | 2.601E+10            | 0.000 |
| 1s 3p <sup>1</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 6.5328E+00    | 2.725E-04 | 6.084E+09            | 6.5062E+00    | 2.680E-04 | 5.982E+09            | 0.000 |
| 1s 4p <sup>3</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 1.8322E+02    | 6.325E-07 | 1.795E+04            | 1.8244E+02    | 6.324E-07 | 1.795E+04            | 0.003 |
| 1s 4p <sup>3</sup> P <sub>2</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 6.5059E+02    | 3.452E-09 | 7.771E+00            | 6.4694E+02    | 3.463E-09 | 7.818E+00            | 0.016 |
| 1s 4p <sup>1</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 8.2895E+02    | 3.954E-10 | 5.482E-01            |               |           |                      | 0.020 |
| 1s 2p <sup>3</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 1.6178E+00    | 8.729E-04 | 4.449E+11            | 1.6111E+00    | 9.021E-04 | 4.597E+11            | 0.001 |
| 1s 2p <sup>3</sup> P <sub>2</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 1.6191E+00    | 1.244E-03 | 6.329E+11            | 1.6123E+00    | 1.269E-03 | 6.460E+11            | 0.000 |
| 1s 2p <sup>1</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 1.7042E+00    | 1.959E-04 | 8.998E+10            | 1.6971E+00    | 1.993E-04 | 9.155E+10            | 0.000 |
| 1s 3p <sup>3</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 1.7124E+00    | 4.103E-04 | 1.867E+11            | 1.7054E+00    | 4.121E-04 | 1.874E+11            | 0.002 |
| 1s 3p <sup>3</sup> P <sub>2</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 6.1266E+00    | 1.521E-03 | 5.406E+10            | 6.1016E+00    | 1.533E-03 | 5.447E+10            | 0.000 |
| 1s 3p <sup>1</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 6.1314E+00    | 2.165E-03 | 7.684E+10            | 6.1062E+00    | 2.172E-03 | 7.706E+10            | 0.000 |
| 1s 3p <sup>3</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 6.4978E+00    | 2.880E-04 | 9.101E+09            | 6.4710E+00    | 2.892E-04 | 9.137E+09            | 0.000 |
| 1s 3p <sup>1</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 6.5317E+00    | 5.991E-04 | 1.874E+10            | 6.5052E+00    | 5.988E-04 | 1.871E+10            | 0.000 |
| 1s 4p <sup>3</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 1.8236E+02    | 1.962E-07 | 7.869E+03            | 1.8158E+02    | 1.960E-07 | 7.865E+03            | 0.002 |
| 1s 4p <sup>3</sup> P <sub>2</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 1.8406E+02    | 2.716E-07 | 1.070E+04            | 1.8322E+02    | 2.717E-07 | 1.070E+04            | 0.003 |
| 1s 4p <sup>3</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 6.3989E+02    | 9.105E-10 | 2.967E+00            | 6.3631E+02    | 9.130E-10 | 2.982E+00            | 0.014 |
| 1s 4p <sup>1</sup> P <sub>0</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 8.1166E+02    | 9.363E-10 | 1.896E+00            | 8.0920E+02    | 9.307E-10 | 1.880E+00            | 0.020 |
| 1s 4f <sup>3</sup> F <sub>3</sub> | 1s 4f <sup>3</sup> F <sub>3</sub> | 3.8916E+04    | 1.030E-14 | 9.073E-09            |               |           |                      | 0.558 |
| 1s <sup>2</sup> S <sub>0</sub>    | 1s 4d <sup>1</sup> D <sub>2</sub> | 3.2740E-01    | 6.231E-04 | 7.755E+12            | 3.2603E-01    | 7.226E-04 | 8.992E+12            | 0.002 |
| 1s 2s <sup>3</sup> S <sub>1</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 1.6017E+00    | 1.591E-04 | 8.273E+10            | 1.5948E+00    | 1.567E-04 | 8.150E+10            | 0.001 |
| 1s 2s <sup>1</sup> S <sub>0</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 1.6194E+00    | 2.277E-04 | 1.158E+11            | 1.6128E+00    | 2.323E-04 | 1.181E+11            | 0.002 |
| 1s 3s <sup>3</sup> S <sub>1</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 6.0634E+00    | 1.094E-03 | 3.969E+10            | 6.0381E+00    | 1.117E-03 | 4.054E+10            | 0.002 |
| 1s 3s <sup>1</sup> S <sub>0</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 6.1308E+00    | 1.677E-03 | 5.953E+10            | 6.1059E+00    | 1.661E-03 | 5.893E+10            | 0.002 |
| 1s 3d <sup>3</sup> D <sub>2</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 6.5262E+00    | 5.168E-05 | 1.619E+09            | 6.4985E+00    | 5.227E-05 | 1.637E+09            | 0.000 |
| 1s 3d <sup>3</sup> D <sub>1</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 6.5313E+00    | 1.191E-04 | 3.724E+09            | 6.5035E+00    | 1.198E-04 | 3.747E+09            | 0.000 |
| 1s 3d <sup>3</sup> D <sub>3</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 6.6532E+00    | 1.372E-04 | 4.134E+09            | 6.6247E+00    | 1.377E-04 | 4.152E+09            | 0.000 |
| 1s 3d <sup>1</sup> D <sub>2</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 6.6582E+00    | 5.591E-04 | 1.683E+10            | 6.6297E+00    | 5.608E-04 | 1.687E+10            | 0.000 |
| 1s 4s <sup>3</sup> S <sub>1</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 1.6177E+02    | 5.455E-07 | 2.781E+04            | 1.6105E+02    | 5.455E-07 | 2.782E+04            | 0.020 |
| 1s 4s <sup>1</sup> S <sub>0</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 1.8350E+02    | 5.750E-07 | 2.278E+04            | 1.8292E+02    | 5.727E-07 | 2.264E+04            | 0.027 |
| 1s 4d <sup>3</sup> D <sub>2</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 7.7722E+02    | 9.379E-10 | 2.071E+00            |               |           |                      | 0.018 |
| 1s 4d <sup>3</sup> D <sub>1</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 8.0779E+02    | 1.943E-09 | 3.972E+00            |               |           |                      | 0.005 |
| 1s 4d <sup>3</sup> D <sub>3</sub> | 1s 4d <sup>1</sup> D <sub>2</sub> | 1.9845E+04    | 1.515E-13 | 5.133E-07            |               |           |                      | 0.342 |
| 1s 2p <sup>3</sup> P <sub>2</sub> | 1s 4f <sup>3</sup> F <sub>4</sub> | 1.7025E+00    | 5.177E-03 | 1.324E+12            | 1.6954E+00    | 5.446E-03 | 1.392E+12            | 0.000 |

(continued on next page)

Table 4 (continued)

| Lower  | Upper  | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|--|--|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|  |  | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 6.4732E+00    | 7.864E-03 | 1.391E+11              | 6.4465E+00    | 7.967E-03 | 1.408E+11              | 0.000 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.6544E+02    | 6.500E-08 | 2.224E+02              | 4.6333E+02    | 6.501E-08 | 2.225E+02              | 0.009 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6355E+03    | 1.450E-10 | 4.017E-02              | 1.6325E+03    | 1.439E-10 | 3.970E-02              | 0.016 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.7073E+03    | 1.015E-11 | 2.582E-03              |               |           |                        | 0.053 |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6162E+00    | 5.484E-06 | 2.001E+09              | 1.6095E+00    | 7.555E-06 | 2.755E+09              | 0.014 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.7025E+00    | 5.783E-04 | 1.901E+11              | 1.6953E+00    | 6.082E-04 | 1.999E+11              | 0.000 |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.7107E+00    | 3.470E-03 | 1.130E+12              | 1.7036E+00    | 3.569E-03 | 1.161E+12              | 0.001 |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 6.1040E+00    | 8.647E-06 | 2.211E+08              | 6.0791E+00    | 9.972E-06 | 2.549E+08              | 0.003 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4472E+00    | 8.785E-04 | 1.998E+10              | 6.4457E+00    | 8.900E-04 | 2.023E+10              | 0.000 |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 6.5060E+00    | 5.198E-03 | 1.170E+11              | 6.4796E+00    | 5.218E-03 | 1.174E+11              | 0.000 |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6424E+02    | 1.482E-09 | 5.234E+01              | 1.6359E+02    | 1.492E-09 | 5.269E+01              | 0.001 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.6135E+02    | 7.452E-09 | 3.336E+01              | 4.5925E+02    | 7.450E-09 | 3.337E+01              | 0.006 |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.4442E+02    | 2.699E-08 | 8.676E+01              | 5.4298E+02    | 2.686E-08 | 8.609E+01              | 0.009 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.5861E+03    | 1.917E-11 | 7.263E-03              |               |           |                        | 0.019 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6535E+03    | 1.021E-10 | 3.557E-02              | 1.6504E+03    | 1.013E-10 | 3.513E-02              | 0.007 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.2510E+04    | 3.365E-15 | 1.163E-09              |               |           |                        | 0.824 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.4473E+00    | 4.378E-12 | 4.647E+03              | 1.4412E+00    | 1.023E-10 | 1.086E+05              | 0.891 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 5s <sup>3</sup> S <sub>1</sub>              | 4.3197E+00    | 7.655E-10 | 9.121E+04              |               |           |                        | 0.164 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5s <sup>3</sup> S <sub>1</sub>              | 4.5495E+00    | 2.933E-05 | 3.150E+09              | 4.5304E+00    | 2.931E-05 | 3.148E+09              | 0.001 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 5s <sup>3</sup> S <sub>1</sub>              | 4.5520E+00    | 2.949E-05 | 3.165E+09              | 4.5328E+00    | 2.930E-05 | 3.144E+09              | 0.003 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5s <sup>3</sup> S <sub>1</sub>              | 4.6109E+00    | 7.001E-05 | 7.322E+09              | 4.5914E+00    | 6.937E-05 | 7.254E+09              | 0.001 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5s <sup>3</sup> S <sub>1</sub>              | 4.6133E+00    | 1.982E-05 | 2.071E+09              | 4.5938E+00    | 1.952E-05 | 2.039E+09              | 0.003 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.3745E+01    | 5.045E-09 | 5.937E+04              |               |           |                        | 0.022 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.4736E+01    | 1.591E-04 | 1.629E+09              | 1.4676E+01    | 1.575E-04 | 1.612E+09              | 0.001 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.4747E+01    | 1.592E-04 | 1.628E+09              | 1.4686E+01    | 1.567E-04 | 1.602E+09              | 0.002 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.5010E+01    | 3.835E-04 | 3.785E+09              | 1.4947E+01    | 3.784E-04 | 3.734E+09              | 0.001 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5s <sup>3</sup> S <sub>1</sub>              | 1.5021E+01    | 1.079E-04 | 1.063E+09              | 1.4959E+01    | 1.059E-04 | 1.044E+09              | 0.002 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.4598E+00    | 3.294E-07 | 3.437E+08              | 1.4537E+00    | 3.558E-07 | 3.711E+08              | 0.007 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.5297E+00    | 5.743E-05 | 5.456E+10              | 1.5233E+00    | 5.632E-05 | 5.350E+10              | 0.003 |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.5364E+00    | 5.106E-05 | 4.809E+10              | 1.5300E+00    | 4.964E-05 | 4.674E+10              | 0.002 |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.3450E+00    | 7.585E-07 | 8.933E+07              | 4.3271E+00    | 8.116E-07 | 9.556E+07              | 0.006 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.5285E+00    | 1.479E-04 | 1.603E+10              | 4.5097E+00    | 1.475E-04 | 1.598E+10              | 0.000 |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.5449E+00    | 1.323E-04 | 1.424E+10              | 4.5263E+00    | 1.309E-04 | 1.408E+10              | 0.000 |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.3810E+01    | 2.420E-06 | 2.821E+07              | 1.3752E+01    | 2.598E-06 | 3.028E+07              | 0.001 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.4601E+01    | 5.296E-04 | 5.524E+09              | 1.4539E+01    | 5.330E-04 | 5.559E+09              | 0.000 |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.4672E+01    | 4.785E-04 | 4.943E+09              | 1.4610E+01    | 4.758E-04 | 4.914E+09              | 0.000 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.4936E+01    | 9.431E-05 | 9.400E+08              | 1.4873E+01    | 9.437E-05 | 9.404E+08              | 0.000 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.4942E+01    | 2.888E-05 | 2.876E+08              | 1.4879E+01    | 2.862E-05 | 2.850E+08              | 0.001 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.5078E+01    | 1.573E-07 | 1.538E+06              | 1.5014E+01    | 1.253E-07 | 1.225E+06              | 0.002 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5s <sup>1</sup> S <sub>0</sub>              | 4.5420E+00    | 1.917E-05 | 6.199E+09              | 4.5228E+00    | 1.941E-05 | 6.277E+09              | 0.001 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5s <sup>1</sup> S <sub>0</sub>              | 4.6055E+00    | 2.999E-05 | 9.431E+09              | 4.5859E+00    | 2.997E-05 | 9.427E+09              | 0.002 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5s <sup>1</sup> S <sub>0</sub>              | 1.4657E+01    | 1.021E-04 | 3.171E+09              | 1.4596E+01    | 1.045E-04 | 3.246E+09              | 0.000 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5s <sup>1</sup> S <sub>0</sub>              | 1.4939E+01    | 1.627E-04 | 4.864E+09              | 1.4876E+01    | 1.658E-04 | 4.956E+09              | 0.001 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.5297E+00    | 3.640E-05 | 1.038E+11              | 1.5233E+00    | 3.564E-05 | 1.015E+11              | 0.000 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.5279E+00    | 9.388E-05 | 3.054E+10              | 4.5092E+00    | 9.356E-05 | 3.043E+10              | 0.000 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.4595E+01    | 3.360E-04 | 1.052E+10              | 1.4534E+01    | 3.399E-04 | 1.064E+10              | 0.000 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.4936E+01    | 4.095E-05 | 1.225E+09              | 1.4874E+01    | 4.095E-05 | 1.224E+09              | 0.001 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.4555E+00    | 6.570E-05 | 4.138E+10              | 1.4495E+00    | 6.694E-05 | 4.214E+10              | 0.002 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.4565E+00    | 4.114E-05 | 2.587E+10              | 1.4505E+00    | 4.181E-05 | 2.628E+10              | 0.001 |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.5251E+00    | 6.889E-05 | 3.951E+10              | 1.5187E+00    | 6.910E-05 | 3.963E+10              | 0.001 |
| 1s 2p <sup>1</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.5317E+00    | 2.611E-05 | 1.485E+10              | 1.5253E+00    | 2.616E-05 | 1.487E+10              | 0.004 |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.3076E+00    | 1.546E-04 | 1.112E+10              | 4.2899E+00    | 1.560E-04 | 1.121E+10              | 0.000 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.3099E+00    | 9.802E-05 | 7.040E+09              | 4.2921E+00    | 9.847E-05 | 7.070E+09              | 0.000 |
| 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4878E+00    | 1.697E-04 | 1.124E+10              | 4.4692E+00    | 1.704E-04 | 1.128E+10              | 0.000 |
| 1s 3p <sup>1</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.5039E+00    | 6.500E-05 | 4.275E+09              | 4.4855E+00    | 6.502E-05 | 4.274E+09              | 0.001 |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.3439E+01    | 4.552E-04 | 3.363E+09              | 1.3383E+01    | 4.582E-04 | 3.384E+09              | 0.000 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.3448E+01    | 2.902E-04 | 2.140E+09              | 1.3392E+01    | 2.890E-04 | 2.131E+09              | 0.000 |
| 1s 4p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.4186E+01    | 5.493E-04 | 3.641E+09              | 1.4127E+01    | 5.527E-04 | 3.663E+09              | 0.000 |
| 1s 4p <sup>1</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.4253E+01    | 2.123E-04 | 1.394E+09              | 1.4194E+01    | 2.117E-04 | 1.390E+09              | 0.000 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.4503E+01    | 1.980E-05 | 1.256E+08              | 1.4442E+01    | 1.963E-05 | 1.245E+08              | 0.001 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.4508E+01    | 4.987E-06 | 3.161E+07              | 1.4447E+01    | 4.933E-06 | 3.126E+07              | 0.000 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.4632E+01    | 1.385E-04 | 8.628E+08              | 1.4571E+01    | 1.367E-04 | 8.519E+08              | 0.000 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.4636E+01    | 1.545E-05 | 9.618E+07              | 1.4575E+01    | 1.522E-05 | 9.479E+07              | 0.000 |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.9993E+02    | 2.211E-07 | 1.180E+03              | 4.9817E+02    | 2.213E-07 | 1.179E+03              | 0.003 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 5.0634E+02    | 1.353E-07 | 7.042E+02              | 5.0434E+02    | 1.354E-07 | 7.042E+02              | 0.002 |
| 1s <sup>2</sup> <sup>1</sup> S <sub>0</sub>    | 1s 5d <sup>3</sup> D <sub>2</sub>              | 3.2010E-01    | 2.358E-04 | 3.069E+12              | 3.1882E-01    | 2.397E-04 | 3.120E+12              | 0.002 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4421E+00    | 4.328E-05 | 2.776E+10              | 1.4360E+00    | 3.977E-05 | 2.551E+10              | 0.000 |
| 1s 2s <sup>1</sup> S <sub>0</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4565E+00    | 2.475E-05 | 1.556E+10              | 1.4506E+00    | 2.497E-05 | 1.569E+10              | 0.003 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.2737E+00    | 2.788E-04 | 2.036E+10              | 4.2558E+00    | 2.762E-04 | 2.017E+10              | 0.002 |
| 1s 3s <sup>1</sup> S <sub>0</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.3071E+00    | 1.759E-04 | 1.265E+10              | 4.2893E+00    | 1.752E-04 | 1.259E+10              | 0.001 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.4985E+00    | 9.377E-05 | 6.182E+09              | 4.4794E+00    | 9.361E-05 | 6.171E+09              | 0.001 |

(continued on next page)

Table 4 (continued)

| Lower  | Upper  | GRASP2K       |           |                  | FAC           |           |                  | dT    |
|--|--|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|  |  | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) |       |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.5010E+00    | 4.110E–05 | 2.707E+09        | 4.4818E+00    | 4.103E–05 | 2.702E+09        | 0.002 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.5585E+00    | 4.574E–05 | 2.936E+09        | 4.5391E+00    | 4.533E–05 | 2.910E+09        | 0.001 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.5609E+00    | 1.111E–05 | 7.124E+08        | 4.5414E+00    | 1.094E–05 | 7.020E+08        | 0.002 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.3290E+01    | 1.104E–03 | 8.339E+09        | 1.3233E+01    | 1.121E–03 | 8.472E+09        | 0.002 |
| 1s 4s <sup>1</sup> S <sub>0</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.3420E+01    | 7.221E–04 | 5.349E+09        | 1.3364E+01    | 7.080E–04 | 5.244E+09        | 0.001 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>1</sup> P <sub>2</sub>              | 1.4214E+01    | 4.446E–04 | 2.936E+09        | 1.4154E+01    | 4.454E–04 | 2.940E+09        | 0.000 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4224E+01    | 1.955E–04 | 1.289E+09        | 1.4164E+01    | 1.954E–04 | 1.288E+09        | 0.000 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4468E+01    | 2.257E–04 | 1.438E+09        | 1.4407E+01    | 2.258E–04 | 1.439E+09        | 0.000 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4479E+01    | 5.540E–05 | 3.525E+08        | 1.4417E+01    | 5.517E–05 | 3.511E+08        | 0.000 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.0118E+02    | 3.701E–07 | 3.067E+03        | 3.9828E+02    | 3.741E–07 | 3.119E+03        | 0.027 |
| 1s 5s <sup>1</sup> S <sub>0</sub>              | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.7039E+02    | 1.499E–07 | 9.037E+02        | 4.6740E+02    | 1.505E–07 | 9.114E+02        | 0.045 |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.4551E+00    | 5.848E–05 | 6.140E+10        | 1.4491E+00    | 5.907E–05 | 6.201E+10        | 0.000 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.5247E+00    | 2.653E–05 | 2.538E+10        | 1.5183E+00    | 2.678E–05 | 2.561E+10        | 0.008 |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.5313E+00    | 3.621E–05 | 3.434E+10        | 1.5249E+00    | 3.560E–05 | 3.375E+10        | 0.002 |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 4.3044E+00    | 1.385E–04 | 1.662E+10        | 4.2867E+00    | 1.391E–04 | 1.669E+10        | 0.000 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 4.4844E+00    | 6.547E–05 | 7.239E+09        | 4.4658E+00    | 6.579E–05 | 7.272E+09        | 0.001 |
| 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 4.5006E+00    | 8.834E–05 | 9.697E+09        | 4.4821E+00    | 8.767E–05 | 9.621E+09        | 0.000 |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.3409E+01    | 4.062E–04 | 5.023E+09        | 1.3352E+01    | 4.085E–04 | 5.051E+09        | 0.000 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.4153E+01    | 2.101E–04 | 2.332E+09        | 1.4093E+01    | 2.121E–04 | 2.355E+09        | 0.000 |
| 1s 4p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.4219E+01    | 2.851E–04 | 3.135E+09        | 1.4160E+01    | 2.846E–04 | 3.130E+09        | 0.000 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.4467E+01    | 4.625E–06 | 4.913E+07        | 1.4407E+01    | 4.908E–06 | 5.213E+07        | 0.000 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.4473E+01    | 1.034E–05 | 1.097E+08        | 1.4412E+01    | 1.028E–05 | 1.091E+08        | 0.001 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.4601E+01    | 9.082E–05 | 9.472E+08        | 1.4539E+01    | 9.153E–05 | 9.546E+08        | 0.000 |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 4.6126E+02    | 2.539E–07 | 2.653E+03        | 4.5925E+02    | 2.534E–07 | 2.649E+03        | 0.004 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 5.9640E+03    | 5.793E–11 | 3.621E–03        |               |           |                  | 0.013 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4421E+00    | 4.306E–05 | 4.604E+10        | 1.4359E+00    | 3.931E–05 | 4.203E+10        | 0.002 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.2732E+00    | 2.771E–04 | 3.375E+10        | 4.2553E+00    | 2.739E–04 | 3.335E+10        | 0.002 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.4980E+00    | 4.080E–05 | 4.484E+09        | 4.4789E+00    | 4.078E–05 | 4.481E+09        | 0.001 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.5005E+00    | 4.016E–05 | 4.408E+09        | 4.4813E+00    | 3.999E–05 | 4.390E+09        | 0.001 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.5580E+00    | 7.478E–06 | 8.003E+08        | 4.5386E+00    | 7.403E–06 | 7.923E+08        | 0.003 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.5603E+00    | 2.632E–05 | 2.814E+09        | 4.5409E+00    | 2.597E–05 | 2.777E+09        | 0.001 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.3285E+01    | 1.095E–03 | 1.380E+10        | 1.3229E+01    | 1.114E–03 | 1.403E+10        | 0.002 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4209E+01    | 1.940E–04 | 2.137E+09        | 1.4150E+01    | 1.951E–04 | 2.149E+09        | 0.000 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4219E+01    | 1.902E–04 | 2.091E+09        | 1.4159E+01    | 1.904E–04 | 2.094E+09        | 0.000 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4463E+01    | 3.687E–05 | 3.919E+08        | 1.4402E+01    | 3.689E–05 | 3.921E+08        | 0.001 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4474E+01    | 1.291E–04 | 1.370E+09        | 1.4412E+01    | 1.289E–04 | 1.368E+09        | 0.000 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 3.9728E+02    | 3.792E–07 | 5.342E+03        | 3.9446E+02    | 3.826E–07 | 5.421E+03        | 0.023 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.0886E+04    | 1.644E–13 | 2.186E–07        |               |           |                  | 0.336 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4408E+00    | 1.204E–04 | 5.525E+10        | 1.4347E+00    | 1.149E–04 | 5.277E+10        | 0.002 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 4.2622E+00    | 6.786E–04 | 3.560E+10        | 4.2443E+00    | 6.795E–04 | 3.563E+10        | 0.002 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 4.4858E+00    | 4.726E–05 | 2.238E+09        | 4.4668E+00    | 4.769E–05 | 2.258E+09        | 0.001 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 4.4882E+00    | 7.661E–06 | 3.624E+08        | 4.4692E+00    | 7.705E–06 | 3.644E+08        | 0.002 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 4.5454E+00    | 1.848E–04 | 8.523E+09        | 4.5261E+00    | 1.847E–04 | 8.521E+09        | 0.001 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 4.5477E+00    | 3.058E–05 | 1.409E+09        | 4.5284E+00    | 3.047E–05 | 1.404E+09        | 0.001 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.3179E+01    | 2.524E–03 | 1.385E+10        | 1.3123E+01    | 2.570E–03 | 1.410E+10        | 0.002 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4088E+01    | 2.165E–04 | 1.040E+09        | 1.4029E+01    | 2.178E–04 | 1.046E+09        | 0.000 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4097E+01    | 3.491E–05 | 1.674E+08        | 1.4038E+01    | 3.507E–05 | 1.681E+08        | 0.000 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4337E+01    | 8.763E–04 | 4.062E+09        | 1.4277E+01    | 8.786E–04 | 4.072E+09        | 0.000 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4348E+01    | 1.443E–04 | 6.680E+08        | 1.4287E+01    | 1.441E–04 | 6.672E+08        | 0.000 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 3.1997E+02    | 1.720E–06 | 1.600E+04        | 3.1810E+02    | 1.730E–06 | 1.615E+04        | 0.020 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.5807E+03    | 3.267E–09 | 1.246E+00        |               |           |                  | 0.003 |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.6443E+03    | 4.714E–10 | 1.661E–01        |               |           |                  | 0.008 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.4538E+00    | 1.563E–03 | 7.049E+11        | 1.4478E+00    | 1.594E–03 | 7.186E+11        | 0.001 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.5232E+00    | 4.174E–04 | 1.714E+11        | 1.5168E+00    | 4.215E–04 | 1.730E+11        | 0.001 |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.5298E+00    | 1.017E–04 | 4.140E+10        | 1.5235E+00    | 9.866E–05 | 4.016E+10        | 0.003 |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 4.2930E+00    | 6.727E–05 | 3.478E+09        | 4.2753E+00    | 6.478E–05 | 3.348E+09        | 0.001 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 4.4720E+00    | 4.140E–06 | 1.972E+08        | 4.4534E+00    | 3.472E–06 | 1.654E+08        | 0.002 |
| 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 4.4880E+00    | 8.259E–07 | 3.907E+07        | 4.4696E+00    | 1.108E–06 | 5.240E+07        | 0.012 |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.3298E+01    | 3.606E–03 | 1.943E+10        | 1.3242E+01    | 3.616E–03 | 1.948E+10        | 0.000 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.4030E+01    | 8.664E–04 | 4.194E+09        | 1.3970E+01    | 8.723E–04 | 4.223E+09        | 0.000 |
| 1s 4p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.4095E+01    | 2.047E–04 | 9.816E+08        | 1.4036E+01    | 2.005E–04 | 9.620E+08        | 0.000 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.4339E+01    | 5.397E–04 | 2.501E+09        | 1.4278E+01    | 5.406E–04 | 2.505E+09        | 0.000 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.4344E+01    | 8.972E–05 | 4.155E+08        | 1.4283E+01    | 8.978E–05 | 4.157E+08        | 0.000 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.4466E+01    | 9.385E–05 | 4.274E+08        | 1.4404E+01    | 9.364E–05 | 4.264E+08        | 0.000 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.4470E+01    | 1.130E–05 | 5.141E+07        | 1.4408E+01    | 1.125E–05 | 5.124E+07        | 0.000 |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 3.5882E+02    | 8.216E–07 | 6.081E+03        | 3.5685E+02    | 8.246E–07 | 6.118E+03        | 0.001 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.2712E+03    | 4.533E–09 | 2.673E+00        | 1.2579E+03    | 4.615E–09 | 2.756E+00        | 0.010 |
| 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.6156E+03    | 5.213E–10 | 1.903E–01        |               |           |                  | 0.012 |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4538E+00    | 4.796E–04 | 3.027E+11        | 1.4478E+00    | 4.936E–04 | 3.115E+11        | 0.001 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4548E+00    | 6.831E–04 | 4.305E+11        | 1.4488E+00    | 6.959E–04 | 4.385E+11        | 0.000 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.5232E+00    | 1.045E–04 | 6.006E+10        | 1.5168E+00    | 1.058E–04 | 6.085E+10        | 0.001 |

(continued on next page)



Table 4 (continued)

| Lower   | Upper   | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|---|---|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|   |   | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.5298E+00    | 2.187E-04 | 1.247E+11              | 1.5234E+00    | 2.185E-04 | 1.245E+11              | 0.002 |
| 1s3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.2928E+00    | 2.075E-05 | 1.502E+09              | 4.2750E+00    | 1.920E-05 | 1.389E+09              | 0.002 |
| 1s3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.2951E+00    | 2.908E-05 | 2.103E+09              | 4.2773E+00    | 2.793E-05 | 2.019E+09              | 0.001 |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4718E+00    | 1.047E-06 | 6.984E+07              | 4.4531E+00    | 8.606E-07 | 5.740E+07              | 0.005 |
| 1s3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4878E+00    | 1.836E-06 | 1.216E+08              | 4.4693E+00    | 1.609E-06 | 1.065E+08              | 0.004 |
| 1s4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3296E+01    | 1.101E-03 | 8.310E+09              | 1.3240E+01    | 1.110E-03 | 8.382E+09              | 0.000 |
| 1s4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3305E+01    | 1.570E-03 | 1.183E+10              | 1.3248E+01    | 1.574E-03 | 1.186E+10              | 0.000 |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4027E+01    | 2.174E-04 | 1.474E+09              | 1.3967E+01    | 2.189E-04 | 1.484E+09              | 0.000 |
| 1s4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4093E+01    | 4.547E-04 | 3.054E+09              | 1.4033E+01    | 4.555E-04 | 3.059E+09              | 0.000 |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4336E+01    | 8.950E-05 | 5.809E+08              | 1.4275E+01    | 8.974E-05 | 5.825E+08              | 0.000 |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4342E+01    | 3.591E-04 | 2.329E+09              | 1.4281E+01    | 3.595E-04 | 2.332E+09              | 0.000 |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4463E+01    | 7.505E-06 | 4.786E+07              | 1.4401E+01    | 7.492E-06 | 4.778E+07              | 0.000 |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4467E+01    | 6.818E-05 | 4.346E+08              | 1.4405E+01    | 6.800E-05 | 4.334E+08              | 0.000 |
| 1s5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.5713E+02    | 2.546E-07 | 2.663E+03              | 3.5518E+02    | 2.555E-07 | 2.679E+03              | 0.001 |
| 1s5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.6039E+02    | 3.530E-07 | 3.626E+03              | 3.5830E+02    | 3.545E-07 | 3.652E+03              | 0.001 |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.2503E+03    | 1.196E-09 | 1.021E+00              | 1.2374E+03    | 1.217E-09 | 1.051E+00              | 0.009 |
| 1s5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.5820E+03    | 1.240E-09 | 6.612E-01              | 1.5673E+03    | 1.256E-09 | 6.767E-01              | 0.013 |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.6009E+04    | 1.358E-14 | 3.135E-09              |               |           |                        | 0.251 |
| 1s <sup>2</sup> <sup>1</sup> S <sub>0</sub>   | 1s5d <sup>1</sup> D <sub>2</sub>              | 3.2000E-01    | 3.384E-04 | 4.406E+12              | 3.1875E-01    | 3.920E-04 | 5.103E+12              | 0.001 |
| 1s2s <sup>3</sup> S <sub>1</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 1.4408E+00    | 3.421E-05 | 2.199E+10              | 1.4346E+00    | 3.238E-05 | 2.081E+10              | 0.001 |
| 1s2s <sup>1</sup> S <sub>0</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 1.4551E+00    | 4.690E-05 | 2.955E+10              | 1.4492E+00    | 4.826E-05 | 3.040E+10              | 0.002 |
| 1s3s <sup>3</sup> S <sub>1</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 4.2617E+00    | 1.913E-04 | 1.405E+10              | 4.2438E+00    | 1.909E-04 | 1.402E+10              | 0.002 |
| 1s3s <sup>1</sup> S <sub>0</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 4.2949E+00    | 2.860E-04 | 2.068E+10              | 4.2772E+00    | 2.874E-04 | 2.078E+10              | 0.001 |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 4.4852E+00    | 1.193E-05 | 7.912E+08              | 4.4662E+00    | 1.201E-05 | 7.964E+08              | 0.000 |
| 1s3d <sup>3</sup> D <sub>1</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 4.4876E+00    | 2.723E-05 | 1.804E+09              | 4.4686E+00    | 2.736E-05 | 1.812E+09              | 0.001 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 4.5449E+00    | 3.039E-05 | 1.963E+09              | 4.5255E+00    | 3.031E-05 | 1.958E+09              | 0.001 |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 4.5472E+00    | 1.242E-04 | 8.013E+09              | 4.5278E+00    | 1.237E-04 | 7.986E+09              | 0.001 |
| 1s4s <sup>3</sup> S <sub>1</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 1.3174E+01    | 7.090E-04 | 5.450E+09              | 1.3118E+01    | 7.220E-04 | 5.550E+09              | 0.002 |
| 1s4s <sup>1</sup> S <sub>0</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 1.3302E+01    | 1.097E-03 | 8.271E+09              | 1.3247E+01    | 1.082E-03 | 8.157E+09              | 0.001 |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 1.4082E+01    | 5.367E-05 | 3.610E+08              | 1.4023E+01    | 5.400E-05 | 3.632E+08              | 0.000 |
| 1s4d <sup>3</sup> D <sub>1</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 1.4092E+01    | 1.243E-04 | 8.352E+08              | 1.4033E+01    | 1.245E-04 | 8.366E+08              | 0.000 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 1.4332E+01    | 1.438E-04 | 9.338E+08              | 1.4271E+01    | 1.442E-04 | 9.366E+08              | 0.000 |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 1.4342E+01    | 5.883E-04 | 3.816E+09              | 1.4282E+01    | 5.895E-04 | 3.823E+09              | 0.000 |
| 1s5s <sup>3</sup> S <sub>1</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 3.1728E+02    | 4.955E-07 | 6.566E+03              | 3.1538E+02    | 4.978E-07 | 6.620E+03              | 0.018 |
| 1s5s <sup>1</sup> S <sub>0</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 3.5905E+02    | 5.277E-07 | 5.460E+03              | 3.5720E+02    | 5.289E-07 | 5.482E+03              | 0.031 |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 1.5170E+03    | 9.109E-10 | 5.280E-01              |               |           |                        | 0.016 |
| 1s5d <sup>3</sup> D <sub>1</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 1.5755E+03    | 1.889E-09 | 1.015E+00              |               |           |                        | 0.003 |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s5d <sup>1</sup> D <sub>2</sub>              | 3.7649E+04    | 1.593E-13 | 1.499E-07              |               |           |                        | 0.285 |
| 1s2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.5225E+00    | 2.780E-03 | 8.890E+11              | 1.5161E+00    | 2.919E-03 | 9.332E+11              | 0.000 |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.4658E+00    | 3.882E-05 | 1.443E+09              | 4.4472E+00    | 3.385E-05 | 1.257E+09              | 0.001 |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.3968E+01    | 5.895E-03 | 2.239E+10              | 1.3909E+01    | 5.959E-03 | 2.263E+10              | 0.000 |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.4275E+01    | 9.254E-05 | 3.366E+08              | 1.4214E+01    | 9.308E-05 | 3.385E+08              | 0.000 |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.4280E+01    | 7.287E-06 | 2.648E+07              | 1.4220E+01    | 7.321E-06 | 2.660E+07              | 0.000 |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.4401E+01    | 7.716E-04 | 1.433E+09              | 1.4339E+01    | 7.730E-04 | 2.762E+09              | 0.000 |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.4404E+01    | 7.051E-05 | 2.519E+08              | 1.4343E+01    | 7.056E-05 | 2.520E+08              | 0.000 |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 9.0890E+02    | 8.517E-08 | 7.641E+01              | 9.0168E+02    | 8.608E-08 | 7.780E+01              | 0.007 |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 3.1889E+03    | 1.921E-10 | 1.400E-02              | 3.1838E+03    | 1.906E-10 | 1.382E-02              | 0.001 |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 3.3285E+03    | 1.343E-11 | 8.982E-04              |               |           |                        | 0.017 |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s5g <sup>3</sup> G <sub>4</sub>              | 4.4792E+00    | 6.254E-03 | 2.310E+11              | 4.4604E+00    | 6.315E-03 | 2.332E+11              | 0.000 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s5g <sup>3</sup> G <sub>4</sub>              | 4.5387E+00    | 6.548E-04 | 2.356E+10              | 4.5195E+00    | 6.553E-04 | 2.357E+10              | 0.000 |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s5g <sup>3</sup> G <sub>4</sub>              | 4.5410E+00    | 5.882E-05 | 2.114E+09              | 4.5219E+00    | 5.907E-05 | 2.122E+09              | 0.000 |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s5g <sup>3</sup> G <sub>4</sub>              | 1.4023E+01    | 5.755E-03 | 2.169E+10              | 1.3966E+01    | 5.765E-03 | 2.172E+10              | 0.000 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s5g <sup>3</sup> G <sub>4</sub>              | 1.4271E+01    | 5.740E-04 | 2.089E+09              | 1.4212E+01    | 5.735E-04 | 2.086E+09              | 0.000 |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s5g <sup>3</sup> G <sub>4</sub>              | 1.4281E+01    | 5.352E-05 | 1.945E+08              | 1.4222E+01    | 5.388E-05 | 1.957E+08              | 0.000 |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s5g <sup>3</sup> G <sub>4</sub>              | 1.0444E+03    | 2.420E-08 | 1.645E+01              | 1.0513E+03    | 2.342E-08 | 1.557E+01              | 0.002 |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s5g <sup>3</sup> G <sub>4</sub>              | 3.0779E+03    | 9.602E-11 | 7.512E-03              | 3.1417E+03    | 8.912E-11 | 6.635E-03              | 0.001 |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s5g <sup>3</sup> G <sub>4</sub>              | 3.3519E+03    | 7.054E-12 | 4.653E-04              |               |           |                        | 0.014 |
| 1s2s <sup>3</sup> S <sub>1</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.4401E+00    | 2.205E-11 | 1.013E+04              | 1.4340E+00    | 5.275E-14 | 2.423E+01              | 0.632 |
| 1s3s <sup>3</sup> S <sub>1</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 4.2561E+00    | 6.131E-09 | 3.225E+05              |               |           |                        | 0.019 |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 4.4791E+00    | 6.989E-04 | 3.319E+10              | 4.4603E+00    | 7.065E-04 | 3.355E+10              | 0.000 |
| 1s3d <sup>3</sup> D <sub>1</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 4.4815E+00    | 4.174E-03 | 1.980E+11              | 4.4627E+00    | 4.206E-03 | 1.995E+11              | 0.000 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 4.5386E+00    | 7.882E-05 | 3.646E+09              | 4.5194E+00    | 7.892E-05 | 3.651E+09              | 0.000 |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 4.5409E+00    | 4.695E-04 | 2.170E+10              | 4.5217E+00    | 4.687E-04 | 2.165E+10              | 0.000 |
| 1s4s <sup>3</sup> S <sub>1</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.3121E+01    | 9.510E-09 | 5.263E+04              |               |           |                        | 0.006 |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.4022E+01    | 6.457E-04 | 3.129E+09              | 1.3965E+01    | 6.475E-04 | 3.137E+09              | 0.000 |
| 1s4d <sup>3</sup> D <sub>1</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.4031E+01    | 3.837E-03 | 1.857E+10              | 1.3974E+01    | 3.841E-03 | 1.858E+10              | 0.000 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.4269E+01    | 6.912E-05 | 3.235E+08              | 1.4210E+01    | 6.907E-05 | 3.231E+08              | 0.000 |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.4280E+01    | 4.090E-04 | 1.912E+09              | 1.4221E+01    | 4.079E-04 | 1.905E+09              | 0.000 |
| 1s5s <sup>3</sup> S <sub>1</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 2.8921E+02    | 1.975E-12 | 2.250E-02              | 2.8822E+02    | 1.905E-12 | 2.167E-02              | 0.069 |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.0362E+03    | 2.785E-09 | 2.471E+00              | 1.0430E+03    | 2.697E-09 | 2.342E+00              | 0.001 |
| 1s5d <sup>3</sup> D <sub>1</sub>              | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.0632E+03    | 1.531E-08 | 1.291E+01              | 1.0701E+03    | 1.482E-08 | 1.222E+01              | 0.002 |

(continued on next page)

Table 4 (continued)

| Lower  | Upper  | GRASP2K       |           |                      | FAC           |           |                      | dT    |
|--|--|---------------|-----------|----------------------|---------------|-----------|----------------------|-------|
|  |  | $\lambda$ (Å) | gf        | A (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | A (s <sup>-1</sup> ) |       |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 5g <sup>3</sup> G <sub>3</sub>              | 3.0082E+03    | 1.239E-11 | 1.304E-03            |               |           |                      | 0.004 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 5g <sup>3</sup> G <sub>3</sub>              | 3.2694E+03    | 5.703E-11 | 5.084E-03            | 3.3474E+03    | 5.238E-11 | 4.417E-03            | 0.014 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 5g <sup>3</sup> G <sub>3</sub>              | 1.3281E+05    | 1.079E-15 | 5.826E-11            |               |           |                      | 0.731 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4532E+00    | 3.021E-06 | 1.363E+09            | 1.4471E+00    | 3.966E-06 | 1.789E+09            | 0.017 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.5225E+00    | 3.106E-04 | 1.277E+11            | 1.5161E+00    | 3.258E-04 | 1.339E+11            | 0.001 |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.5291E+00    | 1.859E-03 | 7.576E+11            | 1.5227E+00    | 1.916E-03 | 7.807E+11            | 0.001 |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.2871E+00    | 1.345E-07 | 6.974E+06            | 4.2694E+00    | 4.281E-08 | 2.219E+06            | 0.026 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.4656E+00    | 4.376E-06 | 2.091E+08            | 4.4470E+00    | 3.777E-06 | 1.804E+08            | 0.001 |
| 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.4815E+00    | 2.232E-05 | 1.059E+09            | 4.4631E+00    | 2.227E-05 | 1.056E+09            | 0.002 |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.3241E+01    | 5.944E-06 | 3.231E+07            | 1.3185E+01    | 6.974E-06 | 3.790E+07            | 0.001 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.3966E+01    | 6.580E-04 | 3.215E+09            | 1.3907E+01    | 6.653E-04 | 3.250E+09            | 0.000 |
| 1s 4p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4031E+01    | 3.910E-03 | 1.892E+10            | 1.3972E+01    | 3.910E-03 | 1.892E+10            | 0.000 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4278E+01    | 1.118E-05 | 5.231E+07            | 1.4212E+01    | 1.125E-05 | 5.265E+07            | 0.000 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4278E+01    | 6.735E-05 | 3.148E+08            | 1.4218E+01    | 6.769E-05 | 3.163E+08            | 0.000 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4398E+01    | 7.046E-05 | 3.239E+08            | 1.4337E+01    | 7.063E-05 | 3.246E+08            | 0.000 |
| 1s 4f <sup>1</sup> F <sub>5</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4402E+01    | 5.838E-04 | 2.682E+09            | 1.4341E+01    | 5.847E-04 | 2.686E+09            | 0.000 |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.2151E+02    | 1.870E-09 | 1.724E+01            | 3.1987E+02    | 1.897E-09 | 1.752E+01            | 0.002 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 9.0084E+02    | 9.762E-09 | 1.146E+01            | 8.9370E+02    | 9.861E-09 | 1.166E+01            | 0.005 |
| 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.0611E+03    | 3.558E-08 | 3.011E+01            | 1.0539E+03    | 3.585E-08 | 3.049E+01            | 0.007 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.0918E+03    | 2.542E-11 | 2.534E-03            |               |           |                      | 0.013 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.2229E+03    | 1.353E-10 | 1.241E-02            | 3.2177E+03    | 1.342E-10 | 1.224E-02            | 0.002 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.0160E+05    | 4.530E-15 | 4.182E-10            |               |           |                      | 0.407 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5g <sup>3</sup> G <sub>5</sub>              | 4.5349E+00    | 8.603E-03 | 2.537E+11            | 4.5157E+00    | 8.751E-03 | 2.580E+11            | 0.000 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5g <sup>3</sup> G <sub>5</sub>              | 1.4233E+01    | 7.663E-03 | 2.294E+10            | 1.4174E+01    | 7.697E-03 | 2.303E+10            | 0.000 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 5g <sup>3</sup> G <sub>5</sub>              | 1.9545E+03    | 5.017E-09 | 7.964E-01            | 1.9786E+03    | 4.774E-09 | 7.332E-01            | 0.001 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 5g <sup>3</sup> G <sub>5</sub>              | 5.3554E+03    | 1.676E-11 | 3.544E-04            | 5.3442E+03    | 1.665E-11 | 3.506E-04            | 0.005 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 5g <sup>3</sup> G <sub>5</sub>              | 5.5804E+03    | 7.076E-13 | 1.378E-05            |               |           |                      | 0.118 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5g <sup>1</sup> G <sub>4</sub>              | 4.4754E+00    | 1.669E-07 | 6.178E+06            |               |           |                      | 0.002 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5g <sup>1</sup> G <sub>4</sub>              | 4.5348E+00    | 5.236E-04 | 1.887E+10            | 4.5156E+00    | 5.326E-04 | 1.919E+10            | 0.000 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5g <sup>1</sup> G <sub>4</sub>              | 4.5371E+00    | 6.519E-03 | 2.347E+11            | 4.5179E+00    | 6.617E-03 | 2.382E+11            | 0.000 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5g <sup>1</sup> G <sub>4</sub>              | 1.3986E+01    | 2.967E-07 | 1.124E+06            |               |           |                      | 0.001 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5g <sup>1</sup> G <sub>4</sub>              | 1.4232E+01    | 4.665E-04 | 1.707E+09            | 1.4173E+01    | 4.686E-04 | 1.714E+09            | 0.000 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5g <sup>1</sup> G <sub>4</sub>              | 1.4242E+01    | 5.798E-03 | 2.119E+10            | 1.4183E+01    | 5.817E-03 | 2.125E+10            | 0.000 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 5g <sup>1</sup> G <sub>4</sub>              | 8.6941E+02    | 2.714E-12 | 2.661E-03            | 8.7388E+02    | 2.967E-12 | 2.855E-03            | 0.022 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 5g <sup>1</sup> G <sub>4</sub>              | 1.9321E+03    | 3.162E-10 | 6.278E-02            | 1.9554E+03    | 3.010E-10 | 5.784E-02            | 0.001 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 5g <sup>1</sup> G <sub>4</sub>              | 2.0366E+03    | 3.358E-09 | 6.000E-01            | 2.0649E+03    | 3.180E-09 | 5.481E-01            | 0.007 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 5g <sup>1</sup> G <sub>4</sub>              | 5.1900E+03    | 1.321E-12 | 3.636E-05            |               |           |                      | 0.045 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 5g <sup>1</sup> G <sub>4</sub>              | 5.4011E+03    | 1.294E-11 | 3.288E-04            | 5.3899E+03    | 1.285E-11 | 3.251E-04            | 0.008 |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 5g <sup>1</sup> G <sub>4</sub>              | 1.6804E+05    | 4.412E-16 | 1.158E-11            |               |           |                      | 0.888 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 1.3696E+00    | 2.953E-10 | 3.501E+05            |               |           |                      | 0.955 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 3.6936E+00    | 9.398E-11 | 1.532E+04            |               |           |                      | 0.701 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 3.8604E+00    | 1.286E-05 | 1.919E+09            | 3.8445E+00    | 1.300E-05 | 1.939E+09            | 0.008 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 3.8622E+00    | 1.310E-05 | 1.952E+09            | 3.8463E+00    | 1.290E-05 | 1.923E+09            | 0.012 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 3.9045E+00    | 3.054E-05 | 4.453E+09            | 3.8883E+00    | 3.041E-05 | 4.435E+09            | 0.008 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 3.9062E+00    | 8.750E-06 | 1.275E+09            | 3.8900E+00    | 8.603E-06 | 1.253E+09            | 0.010 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 8.9291E+00    | 9.105E-10 | 2.539E+04            |               |           |                      | 0.189 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 9.3373E+00    | 4.394E-05 | 1.121E+09            | 9.3006E+00    | 4.402E-05 | 1.122E+09            | 0.001 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 9.3415E+00    | 4.405E-05 | 1.122E+09            | 9.3048E+00    | 4.355E-05 | 1.109E+09            | 0.004 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 9.4463E+00    | 1.037E-04 | 2.583E+09            | 9.4089E+00    | 1.029E-04 | 2.563E+09            | 0.002 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 9.4508E+00    | 2.923E-05 | 7.276E+08            | 9.4135E+00    | 2.897E-05 | 7.208E+08            | 0.003 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 2.5485E+01    | 4.451E-09 | 1.524E+04            |               |           |                      | 0.034 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 2.7214E+01    | 1.771E-04 | 5.316E+08            | 2.7122E+01    | 1.754E-04 | 5.256E+08            | 0.001 |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 2.7232E+01    | 1.769E-04 | 5.303E+08            | 2.7140E+01    | 1.731E-04 | 5.181E+08            | 0.002 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 2.7691E+01    | 4.244E-04 | 1.231E+09            | 2.7596E+01    | 4.178E-04 | 1.209E+09            | 0.001 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 2.7711E+01    | 1.192E-04 | 3.450E+08            | 2.7617E+01    | 1.172E-04 | 3.389E+08            | 0.002 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 6s <sup>3</sup> S <sub>1</sub>              | 2.7948E+01    | 1.280E-10 | 3.644E+02            |               |           |                      | 0.022 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.3810E+00    | 1.717E-07 | 2.002E+08            | 1.3752E+00    | 2.325E-07 | 2.710E+08            | 0.030 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.4434E+00    | 2.896E-05 | 3.090E+10            | 1.4374E+00    | 2.858E-05 | 3.050E+10            | 0.007 |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.4493E+00    | 2.557E-05 | 2.706E+10            | 1.4433E+00    | 2.438E-05 | 2.580E+10            | 0.000 |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 3.7142E+00    | 3.248E-07 | 5.236E+07            | 3.6989E+00    | 4.474E-07 | 7.210E+07            | 0.004 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 3.8474E+00    | 6.170E-05 | 9.267E+09            | 3.8314E+00    | 6.176E-05 | 9.275E+09            | 0.006 |
| 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 3.8593E+00    | 5.498E-05 | 8.208E+09            | 3.8434E+00    | 5.307E-05 | 7.920E+09            | 0.005 |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 8.9685E+00    | 6.588E-07 | 1.821E+07            | 8.9310E+00    | 8.937E-07 | 2.470E+07            | 0.001 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 9.2954E+00    | 1.314E-04 | 3.381E+09            | 9.2564E+00    | 1.331E-04 | 3.424E+09            | 0.001 |
| 1s 4p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 9.3241E+00    | 1.177E-04 | 3.010E+09            | 9.2853E+00    | 1.149E-04 | 2.939E+09            | 0.000 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 9.4302E+00    | 2.483E-05 | 6.209E+08            | 9.3908E+00    | 2.464E-05 | 6.161E+08            | 0.001 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 9.4324E+00    | 7.599E-06 | 1.899E+08            | 9.3930E+00    | 7.633E-06 | 1.907E+08            | 0.001 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 9.4866E+00    | 4.042E-08 | 9.986E+05            | 9.4468E+00    | 5.810E-08 | 1.435E+06            | 0.005 |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 2.5582E+01    | 2.016E-06 | 6.850E+06            | 2.5476E+01    | 2.721E-06 | 9.243E+06            | 0.000 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 2.6962E+01    | 4.480E-04 | 1.370E+09            | 2.6849E+01    | 4.561E-04 | 1.395E+09            | 0.000 |
| 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 2.7084E+01    | 4.051E-04 | 1.228E+09            | 2.6972E+01    | 3.966E-04 | 1.202E+09            | 0.000 |

(continued on next page)

Table 4 (continued)

| Lower          | Upper          | GRASP2K       |           |                  | FAC           |           |                  | dT    |
|----------------|----------------|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|                |                | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) |       |
| 1s5f $^3F_3^o$ | 1s6p $^3P_1^o$ | 2.7546E+01    | 1.673E-04 | 4.903E+08        | 2.7434E+01    | 1.664E-04 | 4.875E+08        | 0.000 |
| 1s5f $^3F_2^o$ | 1s6p $^3P_0^o$ | 2.7556E+01    | 5.120E-05 | 1.499E+08        | 2.7444E+01    | 5.132E-05 | 1.502E+08        | 0.000 |
| 1s5f $^1F_3^o$ | 1s6p $^3P_1^o$ | 2.7794E+01    | 2.736E-07 | 7.876E+05        | 2.7680E+01    | 3.570E-07 | 1.027E+06        | 0.000 |
| 1s3d $^3D_2$   | 1s6s $^1S_0$   | 3.8573E+00    | 8.512E-06 | 3.816E+09        | 3.8418E+00    | 8.554E-06 | 3.833E+09        | 0.004 |
| 1s3d $^1D_2$   | 1s6s $^1S_0$   | 3.9030E+00    | 1.339E-05 | 5.863E+09        | 3.8873E+00    | 1.312E-05 | 5.742E+09        | 0.012 |
| 1s4d $^3D_2$   | 1s6s $^1S_0$   | 9.3190E+00    | 2.867E-05 | 2.202E+09        | 9.2851E+00    | 2.880E-05 | 2.209E+09        | 0.002 |
| 1s4d $^1D_2$   | 1s6s $^1S_0$   | 9.4321E+00    | 4.483E-05 | 3.361E+09        | 9.3976E+00    | 4.468E-05 | 3.346E+09        | 0.002 |
| 1s5d $^3D_2$   | 1s6s $^1S_0$   | 2.7060E+01    | 1.136E-04 | 1.034E+09        | 2.6991E+01    | 1.153E-04 | 1.047E+09        | 0.001 |
| 1s5d $^1D_2$   | 1s6s $^1S_0$   | 2.7551E+01    | 1.808E-04 | 1.589E+09        | 2.7480E+01    | 1.831E-04 | 1.604E+09        | 0.000 |
| 1s2p $^3P_2^o$ | 1s6p $^3P_0^o$ | 1.4434E+00    | 1.839E-05 | 5.887E+10        | 1.4374E+00    | 1.782E-05 | 5.703E+10        | 0.005 |
| 1s3p $^3P_0^o$ | 1s6p $^3P_0^o$ | 3.8472E+00    | 3.921E-05 | 1.767E+10        | 3.8320E+00    | 3.856E-05 | 1.736E+10        | 0.006 |
| 1s4p $^3P_2^o$ | 1s6p $^3P_0^o$ | 9.2942E+00    | 8.350E-05 | 6.448E+09        | 9.2596E+00    | 8.326E-05 | 6.422E+09        | 0.001 |
| 1s4p $^3F_2^o$ | 1s6p $^3P_0^o$ | 9.4312E+00    | 1.079E-05 | 8.090E+08        | 9.3964E+00    | 1.073E-05 | 8.042E+08        | 0.001 |
| 1s5p $^3P_2^o$ | 1s6p $^3P_0^o$ | 2.6952E+01    | 2.844E-04 | 2.612E+09        | 2.6876E+01    | 2.863E-04 | 2.621E+09        | 0.000 |
| 1s5f $^3F_2^o$ | 1s6p $^3P_0^o$ | 2.7545E+01    | 7.268E-05 | 6.390E+08        | 2.7473E+01    | 7.228E-05 | 6.334E+08        | 0.000 |
| 1s2p $^3P_1^o$ | 1s6p $^3P_2^o$ | 1.3788E+00    | 3.430E-05 | 2.407E+10        | 1.3731E+00    | 3.466E-05 | 2.432E+10        | 0.006 |
| 1s2p $^3P_0^o$ | 1s6p $^3P_2^o$ | 1.3797E+00    | 2.139E-05 | 1.499E+10        | 1.3739E+00    | 2.180E-05 | 1.528E+10        | 0.002 |
| 1s2p $^3P_2^o$ | 1s6p $^3P_2^o$ | 1.4410E+00    | 3.551E-05 | 2.281E+10        | 1.4350E+00    | 3.534E-05 | 2.270E+10        | 0.006 |
| 1s2p $^1P_1^o$ | 1s6p $^3P_2^o$ | 1.4469E+00    | 1.342E-05 | 8.551E+09        | 1.4409E+00    | 1.332E-05 | 8.486E+09        | 0.000 |
| 1s3p $^3P_0^o$ | 1s6p $^3P_2^o$ | 3.6983E+00    | 6.924E-05 | 6.753E+09        | 3.6831E+00    | 6.933E-05 | 6.760E+09        | 0.007 |
| 1s3p $^3P_1^o$ | 1s6p $^3P_2^o$ | 3.7000E+00    | 4.378E-05 | 4.266E+09        | 3.6848E+00    | 4.378E-05 | 4.265E+09        | 0.006 |
| 1s3p $^3P_2^o$ | 1s6p $^3P_2^o$ | 3.8304E+00    | 7.355E-05 | 6.688E+09        | 3.8145E+00    | 7.319E-05 | 6.653E+09        | 0.007 |
| 1s3p $^1P_1^o$ | 1s6p $^3P_2^o$ | 3.8422E+00    | 2.807E-05 | 2.536E+09        | 3.8264E+00    | 2.789E-05 | 2.520E+09        | 0.005 |
| 1s4p $^3P_1^o$ | 1s6p $^3P_2^o$ | 8.8767E+00    | 1.362E-04 | 2.306E+09        | 8.8397E+00    | 1.369E-04 | 2.318E+09        | 0.001 |
| 1s4p $^3P_0^o$ | 1s6p $^3P_2^o$ | 8.8807E+00    | 8.680E-05 | 1.465E+09        | 8.8435E+00    | 8.652E-05 | 1.463E+09        | 0.001 |
| 1s4p $^3P_2^o$ | 1s6p $^3P_2^o$ | 9.1968E+00    | 1.504E-04 | 2.372E+09        | 9.1583E+00    | 1.507E-04 | 2.376E+09        | 0.001 |
| 1s4p $^1P_1^o$ | 1s6p $^3P_2^o$ | 9.2248E+00    | 5.772E-05 | 9.049E+08        | 9.1865E+00    | 5.772E-05 | 9.047E+08        | 0.000 |
| 1s4f $^3F_3^o$ | 1s6p $^3P_2^o$ | 9.3286E+00    | 5.477E-06 | 8.396E+07        | 9.2898E+00    | 5.452E-06 | 8.357E+07        | 0.001 |
| 1s4f $^3F_2^o$ | 1s6p $^3P_2^o$ | 9.3309E+00    | 1.379E-06 | 2.113E+07        | 9.2920E+00    | 1.357E-06 | 2.079E+07        | 0.002 |
| 1s4f $^3F_4^o$ | 1s6p $^3P_2^o$ | 9.3822E+00    | 3.795E-05 | 5.752E+08        | 9.3430E+00    | 3.754E-05 | 5.688E+08        | 0.000 |
| 1s4f $^1F_3^o$ | 1s6p $^3P_2^o$ | 9.3838E+00    | 4.233E-06 | 6.413E+07        | 9.3446E+00    | 4.189E-06 | 6.346E+07        | 0.000 |
| 1s5p $^3P_0^o$ | 1s6p $^3P_2^o$ | 2.4849E+01    | 8.840E-04 | 8.296E+08        | 2.4746E+01    | 8.860E-04 | 8.339E+08        | 0.000 |
| 1s5p $^3P_2^o$ | 1s6p $^3P_2^o$ | 2.4864E+01    | 2.449E-04 | 5.284E+08        | 2.4761E+01    | 2.428E-04 | 5.240E+08        | 0.000 |
| 1s5p $^1P_1^o$ | 1s6p $^3P_2^o$ | 2.6148E+01    | 4.645E-04 | 9.063E+08        | 2.6040E+01    | 4.663E-04 | 9.096E+08        | 0.000 |
| 1s5f $^3F_2^o$ | 1s6p $^3P_2^o$ | 2.6264E+01    | 1.798E-04 | 3.477E+08        | 2.6156E+01    | 1.793E-04 | 3.466E+08        | 0.000 |
| 1s5f $^3F_4^o$ | 1s6p $^3P_2^o$ | 2.6698E+01    | 3.580E-05 | 6.700E+07        | 2.6590E+01    | 3.549E-05 | 6.640E+07        | 0.000 |
| 1s5f $^3F_2^o$ | 1s6p $^3P_2^o$ | 2.6707E+01    | 9.011E-06 | 1.685E+07        | 2.6599E+01    | 8.838E-06 | 1.652E+07        | 0.000 |
| 1s5f $^3F_4^o$ | 1s6p $^3P_2^o$ | 2.6923E+01    | 2.493E-04 | 4.588E+08        | 2.6814E+01    | 2.461E-04 | 4.528E+08        | 0.000 |
| 1s5f $^1F_3^o$ | 1s6p $^3P_2^o$ | 2.6930E+01    | 2.780E-05 | 5.113E+07        | 2.6821E+01    | 2.745E-05 | 5.048E+07        | 0.000 |
| 1s6p $^3P_0^o$ | 1s6p $^3P_2^o$ | 8.6654E+02    | 1.895E-07 | 3.367E+02        | 8.6410E+02    | 1.920E-07 | 3.402E+02        | 0.003 |
| 1s6p $^3P_2^o$ | 1s6p $^3P_2^o$ | 8.7749E+02    | 1.161E-07 | 2.012E+02        | 8.3677E+02    | 1.322E-07 | 2.498E+02        | 0.003 |
| 1s2 $^1S_0$    | 1s6d $^3D_2$   | 3.1620E-01    | 1.394E-04 | 1.859E+12        | 3.1497E-01    | 1.398E-04 | 1.864E+12        | 0.002 |
| 1s2s $^3S_1$   | 1s6d $^3D_2$   | 1.3669E+00    | 1.366E-05 | 9.753E+09        | 1.3610E+00    | 1.209E-05 | 8.637E+09        | 0.007 |
| 1s2s $^1S_0$   | 1s6d $^3D_2$   | 1.3798E+00    | 7.380E-06 | 5.171E+09        | 1.3741E+00    | 7.407E-06 | 5.189E+09        | 0.004 |
| 1s3s $^3S_1$   | 1s6d $^3D_2$   | 3.6741E+00    | 8.920E-05 | 8.815E+09        | 3.6587E+00    | 8.805E-05 | 8.701E+09        | 0.004 |
| 1s3s $^1S_0$   | 1s6d $^3D_2$   | 3.6988E+00    | 5.586E-05 | 5.447E+09        | 3.6835E+00    | 5.475E-05 | 5.337E+09        | 0.013 |
| 1s3d $^3D_2$   | 1s6d $^3D_2$   | 3.8391E+00    | 3.737E-05 | 3.822E+09        | 3.713E-05     | 3.822E+09 | 3.713E+09        | 0.003 |
| 1s3d $^3D_1$   | 1s6d $^3D_2$   | 3.8409E+00    | 1.647E-05 | 1.489E+09        | 3.8245E+00    | 1.647E-05 | 1.490E+09        | 0.007 |
| 1s3d $^3D_3$   | 1s6d $^3D_2$   | 3.8827E+00    | 1.797E-05 | 1.590E+09        | 3.8661E+00    | 1.793E-05 | 1.587E+09        | 0.004 |
| 1s3d $^1D_2$   | 1s6d $^3D_2$   | 3.8844E+00    | 4.392E-06 | 3.883E+08        | 3.8678E+00    | 4.140E-06 | 3.661E+08        | 0.010 |
| 1s4s $^3S_1$   | 1s6d $^3D_2$   | 8.8160E+00    | 2.394E-04 | 4.109E+09        | 8.7783E+00    | 2.410E-04 | 4.138E+09        | 0.003 |
| 1s4s $^1S_0$   | 1s6d $^3D_2$   | 8.8733E+00    | 1.533E-04 | 2.598E+09        | 8.8358E+00    | 1.502E-04 | 2.545E+09        | 0.007 |
| 1s4d $^3D_2$   | 1s6d $^3D_2$   | 9.2136E+00    | 1.112E-04 | 1.748E+09        | 9.1745E+00    | 1.107E-04 | 1.740E+09        | 0.001 |
| 1s4d $^3D_1$   | 1s6d $^3D_2$   | 9.2178E+00    | 4.892E-05 | 7.682E+08        | 9.1786E+00    | 4.923E-05 | 7.730E+08        | 0.002 |
| 1s4d $^3D_3$   | 1s6d $^3D_2$   | 9.3198E+00    | 5.465E-05 | 8.393E+08        | 9.2799E+00    | 5.491E-05 | 8.435E+08        | 0.001 |
| 1s4d $^1D_2$   | 1s6d $^3D_2$   | 9.3242E+00    | 1.339E-05 | 2.054E+08        | 9.2843E+00    | 1.284E-05 | 1.970E+08        | 0.003 |
| 1s5s $^3S_1$   | 1s6d $^3D_2$   | 2.4585E+01    | 7.948E-04 | 1.754E+09        | 2.4475E+01    | 8.142E-04 | 1.798E+09        | 0.002 |
| 1s5s $^1S_0$   | 1s6d $^3D_2$   | 2.4809E+01    | 5.211E-04 | 1.130E+09        | 2.4699E+01    | 5.045E-04 | 1.094E+09        | 0.001 |
| 1s5d $^3D_2$   | 1s6d $^3D_2$   | 2.6190E+01    | 4.075E-04 | 7.925E+08        | 2.6077E+01    | 4.066E-04 | 7.910E+08        | 0.000 |
| 1s5d $^3D_1$   | 1s6d $^3D_2$   | 2.6207E+01    | 1.795E-04 | 3.486E+08        | 2.6094E+01    | 1.806E-04 | 3.509E+08        | 0.001 |
| 1s5d $^3D_3$   | 1s6d $^3D_2$   | 2.6631E+01    | 2.076E-04 | 3.904E+08        | 2.6515E+01    | 2.095E-04 | 3.941E+08        | 0.000 |
| 1s5d $^1D_2$   | 1s6d $^3D_2$   | 2.6650E+01    | 5.102E-05 | 9.582E+07        | 2.6534E+01    | 4.929E-05 | 9.260E+07        | 0.001 |
| 1s5g $^3G_4$   | 1s6d $^3D_2$   | 2.6864E+01    | 6.067E-05 | 1.121E+08        | 2.6740E+01    | 6.071E-05 | 1.123E+08        | 0.000 |
| 1s5g $^3G_3$   | 1s6d $^3D_2$   | 2.6869E+01    | 6.827E-06 | 1.262E+07        | 2.6746E+01    | 6.882E-06 | 1.272E+07        | 0.000 |
| 1s5g $^1G_4$   | 1s6d $^3D_2$   | 2.7003E+01    | 4.401E-09 | 8.052E+03        |               |           |                  | 0.005 |
| 1s6s $^3S_1$   | 1s6d $^3D_2$   | 6.9582E+02    | 3.295E-07 | 9.080E+02        | 6.7673E+02    | 3.578E-07 | 1.033E+03        | 0.023 |
| 1s6s $^1S_0$   | 1s6d $^3D_2$   | 8.1469E+02    | 1.337E-07 | 2.688E+02        | 7.7023E+02    | 1.541E-07 | 3.436E+02        | 0.058 |
| 1s2p $^3P_0^o$ | 1s6p $^1P_1^o$ | 1.3786E+00    | 3.042E-05 | 3.559E+10        | 1.3729E+00    | 3.065E-05 | 3.585E+10        | 0.000 |
| 1s2p $^3P_2^o$ | 1s6p $^1P_1^o$ | 1.4408E+00    | 1.370E-05 | 1.468E+10        | 1.4348E+00    | 1.329E-05 | 1.423E+10        | 0.002 |
| 1s2p $^1P_1^o$ | 1s6p $^1P_1^o$ | 1.4467E+00    | 1.830E-05 | 1.952E+10        | 1.4407E+00    | 1.863E-05 | 1.979E+10        | 0.007 |
| 1s3p $^3P_0^o$ | 1s6p $^1P_1^o$ | 3.6970E+00    | 6.212E-05 | 1.010E+10        | 3.6819E+00    | 6.180E-05 | 1.005E+10        | 0.006 |

(continued on next page)

Table 4 (continued)

| Lower  | Upper  | GRASP2K       |           |                      | FAC           |            |                      | dT    |
|--|--|---------------|-----------|----------------------|---------------|------------|----------------------|-------|
|  |  | $\lambda$ (Å) | gf        | A (s <sup>-1</sup> ) | $\lambda$ (Å) | gf         | A (s <sup>-1</sup> ) |       |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.8290E+00    | 2.847E-05 | 4.318E+09            | 3.8133E+00    | 2.744E-05  | 4.160E+09            | 0.005 |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.8407E+00    | 3.813E-05 | 5.747E+09            | 3.8251E+00    | 3.860E-05  | 5.816E+09            | 0.003 |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 8.8691E+00    | 1.223E-04 | 3.458E+09            | 8.8329E+00    | 1.223E-04  | 3.455E+09            | 0.001 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 9.1886E+00    | 5.804E-05 | 1.529E+09            | 9.1511E+00    | 5.631E-05  | 1.482E+09            | 0.001 |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 9.2166E+00    | 7.802E-05 | 2.042E+09            | 9.1793E+00    | 7.959E-05  | 2.082E+09            | 0.000 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 9.3203E+00    | 1.284E-06 | 3.286E+07            | 9.2824E+00    | 1.452E-06  | 3.715E+07            | 0.003 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 9.3225E+00    | 2.872E-06 | 7.347E+07            | 9.2846E+00    | 2.760E-06  | 7.058E+07            | 0.001 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 9.3754E+00    | 2.499E-05 | 6.322E+08            | 9.3371E+00    | 2.499E-05  | 6.319E+08            | 0.001 |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.4789E+01    | 3.429E-04 | 1.241E+09            | 2.4694E+01    | 3.435E-04  | 1.241E+09            | 0.000 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.6083E+01    | 1.778E-04 | 5.810E+08            | 2.5981E+01    | 1.727E-04  | 5.643E+08            | 0.000 |
| 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.6197E+01    | 2.407E-04 | 7.798E+08            | 2.6097E+01    | 2.471E-04  | 8.000E+08            | 0.000 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.6629E+01    | 8.342E-06 | 2.616E+07            | 2.6529E+01    | 9.671E-06  | 3.029E+07            | 0.000 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.6638E+01    | 1.871E-05 | 5.863E+07            | 2.6539E+01    | 1.789E-05  | 5.600E+07            | 0.000 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.6860E+01    | 1.637E-04 | 5.046E+08            | 2.6759E+01    | 1.646E-04  | 5.067E+08            | 0.000 |
| 1s 6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.9973E+02    | 2.175E-07 | 7.560E+02            | 8.0416E+02    | 2.068E-07  | 7.051E+02            | 0.003 |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.0374E+04    | 4.887E-11 | 1.010E-03            |               |            |                      | 0.005 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 1.3668E+00    | 1.350E-05 | 1.607E+10            | 1.3611E+00    | 1.183E-05  | 1.408E+10            | 0.004 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 3.6740E+00    | 8.868E-05 | 1.461E+10            | 3.6587E+00    | 8.652E-05  | 1.424E+10            | 0.006 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 3.8389E+00    | 1.627E-05 | 2.454E+09            | 3.8228E+00    | 1.618E-05  | 2.441E+09            | 0.005 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 3.8407E+00    | 1.611E-05 | 2.429E+09            | 3.8246E+00    | 1.597E-05  | 2.408E+09            | 0.005 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 3.8825E+00    | 2.940E-06 | 4.336E+08            | 3.8625E+00    | 2.932E-06  | 4.324E+08            | 0.006 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 3.8842E+00    | 1.041E-05 | 1.534E+09            | 3.8678E+00    | 1.015E-05  | 1.496E+09            | 0.005 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 8.8149E+00    | 2.379E-04 | 6.807E+09            | 8.7785E+00    | 2.371E-04  | 6.783E+09            | 0.004 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 9.2124E+00    | 4.864E-05 | 1.274E+09            | 9.1748E+00    | 4.850E-05  | 1.270E+09            | 0.002 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 9.2166E+00    | 4.770E-05 | 1.249E+09            | 9.1789E+00    | 4.769E-05  | 1.247E+09            | 0.002 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 9.3186E+00    | 8.922E-06 | 2.284E+08            | 9.2802E+00    | 8.978E-06  | 2.298E+08            | 0.002 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 9.3230E+00    | 3.131E-05 | 8.010E+08            | 9.2846E+00    | 3.094E-05  | 7.914E+08            | 0.001 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.4577E+01    | 7.884E-04 | 2.902E+09            | 2.4477E+01    | 8.016E-04  | 2.949E+09            | 0.003 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6180E+01    | 1.783E-04 | 5.784E+08            | 2.6079E+01    | 1.784E-04  | 5.784E+08            | 0.001 |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6197E+01    | 1.744E-04 | 5.652E+08            | 2.6096E+01    | 1.750E-04  | 5.667E+08            | 0.000 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6621E+01    | 3.384E-05 | 1.062E+08            | 2.6517E+01    | 3.426E-05  | 1.074E+08            | 0.001 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6640E+01    | 1.185E-04 | 3.712E+08            | 2.6536E+01    | 1.178E-04  | 3.688E+08            | 0.000 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6859E+01    | 4.044E-05 | 1.246E+08            | 2.6748E+01    | 4.053E-05  | 1.248E+08            | 0.000 |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 6.8911E+02    | 3.374E-07 | 1.580E+03            | 6.7829E+02    | 3.486E-07  | 1.670E+03            | 0.016 |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>1</sub>              | 7.1428E+04    | 1.468E-13 | 6.396E-08            |               |            |                      | 0.467 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 1.3662E+00    | 4.040E-05 | 2.062E+10            | 1.3604E+00    | 3.740E-05  | 1.909E+10            | 0.001 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 3.6692E+00    | 2.239E-04 | 1.585E+10            | 3.6538E+00    | 2.222E-04  | 1.572E+10            | 0.005 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 3.8337E+00    | 1.908E-05 | 1.237E+09            | 3.8174E+00    | 1.928E-05  | 1.250E+09            | 0.004 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 3.8355E+00    | 3.117E-06 | 2.019E+08            | 3.8192E+00    | 3.126E-06  | 2.025E+08            | 0.005 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 3.8772E+00    | 7.363E-05 | 4.667E+09            | 3.8607E+00    | 7.364E-05  | 4.668E+09            | 0.004 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 3.8789E+00    | 1.225E-05 | 7.761E+08            | 3.8624E+00    | 1.214E-05  | 7.694E+08            | 0.005 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 8.7877E+00    | 5.723E-04 | 7.062E+09            | 8.7503E+00    | 5.746E-04  | 7.090E+09            | 0.004 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.1827E+00    | 5.597E-05 | 6.325E+08            | 9.1440E+00    | 5.630E-05  | 6.362E+08            | 0.001 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.1868E+00    | 9.054E-06 | 1.022E+08            | 9.1480E+00    | 9.077E-06  | 1.024E+08            | 0.001 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.2881E+00    | 2.193E-04 | 2.423E+09            | 9.2486E+00    | 2.195E-04  | 2.424E+09            | 0.001 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.2925E+00    | 3.614E-05 | 3.988E+08            | 9.2530E+00    | 3.603E-05  | 3.976E+08            | 0.002 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.4366E+01    | 1.808E-03 | 2.903E+09            | 2.4258E+01    | 1.840E-03  | 2.955E+09            | 0.002 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.5941E+01    | 1.985E-04 | 2.811E+08            | 2.5832E+01    | 1.994E-04  | 2.823E+08            | 0.000 |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.5958E+01    | 3.202E-05 | 4.528E+07            | 2.5848E+01    | 3.209E-05  | 4.538E+07            | 0.000 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.6374E+01    | 8.038E-04 | 1.101E+09            | 2.6261E+01    | 8.056E-04  | 1.103E+09            | 0.000 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.6393E+01    | 1.321E-04 | 1.808E+08            | 2.6280E+01    | 1.319E-04  | 1.804E+08            | 0.000 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.6602E+01    | 5.844E-06 | 7.869E+06            | 2.6482E+01    | 5.860E-06  | 7.894E+06            | 0.000 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.6608E+01    | 7.044E-07 | 9.481E+05            | 2.6488E+01    | 7.042E-07  | 9.483E+05            | 0.000 |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.6735E+01    | 7.898E-05 | 1.053E+08            | 2.6614E+01    | 7.896E-05  | 1.053E+08            | 0.000 |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.6739E+01    | 4.809E-06 | 6.409E+06            | 2.6619E+01    | 4.803E-06  | 6.404E+06            | 0.000 |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 5.5466E+02    | 1.528E-06 | 4.732E+03            | 5.4291E+02    | 1.608E-06  | 5.157E+03            | 0.017 |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.7340E+03    | 3.001E-09 | 3.826E-01            |               |            |                      | 0.003 |
| 1s 6d <sup>3</sup> D <sub>1</sub>              | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.8428E+03    | 4.330E-10 | 5.106E-02            |               |            |                      | 0.008 |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.3779E+00    | 9.054E-04 | 4.544E+11            | 1.3722E+00    | 9.227E-04  | 4.630E+11            | 0.001 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4401E+00    | 2.384E-04 | 1.095E+11            | 1.4340E+00    | 2.412E-04  | 1.108E+11            | 0.001 |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4460E+00    | 5.807E-05 | 2.646E+10            | 1.4400E+00    | 5.515E-05  | 2.513E+10            | 0.001 |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.6921E+00    | 3.684E-06 | 2.575E+08            | 3.6768E+00    | 4.342E-06  | 3.035E+08            | 0.024 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.8237E+00    | 6.010E-06 | 3.917E+08            | 3.8077E+00    | 6.772E-06  | 4.413E+08            | 0.007 |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.8355E+00    | 1.590E-06 | 1.030E+08            | 3.8195E+00    | 1.275E-06  | 8.258E+07            | 0.008 |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 8.8410E+00    | 3.538E-04 | 4.314E+09            | 8.8032E+00    | 3.5117E-04 | 4.288E+09            | 0.000 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 9.1585E+00    | 6.227E-05 | 7.074E+08            | 9.1192E+00    | 6.110E-05  | 6.942E+08            | 0.000 |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 9.1863E+00    | 1.425E-05 | 1.609E+08            | 9.1472E+00    | 1.460E-05  | 1.649E+08            | 0.000 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 9.2892E+00    | 1.116E-04 | 1.233E+09            | 9.2496E+00    | 1.113E-04  | 1.229E+09            | 0.001 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 9.2914E+00    | 1.854E-05 | 2.047E+08            | 9.2518E+00    | 1.857E-05  | 2.050E+08            | 0.001 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 9.3423E+00    | 1.905E-05 | 2.080E+08            | 9.3023E+00    | 1.898E-05  | 2.072E+08            | 0.001 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 9.3440E+00    | 2.289E-06 | 2.499E+07            | 9.3039E+00    | 2.187E-06  | 2.387E+07            | 0.001 |

(continued on next page)

Table 4 (continued)

| Lower   | Upper   | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|---|---|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|   |   | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.4571E+01    | 2.580E-03 | 4.072E+09              | 2.4463E+01    | 2.587E-03 | 4.085E+09              | 0.000 |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.5841E+01    | 6.351E-04 | 9.063E+08              | 2.5726E+01    | 6.431E-04 | 9.181E+08              | 0.000 |
| 1s5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.5954E+01    | 1.498E-04 | 2.119E+08              | 2.5839E+01    | 1.432E-04 | 2.027E+08              | 0.000 |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.6377E+01    | 6.346E-04 | 8.692E+08              | 2.6263E+01    | 6.351E-04 | 8.700E+08              | 0.000 |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.6386E+01    | 1.056E-04 | 1.445E+08              | 2.6272E+01    | 1.060E-04 | 1.451E+08              | 0.000 |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.6597E+01    | 1.106E-04 | 1.490E+08              | 2.6482E+01    | 1.110E-04 | 1.495E+08              | 0.000 |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.6604E+01    | 1.332E-05 | 1.793E+07              | 2.6488E+01    | 1.282E-05 | 1.727E+07              | 0.000 |
| 1s6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 6.2157E+02    | 8.428E-07 | 2.079E+03              | 6.1517E+02    | 8.540E-07 | 2.132E+03              | 0.002 |
| 1s6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.1987E+03    | 4.683E-09 | 9.231E-01              | 2.1353E+03    | 5.072E-09 | 1.051E+00              | 0.014 |
| 1s6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.7901E+03    | 5.400E-10 | 6.610E-02              |               |           |                        | 0.014 |
| 1s2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3779E+00    | 2.777E-04 | 1.951E+11              | 1.3722E+00    | 2.854E-04 | 2.005E+11              | 0.001 |
| 1s2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3788E+00    | 3.955E-04 | 2.775E+11              | 1.3730E+00    | 4.024E-04 | 2.823E+11              | 0.000 |
| 1s2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4401E+00    | 5.965E-05 | 3.838E+10              | 1.4340E+00    | 6.023E-05 | 3.874E+10              | 0.002 |
| 1s2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4459E+00    | 1.248E-04 | 7.961E+10              | 1.4400E+00    | 1.244E-04 | 7.940E+10              | 0.002 |
| 1s3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.6920E+00    | 1.087E-06 | 1.064E+08              | 3.6768E+00    | 1.477E-06 | 1.445E+08              | 0.029 |
| 1s3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.6937E+00    | 1.645E-06 | 1.609E+08              | 3.6784E+00    | 1.937E-06 | 1.893E+08              | 0.023 |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.8236E+00    | 1.498E-06 | 1.367E+08              | 3.8077E+00    | 1.691E-06 | 1.543E+08              | 0.012 |
| 1s3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.8353E+00    | 3.469E-06 | 3.146E+08              | 3.8195E+00    | 3.746E-06 | 3.396E+08              | 0.003 |
| 1s4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 8.8404E+00    | 1.083E-04 | 1.849E+09              | 8.8032E+00    | 1.065E-04 | 1.819E+09              | 0.001 |
| 1s4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 8.8444E+00    | 1.537E-04 | 2.622E+09              | 8.8071E+00    | 1.527E-04 | 2.605E+09              | 0.000 |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 9.1578E+00    | 1.565E-05 | 2.489E+08              | 9.1192E+00    | 1.529E-05 | 2.432E+08              | 0.001 |
| 1s4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 9.1856E+00    | 3.180E-05 | 5.028E+08              | 9.1472E+00    | 3.119E-05 | 4.931E+08              | 0.000 |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 9.2886E+00    | 1.855E-05 | 2.868E+08              | 9.2496E+00    | 1.847E-05 | 2.856E+08              | 0.001 |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 9.2908E+00    | 7.429E-05 | 1.148E+09              | 9.2518E+00    | 7.409E-05 | 1.145E+09              | 0.000 |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 9.3416E+00    | 1.524E-06 | 2.329E+07              | 9.3023E+00    | 1.517E-06 | 2.318E+07              | 0.001 |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 9.3433E+00    | 1.384E-05 | 2.116E+08              | 9.3039E+00    | 1.371E-05 | 2.095E+08              | 0.001 |
| 1s5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 2.4566E+01    | 7.873E-04 | 1.740E+09              | 2.4463E+01    | 7.936E-04 | 1.754E+09              | 0.000 |
| 1s5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 2.4582E+01    | 1.123E-03 | 2.479E+09              | 2.4477E+01    | 1.126E-03 | 2.486E+09              | 0.000 |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 2.5836E+01    | 1.593E-04 | 3.185E+08              | 2.5726E+01    | 1.609E-04 | 3.216E+08              | 0.000 |
| 1s5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 2.5948E+01    | 3.343E-04 | 6.624E+08              | 2.5839E+01    | 3.349E-04 | 6.635E+08              | 0.000 |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 2.6372E+01    | 1.053E-04 | 2.020E+08              | 2.6263E+01    | 1.054E-04 | 2.022E+08              | 0.000 |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 2.6381E+01    | 4.223E-04 | 8.094E+08              | 2.6272E+01    | 4.226E-04 | 8.098E+08              | 0.000 |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 2.6592E+01    | 8.828E-06 | 1.665E+07              | 2.6482E+01    | 8.872E-06 | 1.673E+07              | 0.000 |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 2.6599E+01    | 8.031E-05 | 1.514E+08              | 2.6489E+01    | 8.015E-05 | 1.511E+08              | 0.000 |
| 1s6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 6.1864E+02    | 2.611E-07 | 9.100E+02              | 6.1520E+02    | 2.653E-07 | 9.272E+02              | 0.001 |
| 1s6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 6.2421E+02    | 3.621E-07 | 1.240E+03              | 6.0122E+02    | 4.004E-07 | 1.465E+03              | 0.001 |
| 1s6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 2.1625E+03    | 1.236E-09 | 3.526E-01              | 2.1357E+03    | 1.266E-09 | 3.671E-01              | 0.013 |
| 1s6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 2.7321E+03    | 1.288E-09 | 2.302E-01              | 2.6181E+03    | 1.394E-09 | 2.690E-01              | 0.017 |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3144E+05    | 1.419E-14 | 1.096E-09              |               |           |                        | 0.139 |
| 1s <sup>2</sup> <sup>1</sup> S <sub>0</sub>   | 1s6d <sup>1</sup> D <sub>2</sub>              | 3.1620E-01    | 2.010E-04 | 2.681E+12              | 3.1493E-01    | 2.346E-04 | 3.129E+12              | 0.002 |
| 1s2s <sup>3</sup> S <sub>1</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 1.3661E+00    | 1.156E-05 | 8.265E+09              | 1.3604E+00    | 1.042E-05 | 7.448E+09              | 0.008 |
| 1s2s <sup>1</sup> S <sub>0</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 1.3791E+00    | 1.520E-05 | 1.066E+10              | 1.3734E+00    | 1.583E-05 | 1.110E+10              | 0.002 |
| 1s3s <sup>3</sup> S <sub>1</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 3.6690E+00    | 6.320E-05 | 6.263E+09              | 3.6537E+00    | 6.164E-05 | 6.108E+09              | 0.004 |
| 1s3s <sup>1</sup> S <sub>0</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 3.6936E+00    | 9.420E-05 | 9.212E+09              | 3.6785E+00    | 9.501E-05 | 9.288E+09              | 0.013 |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 3.8335E+00    | 4.853E-06 | 4.406E+08              | 3.8174E+00    | 4.999E-06 | 4.537E+08              | 0.001 |
| 1s3d <sup>3</sup> D <sub>1</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 3.8353E+00    | 1.105E-05 | 1.002E+09              | 3.8191E+00    | 1.091E-05 | 9.901E+08              | 0.006 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 3.8770E+00    | 1.211E-05 | 1.075E+09              | 3.8606E+00    | 1.192E-05 | 1.058E+09              | 0.005 |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 3.8787E+00    | 4.990E-05 | 4.425E+09              | 3.8623E+00    | 4.949E-05 | 4.388E+09              | 0.006 |
| 1s4s <sup>3</sup> S <sub>1</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 8.7865E+00    | 1.610E-04 | 2.782E+09              | 8.7499E+00    | 1.592E-04 | 2.751E+09              | 0.003 |
| 1s4s <sup>1</sup> S <sub>0</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 8.8434E+00    | 2.451E-04 | 4.180E+09              | 8.8071E+00    | 2.460E-04 | 4.195E+09              | 0.007 |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 9.1814E+00    | 1.395E-05 | 2.208E+08              | 9.1435E+00    | 1.436E-05 | 2.272E+08              | 0.000 |
| 1s4d <sup>3</sup> D <sub>1</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 9.1855E+00    | 3.215E-05 | 5.084E+08              | 9.1476E+00    | 3.177E-05 | 5.021E+08              | 0.002 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 9.2868E+00    | 3.602E-05 | 5.571E+08              | 9.2482E+00    | 3.553E-05 | 5.496E+08              | 0.002 |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 9.2911E+00    | 1.477E-04 | 2.282E+09              | 9.2526E+00    | 1.477E-04 | 2.282E+09              | 0.002 |
| 1s5s <sup>3</sup> S <sub>1</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 2.4357E+01    | 5.073E-04 | 1.141E+09              | 2.4255E+01    | 5.096E-04 | 1.145E+09              | 0.003 |
| 1s5s <sup>1</sup> S <sub>0</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 2.4576E+01    | 7.897E-04 | 1.744E+09              | 2.4475E+01    | 7.829E-04 | 1.728E+09              | 0.001 |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 2.5931E+01    | 4.900E-05 | 9.721E+07              | 2.5828E+01    | 5.056E-05 | 1.002E+08              | 0.000 |
| 1s5d <sup>3</sup> D <sub>1</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 2.5947E+01    | 1.137E-04 | 2.253E+08              | 2.5844E+01    | 1.121E-04 | 2.221E+08              | 0.000 |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 2.6363E+01    | 1.317E-04 | 2.529E+08              | 2.6257E+01    | 1.303E-04 | 2.519E+08              | 0.000 |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 2.6382E+01    | 5.402E-04 | 1.035E+09              | 2.6276E+01    | 5.422E-04 | 1.038E+09              | 0.000 |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 2.6591E+01    | 5.584E-07 | 1.054E+06              | 2.6478E+01    | 6.309E-07 | 1.190E+06              | 0.000 |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 2.6597E+01    | 4.150E-06 | 7.826E+06              | 2.6484E+01    | 4.105E-06 | 7.742E+06              | 0.000 |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 2.6728E+01    | 5.969E-05 | 1.115E+08              | 2.6615E+01    | 5.978E-05 | 1.116E+08              | 0.000 |
| 1s6s <sup>3</sup> S <sub>1</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 5.4990E+02    | 4.398E-07 | 1.940E+03              | 5.4127E+02    | 4.505E-07 | 2.034E+03              | 0.014 |
| 1s6s <sup>1</sup> S <sub>0</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 6.2157E+02    | 4.706E-07 | 1.625E+03              | 5.9948E+02    | 5.219E-07 | 1.921E+03              | 0.040 |
| 1s6d <sup>3</sup> D <sub>2</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 2.6222E+03    | 8.371E-10 | 1.624E-01              |               |           |                        | 0.019 |
| 1s6d <sup>3</sup> D <sub>1</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 2.7221E+03    | 1.737E-09 | 3.127E-01              |               |           |                        | 0.001 |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s6d <sup>1</sup> D <sub>2</sub>              | 6.4120E+04    | 1.525E-13 | 4.950E-08              |               |           |                        | 0.345 |
| 1s2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.4397E+00    | 1.592E-03 | 5.693E+11              | 1.4336E+00    | 1.671E-03 | 5.974E+11              | 0.001 |
| 1s3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 3.8211E+00    | 3.236E-05 | 1.643E+09              | 3.8051E+00    | 3.745E-05 | 1.901E+09              | 0.010 |
| 1s4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 9.1433E+00    | 4.491E-04 | 3.981E+09              | 9.1041E+00    | 4.417E-04 | 3.916E+09              | 0.000 |

(continued on next page)

Table 4 (continued)

| Lower           | Upper           | GRASP2K       |           |                | FAC           |           |                | dT    |
|-----------------|-----------------|---------------|-----------|----------------|---------------|-----------|----------------|-------|
|                 |                 | $\lambda$ (Å) | gf        | A ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | A ( $s^{-1}$ ) |       |
| 1s 4f $^3F_3^0$ | 1s 6f $^3F_4^0$ | 9.2736E+00    | 1.951E-05 | 1.681E+08      | 9.2341E+00    | 1.958E-05 | 1.688E+08      | 0.001 |
| 1s 4f $^3F_2^0$ | 1s 6f $^3F_4^0$ | 9.2758E+00    | 1.549E-06 | 1.335E+07      | 9.2363E+00    | 1.553E-06 | 1.338E+07      | 0.001 |
| 1s 4f $^3F_4^0$ | 1s 6f $^3F_4^0$ | 9.3265E+00    | 1.596E-04 | 1.360E+09      | 9.2866E+00    | 1.593E-04 | 1.358E+09      | 0.000 |
| 1s 4f $^1F_3^0$ | 1s 6f $^3F_4^0$ | 9.3281E+00    | 1.458E-05 | 1.242E+08      | 9.2883E+00    | 1.455E-05 | 1.239E+08      | 0.000 |
| 1s 5p $^3P_2^0$ | 1s 6f $^3F_4^0$ | 2.5720E+01    | 4.305E-03 | 4.823E+09      | 2.5607E+01    | 4.350E-03 | 4.875E+09      | 0.000 |
| 1s 5f $^3F_3^0$ | 1s 6f $^3F_4^0$ | 2.6252E+01    | 1.086E-04 | 1.168E+08      | 2.6139E+01    | 1.090E-04 | 1.172E+08      | 0.000 |
| 1s 5f $^3F_2^0$ | 1s 6f $^3F_4^0$ | 2.6261E+01    | 8.548E-06 | 9.187E+06      | 2.6148E+01    | 8.573E-06 | 9.214E+06      | 0.000 |
| 1s 5f $^3F_4^0$ | 1s 6f $^3F_4^0$ | 2.6469E+01    | 9.072E-04 | 9.597E+08      | 2.6355E+01    | 9.087E-04 | 9.613E+08      | 0.000 |
| 1s 5f $^1F_3^0$ | 1s 6f $^3F_4^0$ | 2.6476E+01    | 8.289E-05 | 8.763E+07      | 2.6362E+01    | 8.292E-05 | 8.768E+07      | 0.000 |
| 1s 6p $^3P_2^0$ | 1s 6f $^3F_4^0$ | 1.5714E+03    | 8.788E-08 | 2.638E+01      | 1.5399E+03    | 9.216E-08 | 2.856E+01      | 0.009 |
| 1s 6f $^3F_3^0$ | 1s 6f $^3F_4^0$ | 5.5078E+03    | 2.014E-10 | 4.921E-03      | 5.5226E+03    | 1.981E-10 | 4.774E-03      | 0.002 |
| 1s 6f $^3F_2^0$ | 1s 6f $^3F_4^0$ | 5.7487E+03    | 1.406E-11 | 3.153E-04      |               |           |                | 0.005 |
| 1s 3d $^3D_2$   | 1s 6g $^3G_4$   | 3.8309E+00    | 3.357E-03 | 1.695E+11      | 3.8148E+00    | 3.386E-03 | 1.709E+11      | 0.000 |
| 1s 3d $^3D_3$   | 1s 6g $^3G_4$   | 3.8744E+00    | 3.474E-04 | 1.715E+10      | 3.8580E+00    | 3.479E-04 | 1.717E+10      | 0.000 |
| 1s 3d $^1D_2$   | 1s 6g $^3G_4$   | 3.8761E+00    | 3.116E-05 | 1.537E+09      | 3.8597E+00    | 3.004E-05 | 1.481E+09      | 0.001 |
| 1s 4d $^3D_2$   | 1s 6g $^3G_4$   | 9.1668E+00    | 7.908E-05 | 6.975E+08      | 9.1289E+00    | 8.154E-05 | 7.190E+08      | 0.001 |
| 1s 4d $^3D_3$   | 1s 6g $^3G_4$   | 9.2719E+00    | 1.137E-05 | 9.800E+07      | 9.2332E+00    | 1.167E-05 | 1.006E+08      | 0.001 |
| 1s 4d $^1D_2$   | 1s 6g $^3G_4$   | 9.2762E+00    | 1.073E-06 | 9.238E+06      | 9.2375E+00    | 1.032E-06 | 8.892E+06      | 0.003 |
| 1s 5d $^3D_2$   | 1s 6g $^3G_4$   | 2.5815E+01    | 5.070E-03 | 5.639E+09      | 2.5711E+01    | 5.076E-03 | 5.642E+09      | 0.000 |
| 1s 5d $^3D_3$   | 1s 6g $^3G_4$   | 2.6244E+01    | 5.114E-04 | 5.504E+08      | 2.6137E+01    | 5.132E-04 | 5.520E+08      | 0.000 |
| 1s 5d $^1D_2$   | 1s 6g $^3G_4$   | 2.6262E+01    | 4.852E-05 | 5.214E+07      | 2.6155E+01    | 4.698E-05 | 5.047E+07      | 0.000 |
| 1s 5g $^3G_4$   | 1s 6g $^3G_4$   | 2.6470E+01    | 5.388E-04 | 5.699E+08      | 2.6356E+01    | 5.393E-04 | 5.705E+08      | 0.000 |
| 1s 5g $^3G_3$   | 1s 6g $^3G_4$   | 2.6475E+01    | 4.880E-05 | 5.160E+07      | 2.6361E+01    | 4.899E-05 | 5.180E+07      | 0.000 |
| 1s 5g $^3G_5$   | 1s 6g $^3G_4$   | 2.6601E+01    | 4.984E-05 | 5.220E+07      | 2.6487E+01    | 4.993E-05 | 5.231E+07      | 0.000 |
| 1s 5g $^1G_4$   | 1s 6g $^3G_4$   | 2.6605E+01    | 3.575E-06 | 3.744E+06      | 2.6491E+01    | 3.402E-06 | 3.562E+06      | 0.000 |
| 1s 6d $^3D_2$   | 1s 6g $^3G_4$   | 1.8045E+03    | 3.645E-08 | 8.298E+00      | 1.8335E+03    | 3.427E-08 | 7.491E+00      | 0.002 |
| 1s 6d $^3D_3$   | 1s 6g $^3G_4$   | 5.3075E+03    | 1.458E-10 | 3.836E-03      | 5.5194E+03    | 1.284E-10 | 3.097E-03      | 0.000 |
| 1s 6d $^1D_2$   | 1s 6g $^3G_4$   | 5.7864E+03    | 1.077E-11 | 2.384E-04      |               |           |                | 0.038 |
| 1s 2s $^3S_1$   | 1s 6g $^3G_3$   | 1.3658E+00    | 5.739E-11 | 2.931E+04      |               |           |                | 0.903 |
| 1s 3s $^3S_1$   | 1s 6g $^3G_3$   | 3.6666E+00    | 3.747E-09 | 2.656E+05      |               |           |                | 0.102 |
| 1s 3d $^3D_2$   | 1s 6g $^3G_3$   | 3.8309E+00    | 3.753E-04 | 2.437E+10      | 3.8148E+00    | 3.787E-04 | 2.459E+10      | 0.000 |
| 1s 3d $^3D_1$   | 1s 6g $^3G_3$   | 3.8326E+00    | 2.240E-03 | 1.453E+11      | 3.8166E+00    | 2.255E-03 | 1.463E+11      | 0.000 |
| 1s 3d $^3D_3$   | 1s 6g $^3G_3$   | 3.8743E+00    | 4.181E-05 | 2.654E+09      | 3.8580E+00    | 4.175E-05 | 2.650E+09      | 0.000 |
| 1s 3d $^1D_2$   | 1s 6g $^3G_3$   | 3.8760E+00    | 2.490E-04 | 1.579E+10      | 3.8597E+00    | 2.479E-04 | 1.572E+10      | 0.000 |
| 1s 4s $^3S_1$   | 1s 6g $^3G_3$   | 8.7728E+00    | 1.855E-11 | 2.297E+02      |               |           |                | 0.573 |
| 1s 4d $^3D_2$   | 1s 6g $^3G_3$   | 9.1665E+00    | 8.833E-06 | 1.002E+08      | 9.1289E+00    | 9.173E-06 | 1.039E+08      | 0.000 |
| 1s 4d $^3D_1$   | 1s 6g $^3G_3$   | 9.1706E+00    | 5.325E-05 | 6.034E+08      | 9.1329E+00    | 5.436E-05 | 6.157E+08      | 0.002 |
| 1s 4d $^3D_3$   | 1s 6g $^3G_3$   | 9.2715E+00    | 1.365E-06 | 1.513E+07      | 9.2332E+00    | 1.401E-06 | 1.553E+07      | 0.000 |
| 1s 4d $^1D_2$   | 1s 6g $^3G_3$   | 9.2759E+00    | 8.174E-06 | 9.052E+07      | 9.2375E+00    | 8.299E-06 | 9.189E+07      | 0.001 |
| 1s 5s $^3S_1$   | 1s 6g $^3G_3$   | 2.4252E+01    | 9.019E-09 | 1.461E+04      |               |           |                | 0.014 |
| 1s 5d $^3D_2$   | 1s 6g $^3G_3$   | 2.5812E+01    | 5.697E-04 | 8.147E+08      | 2.5711E+01    | 5.708E-04 | 8.158E+08      | 0.000 |
| 1s 5d $^3D_1$   | 1s 6g $^3G_3$   | 2.5829E+01    | 3.383E-03 | 4.832E+09      | 2.5727E+01    | 3.382E-03 | 4.827E+09      | 0.000 |
| 1s 5d $^3D_3$   | 1s 6g $^3G_3$   | 2.6241E+01    | 6.159E-05 | 8.523E+07      | 2.6137E+01    | 6.159E-05 | 8.518E+07      | 0.000 |
| 1s 5d $^1D_2$   | 1s 6g $^3G_3$   | 2.6259E+01    | 3.639E-04 | 5.028E+08      | 2.6155E+01    | 3.629E-04 | 5.012E+08      | 0.000 |
| 1s 5g $^3G_4$   | 1s 6g $^3G_3$   | 2.6467E+01    | 4.878E-05 | 6.636E+07      | 2.6356E+01    | 4.884E-05 | 6.644E+07      | 0.000 |
| 1s 5g $^3G_3$   | 1s 6g $^3G_3$   | 2.6472E+01    | 4.079E-04 | 5.547E+08      | 2.6361E+01    | 4.082E-04 | 5.550E+08      | 0.000 |
| 1s 5g $^3G_5$   | 1s 6g $^3G_3$   | 2.6598E+01    | 2.379E-06 | 3.205E+06      | 2.6487E+01    | 2.378E-06 | 3.202E+06      | 0.001 |
| 1s 5g $^1G_4$   | 1s 6g $^3G_3$   | 2.6602E+01    | 3.946E-05 | 5.314E+07      | 2.6491E+01    | 3.938E-05 | 5.302E+07      | 0.000 |
| 1s 6s $^3S_1$   | 1s 6g $^3G_3$   | 5.0108E+02    | 3.106E-12 | 1.179E-02      |               |           |                | 0.128 |
| 1s 6d $^3D_2$   | 1s 6g $^3G_3$   | 1.7904E+03    | 4.198E-09 | 1.248E+00      | 1.8335E+03    | 3.889E-09 | 1.093E+00      | 0.003 |
| 1s 6d $^3D_1$   | 1s 6g $^3G_3$   | 1.8364E+03    | 2.308E-08 | 6.523E+00      | 1.8221E+03    | 2.333E-08 | 6.639E+00      | 0.002 |
| 1s 6d $^3D_3$   | 1s 6g $^3G_3$   | 5.1873E+03    | 1.881E-11 | 6.661E-04      |               |           |                | 0.003 |
| 1s 6d $^1D_2$   | 1s 6g $^3G_3$   | 5.6439E+03    | 8.622E-11 | 2.579E-03      | 5.6946E+03    | 8.174E-11 | 2.381E-03      | 0.011 |
| 1s 6g $^3G_4$   | 1s 6g $^3G_3$   | 2.2908E+05    | 1.468E-15 | 2.666E-11      |               |           |                | 0.552 |
| 1s 2p $^3P_1^0$ | 1s 6f $^1F_3^0$ | 1.3775E+00    | 1.744E-06 | 8.756E+08      | 1.3718E+00    | 2.023E-06 | 1.016E+09      | 0.014 |
| 1s 2p $^3P_2^0$ | 1s 6f $^1F_3^0$ | 1.4397E+00    | 1.779E-04 | 8.177E+10      | 1.4336E+00    | 1.854E-04 | 8.523E+10      | 0.000 |
| 1s 2p $^1P_1^0$ | 1s 6f $^1F_3^0$ | 1.4456E+00    | 1.064E-03 | 4.851E+11      | 1.4396E+00    | 1.098E-03 | 5.009E+11      | 0.001 |
| 1s 3p $^3P_1^0$ | 1s 6f $^1F_3^0$ | 3.6895E+00    | 3.092E-09 | 2.165E+05      | 3.6743E+00    | 3.901E-08 | 2.730E+06      | 0.011 |
| 1s 3p $^3P_2^0$ | 1s 6f $^1F_3^0$ | 3.8210E+00    | 3.586E-06 | 2.340E+08      | 3.8051E+00    | 4.156E-06 | 3.8711E+08     | 0.011 |
| 1s 3p $^1P_1^0$ | 1s 6f $^1F_3^0$ | 3.8327E+00    | 2.406E-05 | 1.561E+09      | 3.8169E+00    | 2.471E-05 | 1.602E+09      | 0.008 |
| 1s 4p $^3P_1^0$ | 1s 6f $^1F_3^0$ | 8.8264E+00    | 6.111E-07 | 7.475E+06      | 8.7892E+00    | 4.307E-07 | 5.268E+06      | 0.001 |
| 1s 4p $^3P_2^0$ | 1s 6f $^1F_3^0$ | 9.1428E+00    | 5.020E-05 | 5.723E+08      | 9.1041E+00    | 4.900E-05 | 5.585E+08      | 0.001 |
| 1s 4p $^1P_1^0$ | 1s 6f $^1F_3^0$ | 9.1705E+00    | 2.897E-04 | 3.283E+09      | 9.1320E+00    | 2.914E-04 | 3.302E+09      | 0.000 |
| 1s 4f $^3F_3^0$ | 1s 6f $^1F_3^0$ | 9.2731E+00    | 2.362E-06 | 2.618E+07      | 9.2341E+00    | 2.453E-06 | 2.718E+07      | 0.001 |
| 1s 4f $^3F_2^0$ | 1s 6f $^1F_3^0$ | 9.2753E+00    | 1.418E-05 | 1.571E+08      | 9.2363E+00    | 1.414E-05 | 1.566E+08      | 0.001 |
| 1s 4f $^3F_4^0$ | 1s 6f $^1F_3^0$ | 9.3260E+00    | 1.458E-05 | 1.598E+08      | 9.2866E+00    | 1.446E-05 | 1.585E+08      | 0.000 |
| 1s 4f $^1F_3^0$ | 1s 6f $^1F_3^0$ | 9.3276E+00    | 1.208E-04 | 1.323E+09      | 9.2883E+00    | 1.206E-04 | 1.320E+09      | 0.000 |
| 1s 5p $^3P_1^0$ | 1s 6f $^1F_3^0$ | 2.4458E+01    | 4.144E-06 | 6.601E+06      | 2.4355E+01    | 4.367E-06 | 6.957E+06      | 0.000 |
| 1s 5p $^3P_2^0$ | 1s 6f $^1F_3^0$ | 2.5717E+01    | 4.804E-04 | 6.921E+08      | 2.5607E+01    | 4.825E-04 | 6.952E+08      | 0.000 |
| 1s 5p $^1P_1^0$ | 1s 6f $^1F_3^0$ | 2.5828E+01    | 2.861E-03 | 4.087E+09      | 2.5719E+01    | 2.859E-03 | 4.084E+09      | 0.000 |
| 1s 5f $^3F_3^0$ | 1s 6f $^1F_3^0$ | 2.6248E+01    | 1.311E-05 | 1.813E+07      | 2.6139E+01    | 1.363E-05 | 1.885E+07      | 0.000 |

(continued on next page)

Table 4 (continued)

| Lower   | Upper   | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|---|---|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|   |   | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.6257E+01    | 7.903E-05 | 1.092E+08              | 2.6148E+01    | 7.877E-05 | 1.088E+08              | 0.000 |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.6465E+01    | 8.283E-05 | 1.127E+08              | 2.6355E+01    | 8.250E-05 | 1.122E+08              | 0.000 |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.6472E+01    | 6.865E-04 | 9.335E+08              | 2.6362E+01    | 6.876E-04 | 9.348E+08              | 0.000 |
| 1s6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.5676E+02    | 1.886E-09 | 5.797E+00              | 5.5347E+02    | 2.833E-09 | 8.739E+00              | 0.006 |
| 1s6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.5574E+03    | 1.007E-08 | 3.956E+00              | 1.5396E+03    | 1.023E-08 | 4.078E+00              | 0.008 |
| 1s6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.8325E+03    | 3.684E-08 | 1.045E+01              | 1.7754E+03    | 4.001E-08 | 1.199E+01              | 0.009 |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.3394E+03    | 2.665E-11 | 8.908E-04              |               |           |                        | 0.009 |
| 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.5655E+03    | 1.419E-10 | 4.365E-03              | 5.5161E+03    |           | 4.435E-03              | 0.004 |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.7466E+05    | 4.802E-15 | 1.500E-10              |               | 1.428E-10 |                        | 0.228 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s6g <sup>3</sup> G <sub>5</sub>              | 3.8728E+00    | 4.582E-03 | 1.853E+11              | 3.8564E+00    | 4.660E-03 | 1.884E+11              | 0.000 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s6g <sup>3</sup> G <sub>5</sub>              | 9.2626E+00    | 1.359E-04 | 9.604E+08              | 9.2240E+00    | 1.404E-04 | 9.926E+08              | 0.001 |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s6g <sup>3</sup> G <sub>5</sub>              | 2.6170E+01    | 6.805E-03 | 6.026E+09              | 2.6063E+01    | 6.824E-03 | 6.040E+09              | 0.000 |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s6g <sup>3</sup> G <sub>5</sub>              | 2.6394E+01    | 4.948E-05 | 4.307E+07              | 2.6281E+01    | 4.968E-05 | 4.325E+07              | 0.000 |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s6g <sup>3</sup> G <sub>5</sub>              | 2.6399E+01    | 2.359E-06 | 2.053E+06              | 2.6286E+01    | 2.367E-06 | 2.059E+06              | 0.000 |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s6g <sup>3</sup> G <sub>5</sub>              | 2.6525E+01    | 6.910E-04 | 5.955E+08              | 2.6411E+01    | 6.918E-04 | 5.963E+08              | 0.000 |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s6g <sup>3</sup> G <sub>5</sub>              | 2.6529E+01    | 4.004E-05 | 3.450E+07              | 2.6415E+01    | 4.006E-05 | 3.452E+07              | 0.000 |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s6g <sup>3</sup> G <sub>5</sub>              | 3.3718E+03    | 7.594E-09 | 4.050E-01              | 3.4576E+03    | 6.952E-09 | 3.496E-01              | 0.001 |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s6g <sup>3</sup> G <sub>5</sub>              | 9.2456E+03    | 2.278E-11 | 1.616E-04              | 9.2559E+03    | 2.249E-11 | 1.578E-04              | 0.004 |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s6g <sup>3</sup> G <sub>5</sub>              | 9.6344E+03    | 9.609E-13 | 6.277E-06              |               |           |                        | 0.063 |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 9.2643E+00    | 9.005E-03 | 6.362E+10              | 9.2249E+00    | 9.057E-03 | 6.399E+10              | 0.000 |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 9.3170E+00    | 5.230E-04 | 3.653E+09              | 9.2773E+00    | 5.243E-04 | 3.662E+09              | 0.000 |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 9.3187E+00    | 2.439E-05 | 1.703E+08              | 9.2790E+00    | 2.295E-05 | 1.602E+08              | 0.000 |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 2.6177E+01    | 5.783E-03 | 5.118E+09              | 2.6065E+01    | 5.792E-03 | 5.126E+09              | 0.000 |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 2.6394E+01    | 3.283E-04 | 2.858E+08              | 2.6281E+01    | 3.291E-04 | 2.864E+08              | 0.000 |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 2.6400E+01    | 1.539E-05 | 1.339E+07              | 2.6287E+01    | 1.448E-05 | 1.259E+07              | 0.000 |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 3.4460E+03    | 2.908E-09 | 1.485E-01              | 3.4619E+03    | 2.830E-09 | 1.420E-01              | 0.000 |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 9.2055E+03    | 8.735E-12 | 6.251E-05              | 9.2780E+03    | 8.447E-12 | 5.900E-05              | 0.006 |
| 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 9.7177E+03    | 3.492E-13 | 2.242E-06              |               |           |                        | 0.010 |
| 1s2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.4395E+00    | 2.079E-12 | 7.436E+02              |               |           |                        | 0.948 |
| 1s3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 3.8195E+00    | 1.741E-13 | 8.847E+00              |               |           |                        | 0.800 |
| 1s4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 9.1340E+00    | 7.955E-10 | 7.067E+03              |               |           |                        | 0.008 |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 9.2640E+00    | 5.435E-04 | 4.694E+09              | 9.2249E+00    | 5.467E-04 | 4.721E+09              | 0.000 |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 9.2662E+00    | 6.821E-03 | 5.888E+10              | 9.2271E+00    | 6.855E-03 | 5.917E+10              | 0.000 |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 9.3168E+00    | 3.746E-05 | 3.198E+08              | 9.2773E+00    | 3.745E-05 | 3.197E+08              | 0.000 |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 9.3184E+00    | 4.142E-04 | 3.535E+09              | 9.2790E+00    | 4.138E-04 | 3.531E+09              | 0.000 |
| 1s5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 2.5647E+01    | 9.502E-10 | 1.071E+03              |               |           |                        | 0.001 |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 2.6175E+01    | 3.493E-04 | 3.778E+08              | 2.6065E+01    | 3.497E-04 | 3.783E+08              | 0.000 |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 2.6184E+01    | 4.378E-03 | 4.733E+09              | 2.6074E+01    | 4.383E-03 | 4.737E+09              | 0.000 |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 2.6392E+01    | 2.352E-05 | 2.503E+07              | 2.6281E+01    | 2.350E-05 | 2.501E+07              | 0.000 |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 2.6398E+01    | 2.598E-04 | 2.763E+08              | 2.6287E+01    | 2.595E-04 | 2.760E+08              | 0.000 |
| 1s6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.3372E+03    | 1.003E-14 | 4.157E-06              |               |           |                        | 0.006 |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 3.4128E+03    | 1.808E-10 | 1.151E-02              | 3.4619E+03    | 1.717E-10 | 1.053E-02              | 0.001 |
| 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 3.5038E+03    | 2.095E-09 | 1.265E-01              | 3.4609E+03    | 2.146E-09 | 1.317E-01              | 0.000 |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 8.9725E+03    | 6.759E-13 | 6.222E-06              |               |           |                        | 0.002 |
| 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 9.4584E+03    | 6.374E-12 | 5.281E-05              | 9.2889E+03    | 6.605E-12 | 5.625E-05              | 0.006 |
| 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 3.5443E+05    | 1.836E-16 | 1.083E-12              |               |           |                        | 0.747 |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 3.8293E+00    | 9.113E-08 | 4.606E+06              |               |           |                        | 0.015 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 3.8727E+00    | 2.790E-04 | 1.379E+10              | 3.8564E+00    | 2.824E-04 | 1.395E+10              | 0.000 |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 3.8744E+00    | 3.470E-03 | 1.713E+11              | 3.8580E+00    | 3.526E-03 | 1.740E+11              | 0.000 |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 9.1575E+00    | 3.631E-09 | 3.209E+04              |               |           |                        | 0.043 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 9.2623E+00    | 8.247E-06 | 7.125E+07              | 9.2240E+00    | 8.512E-06 | 7.352E+07              | 0.000 |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 9.2666E+00    | 1.039E-04 | 8.965E+08              | 9.2283E+00    | 1.062E-04 | 9.168E+08              | 0.001 |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.5741E+01    | 3.250E-07 | 3.635E+05              |               |           |                        | 0.002 |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.6167E+01    | 4.142E-04 | 4.484E+08              | 2.6063E+01    | 4.135E-04 | 4.474E+08              | 0.000 |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.6185E+01    | 5.151E-03 | 5.567E+09              | 2.6082E+01    | 5.158E-03 | 5.572E+09              | 0.000 |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.6392E+01    | 3.549E-06 | 3.777E+06              | 2.6281E+01    | 3.733E-06 | 3.972E+06              | 0.000 |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.6397E+01    | 3.919E-05 | 4.168E+07              | 2.6286E+01    | 3.914E-05 | 4.163E+07              | 0.000 |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.6522E+01    | 4.003E-05 | 4.218E+07              | 2.6411E+01    | 3.991E-05 | 4.205E+07              | 0.000 |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.6527E+01    | 5.878E-04 | 5.875E+08              | 2.6415E+01    | 5.883E-04 | 5.880E+08              | 0.000 |
| 1s6d <sup>3</sup> D <sub>2</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 1.5020E+03    | 4.543E-12 | 1.492E-03              | 1.5304E+03    | 8.482E-12 | 2.661E-03              | 0.073 |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 3.3331E+03    | 4.786E-10 | 3.193E-02              | 3.4576E+03    | 4.213E-10 | 2.590E-02              | 0.003 |
| 1s6d <sup>1</sup> D <sub>2</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 3.5158E+03    | 5.072E-09 | 3.041E-01              | 3.5255E+03    | 4.967E-09 | 2.936E-01              | 0.007 |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 8.9597E+03    | 1.796E-12 | 1.658E-05              |               |           |                        | 0.031 |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 9.3244E+03    | 1.758E-11 | 1.499E-04              | 9.2557E+03    | 1.767E-11 | 1.515E-04              | 0.005 |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.8974E+05    | 5.995E-16 | 5.293E-12              |               |           |                        | 0.672 |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 9.3108E+00    | 1.132E-02 | 6.701E+10              | 9.2712E+00    | 1.142E-02 | 6.763E+10              | 0.000 |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 2.6344E+01    | 7.177E-03 | 5.306E+09              | 2.6231E+01    | 7.197E-03 | 5.321E+09              | 0.000 |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 5.5410E+03    | 8.762E-10 | 1.464E-02              | 5.5692E+03    | 8.520E-10 | 1.397E-02              | 0.003 |
| 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1.3919E+04    | 3.060E-12 | 8.104E-06              | 1.3932E+04    | 3.021E-12 | 7.919E-06              | 0.005 |
| 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1.4488E+04    | 8.641E-14 | 2.112E-07              |               |           |                        | 0.178 |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 9.2579E+00    | 3.678E-09 | 2.602E+04              |               |           |                        | 0.007 |

(continued on next page)

Table 4 (continued)

| Lower  | Upper  | GRASP2K       |           |                      | FAC           |           |                      | dT    |
|--|--|---------------|-----------|----------------------|---------------|-----------|----------------------|-------|
|  |  | $\lambda$ (Å) | gf        | A (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | A (s <sup>-1</sup> ) |       |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 9.3106E+00    | 4.369E-04 | 3.056E+09            | 9.2712E+00    | 4.395E-04 | 3.074E+09            | 0.000 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 9.3123E+00    | 9.144E-03 | 6.394E+10            | 9.2728E+00    | 9.224E-03 | 6.450E+10            | 0.000 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.6126E+01    | 1.462E-09 | 1.299E+03            |               |           |                      | 0.002 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.6342E+01    | 2.770E-04 | 2.421E+08            | 2.6231E+01    | 2.768E-04 | 2.419E+08            | 0.000 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.6349E+01    | 5.794E-03 | 5.061E+09            | 2.6238E+01    | 5.809E-03 | 5.073E+09            | 0.000 |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.7445E+03    | 1.003E-15 | 8.072E-08            |               |           |                      | 0.007 |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 5.4702E+03    | 3.515E-11 | 7.124E-04            | 5.5692E+03    | 3.276E-11 | 6.352E-04            | 0.001 |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 5.6471E+03    | 6.685E-10 | 1.271E-02            | 5.5731E+03    | 6.867E-10 | 1.329E-02            | 0.002 |
| 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.3481E+04    | 1.610E-13 | 5.370E-07            |               |           |                      | 0.045 |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.4014E+04    | 2.491E-12 | 7.690E-06            | 1.3932E+04    | 2.494E-12 | 7.725E-06            | 0.008 |
| 1s 6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.2819E+05    | 8.864E-17 | 2.932E-13            |               |           |                      | 0.869 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 1.3268E+00    | 4.817E-10 | 6.084E+05            |               |           |                      | 0.985 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 3.3983E+00    | 2.685E-10 | 5.170E+04            |               |           |                      | 0.385 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 3.5389E+00    | 6.769E-06 | 1.202E+09            | 3.5242E+00    | 7.076E-06 | 1.256E+09            | 0.040 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 3.5404E+00    | 7.411E-06 | 1.315E+09            | 3.5257E+00    | 7.024E-06 | 1.245E+09            | 0.056 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 3.5760E+00    | 1.602E-05 | 2.785E+09            | 3.5610E+00    | 1.650E-05 | 2.868E+09            | 0.040 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 3.5774E+00    | 4.893E-06 | 8.502E+08            | 3.5624E+00    | 4.667E-06 | 8.108E+08            | 0.044 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 7.3787E+00    | 3.123E-11 | 1.275E+03            |               |           |                      | 0.933 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 7.6552E+00    | 1.969E-05 | 7.471E+08            | 7.6242E+00    | 2.005E-05 | 7.606E+08            | 0.015 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 7.6581E+00    | 2.030E-05 | 7.698E+08            | 7.6271E+00    | 1.984E-05 | 7.521E+08            | 0.023 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 7.7284E+00    | 4.617E-05 | 1.719E+09            | 7.6969E+00    | 4.658E-05 | 1.733E+09            | 0.015 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 7.7314E+00    | 1.334E-05 | 4.961E+08            | 7.6999E+00    | 1.311E-05 | 4.876E+08            | 0.017 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 1.5931E+01    | 6.722E-10 | 5.899E+03            |               |           |                      | 0.419 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 1.6590E+01    | 4.953E-05 | 4.001E+08            | 1.6526E+01    | 4.980E-05 | 4.020E+08            | 0.004 |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 1.6597E+01    | 4.987E-05 | 4.025E+08            | 1.6532E+01    | 4.920E-05 | 3.968E+08            | 0.010 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 1.6766E+01    | 1.160E-04 | 9.178E+08            | 1.6700E+01    | 1.158E-04 | 9.160E+08            | 0.004 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 1.6773E+01    | 3.281E-05 | 2.593E+08            | 1.6708E+01    | 3.254E-05 | 2.570E+08            | 0.007 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 1.6860E+01    | 3.065E-11 | 2.398E+02            |               |           |                      | 0.060 |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 4.2495E+01    | 3.689E-09 | 4.543E+03            |               |           |                      | 0.102 |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 4.5259E+01    | 1.803E-04 | 1.957E+08            | 4.5119E+01    | 1.799E-04 | 1.949E+08            | 0.001 |
| 1s 6d <sup>3</sup> D <sub>1</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 4.5288E+01    | 1.801E-04 | 1.952E+08            | 4.5112E+01    | 1.765E-04 | 1.912E+08            | 0.004 |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 4.6021E+01    | 4.306E-04 | 4.520E+08            | 4.5873E+01    | 4.241E-04 | 4.443E+08            | 0.001 |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 4.6054E+01    | 1.209E-04 | 1.267E+08            | 4.5885E+01    | 1.177E-04 | 1.232E+08            | 0.003 |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7s <sup>3</sup> S <sub>1</sub>              | 4.6433E+01    | 2.618E-10 | 2.700E+02            |               |           |                      | 0.039 |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.3376E+00    | 4.582E-08 | 5.693E+07            | 1.3321E+00    | 1.353E-07 | 1.681E+08            | 0.537 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.3961E+00    | 1.583E-05 | 1.805E+10            | 1.3903E+00    | 1.652E-05 | 1.885E+10            | 0.058 |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.4017E+00    | 1.535E-05 | 1.738E+10            | 1.3959E+00    | 1.409E-05 | 1.595E+10            | 0.029 |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 3.4164E+00    | 2.188E-07 | 4.169E+07            | 3.4024E+00    | 2.384E-07 | 4.540E+07            | 0.201 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.5289E+00    | 3.518E-05 | 6.282E+09            | 3.5142E+00    | 3.240E-05 | 5.784E+09            | 0.079 |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 3.5388E+00    | 3.051E-05 | 5.417E+09            | 3.5243E+00    | 2.782E-05 | 4.939E+09            | 0.053 |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 7.4094E+00    | 3.166E-07 | 1.282E+07            | 7.3785E+00    | 3.980E-07 | 1.611E+07            | 0.067 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.6311E+00    | 5.802E-05 | 2.215E+09            | 7.5991E+00    | 5.725E-05 | 2.185E+09            | 0.017 |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 7.6504E+00    | 5.135E-05 | 1.951E+09            | 7.6186E+00    | 4.936E-05 | 1.874E+09            | 0.007 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 7.7217E+00    | 1.128E-05 | 4.205E+08            | 7.6895E+00    | 1.078E-05 | 4.020E+08            | 0.032 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 7.7232E+00    | 3.454E-06 | 1.288E+08            | 7.6910E+00    | 3.342E-06 | 1.245E+08            | 0.033 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 7.7595E+00    | 1.761E-08 | 6.504E+05            | 7.7270E+00    | 2.587E-08 | 9.555E+05            | 0.017 |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.5987E+01    | 5.833E-07 | 5.075E+06            | 1.5920E+01    | 7.664E-07 | 6.666E+06            | 0.015 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6515E+01    | 1.159E-04 | 9.447E+08            | 1.6446E+01    | 1.167E-04 | 9.520E+08            | 0.003 |
| 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.6561E+01    | 1.036E-04 | 8.397E+08            | 1.6492E+01    | 1.010E-04 | 8.193E+08            | 0.006 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.6732E+01    | 4.609E-05 | 3.661E+08            | 1.6664E+01    | 4.535E-05 | 3.601E+08            | 0.002 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.6736E+01    | 1.410E-05 | 1.119E+08            | 1.6667E+01    | 1.404E-05 | 1.114E+08            | 0.002 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.6823E+01    | 7.450E-08 | 5.853E+05            | 1.6754E+01    | 1.071E-07 | 8.412E+05            | 0.002 |
| 1s 6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.2622E+01    | 1.744E-06 | 2.135E+06            | 4.2444E+01    | 2.994E-06 | 3.664E+06            | 0.005 |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4826E+01    | 3.888E-04 | 4.302E+08            | 4.4636E+01    | 3.931E-04 | 4.350E+08            | 0.001 |
| 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.5021E+01    | 3.515E-04 | 3.856E+08            | 4.4809E+01    | 3.422E-04 | 3.757E+08            | 0.000 |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.5759E+01    | 2.138E-04 | 2.270E+08            | 4.5589E+01    | 2.114E-04 | 2.242E+08            | 0.002 |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.5775E+01    | 6.539E-05 | 6.939E+07            | 4.5589E+01    | 6.507E-05 | 6.902E+07            | 0.002 |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.6155E+01    | 3.481E-07 | 3.633E+05            | 4.5969E+01    | 4.043E-07 | 4.218E+05            | 0.001 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7s <sup>1</sup> S <sub>0</sub>              | 3.5373E+00    | 4.635E-06 | 2.471E+09            | 3.5228E+00    | 4.652E-06 | 2.479E+09            | 0.016 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7s <sup>1</sup> S <sub>0</sub>              | 3.5757E+00    | 7.727E-06 | 4.031E+09            | 3.5610E+00    | 7.113E-06 | 3.709E+09            | 0.063 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7s <sup>1</sup> S <sub>0</sub>              | 7.6475E+00    | 1.316E-05 | 1.501E+09            | 7.6177E+00    | 1.309E-05 | 1.492E+09            | 0.007 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7s <sup>1</sup> S <sub>0</sub>              | 7.7235E+00    | 2.094E-05 | 2.341E+09            | 7.6933E+00    | 2.017E-05 | 2.254E+09            | 0.024 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7s <sup>1</sup> S <sub>0</sub>              | 1.6554E+01    | 3.255E-05 | 7.924E+08            | 1.6495E+01    | 3.248E-05 | 7.896E+08            | 0.005 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7s <sup>1</sup> S <sub>0</sub>              | 1.6736E+01    | 5.105E-05 | 1.216E+09            | 1.6677E+01    | 5.040E-05 | 1.198E+09            | 0.006 |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7s <sup>1</sup> S <sub>0</sub>              | 4.4992E+01    | 1.160E-04 | 3.821E+08            | 4.4893E+01    | 1.158E-04 | 3.801E+08            | 0.003 |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7s <sup>1</sup> S <sub>0</sub>              | 4.5777E+01    | 1.847E-04 | 5.978E+08            | 4.5651E+01    | 1.878E-04 | 5.862E+08            | 0.000 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.3961E+00    | 1.007E-05 | 3.447E+10            | 1.3903E+00    | 1.030E-05 | 3.524E+10            | 0.058 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.5287E+00    | 2.240E-05 | 1.200E+10            | 3.5145E+00    | 2.021E-05 | 1.082E+10            | 0.080 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.6306E+00    | 3.690E-05 | 4.228E+09            | 7.6005E+00    | 3.577E-05 | 4.096E+09            | 0.017 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.7227E+00    | 4.908E-06 | 5.498E+08            | 7.6924E+00    | 4.701E-06 | 5.254E+08            | 0.033 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6512E+01    | 7.368E-05 | 1.802E+09            | 1.6452E+01    | 7.311E-05 | 1.786E+09            | 0.003 |

(continued on next page)



Table 4 (continued)

| Lower   | Upper   | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|---|---|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|   |   | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.6733E+01    | 2.004E-05 | 4.773E+08              | 1.6674E+01    | 1.976E-05 | 4.701E+08              | 0.002 |
| 1s6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.4808E+01    | 2.469E-04 | 8.203E+08              | 4.4683E+01    | 2.466E-04 | 8.170E+08              | 0.001 |
| 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.5756E+01    | 9.289E-05 | 2.959E+08              | 4.5638E+01    | 9.204E-05 | 2.922E+08              | 0.002 |
| 1s2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.3363E+00    | 1.951E-05 | 1.457E+10              | 1.3308E+00    | 2.048E-05 | 1.529E+10              | 0.042 |
| 1s2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.3372E+00    | 1.256E-05 | 9.370E+09              | 1.3316E+00    | 1.289E-05 | 9.615E+09              | 0.014 |
| 1s2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.3947E+00    | 1.980E-05 | 1.358E+10              | 1.3889E+00    | 2.069E-05 | 1.419E+10              | 0.052 |
| 1s2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.4002E+00    | 7.809E-06 | 5.313E+09              | 1.3944E+00    | 7.795E-06 | 5.303E+09              | 0.015 |
| 1s3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.4080E+00    | 4.148E-05 | 4.764E+09              | 3.3940E+00    | 3.776E-05 | 4.336E+09              | 0.093 |
| 1s3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.4095E+00    | 2.597E-05 | 2.980E+09              | 3.3954E+00    | 2.386E-05 | 2.738E+09              | 0.083 |
| 1s3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.5199E+00    | 4.316E-05 | 4.648E+09              | 3.5053E+00    | 3.919E-05 | 4.219E+09              | 0.088 |
| 1s3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.5298E+00    | 1.624E-05 | 1.739E+09              | 3.5153E+00    | 1.492E-05 | 1.597E+09              | 0.074 |
| 1s4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.3699E+00    | 6.450E-05 | 1.584E+09              | 7.3391E+00    | 6.330E-05 | 1.554E+09              | 0.017 |
| 1s4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.3726E+00    | 4.081E-05 | 1.002E+09              | 7.3418E+00    | 4.004E-05 | 9.826E+08              | 0.013 |
| 1s4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.5892E+00    | 6.902E-05 | 1.599E+09              | 7.5574E+00    | 6.734E-05 | 1.559E+09              | 0.019 |
| 1s4p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.6083E+00    | 2.631E-05 | 6.063E+08              | 7.5766E+00    | 2.576E-05 | 5.936E+08              | 0.014 |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.6787E+00    | 2.525E-06 | 5.713E+07              | 7.6467E+00    | 2.419E-06 | 5.473E+07              | 0.035 |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.6803E+00    | 6.368E-07 | 1.440E+07              | 7.6482E+00    | 6.023E-07 | 1.362E+07              | 0.038 |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.7150E+00    | 1.674E-05 | 3.753E+08              | 7.6827E+00    | 1.660E-05 | 3.721E+08              | 0.011 |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.7161E+00    | 1.866E-06 | 4.181E+07              | 7.6838E+00    | 1.853E-06 | 4.152E+07              | 0.012 |
| 1s5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.5804E+01    | 1.192E-04 | 6.370E+08              | 1.5738E+01    | 1.193E-04 | 6.376E+08              | 0.006 |
| 1s5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.5810E+01    | 7.580E-05 | 4.046E+08              | 1.5744E+01    | 7.546E-05 | 4.027E+08              | 0.007 |
| 1s5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6320E+01    | 1.324E-04 | 6.632E+08              | 1.6251E+01    | 1.318E-04 | 6.605E+08              | 0.003 |
| 1s5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6364E+01    | 5.081E-05 | 2.531E+08              | 1.6297E+01    | 5.059E-05 | 2.519E+08              | 0.005 |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6532E+01    | 1.040E-05 | 5.079E+07              | 1.6464E+01    | 1.026E-05 | 5.006E+07              | 0.002 |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6535E+01    | 2.619E-06 | 1.278E+07              | 1.6468E+01    | 2.556E-06 | 1.246E+07              | 0.003 |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6618E+01    | 7.173E-05 | 3.465E+08              | 1.6550E+01    | 7.050E-05 | 3.404E+08              | 0.000 |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6621E+01    | 7.995E-06 | 3.861E+07              | 1.6552E+01    | 7.865E-06 | 3.797E+07              | 0.000 |
| 1s6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.1345E+01    | 3.330E-04 | 2.599E+08              | 4.1174E+01    | 3.369E-04 | 2.629E+08              | 0.002 |
| 1s6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.1369E+01    | 2.124E-04 | 1.656E+08              | 4.1110E+01    | 2.102E-04 | 1.645E+08              | 0.002 |
| 1s6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.3416E+01    | 4.033E-04 | 2.854E+08              | 4.3234E+01    | 4.015E-04 | 2.841E+08              | 0.002 |
| 1s6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.3599E+01    | 1.561E-04 | 1.096E+08              | 4.3396E+01    | 1.504E-04 | 1.056E+08              | 0.001 |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4291E+01    | 4.633E-05 | 3.151E+07              | 4.4127E+01    | 4.585E-05 | 3.114E+07              | 0.002 |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4306E+01    | 1.166E-05 | 7.924E+06              | 4.4127E+01    | 1.145E-05 | 7.778E+06              | 0.002 |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4650E+01    | 3.218E-04 | 2.154E+08              | 4.4483E+01    | 3.160E-04 | 2.112E+08              | 0.002 |
| 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4661E+01    | 3.588E-05 | 2.400E+07              | 4.4483E+01    | 3.507E-05 | 2.344E+07              | 0.002 |
| 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4873E+01    | 1.000E-11 | 6.626E+00              |               |           |                        | 0.004 |
| 1s7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.3800E+03    | 1.615E-07 | 1.131E+02              | 1.3760E+03    | 1.671E-07 | 1.167E+02              | 0.050 |
| 1s7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.3975E+03    | 9.892E-08 | 6.757E+01              | 1.3328E+03    | 1.150E-07 | 8.569E+01              | 0.056 |
| 1s <sup>2</sup> 1S <sub>0</sub>               | 1s7d <sup>3</sup> D <sub>2</sub>              | 3.1400E-01    | 8.874E-05 | 1.201E+12              | 3.1269E-01    | 8.899E-05 | 1.203E+12              | 0.003 |
| 1s2s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.3252E+00    | 5.634E-06 | 4.804E+09              | 1.3196E+00    | 4.807E-06 | 3.652E+09              | 0.011 |
| 1s2s <sup>1</sup> S <sub>0</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.3374E+00    | 2.905E-06 | 2.166E+09              | 1.3319E+00    | 2.936E-06 | 2.189E+09              | 0.005 |
| 1s3s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 3.3879E+00    | 3.868E-05 | 4.496E+09              | 3.3736E+00    | 3.838E-05 | 4.460E+09              | 0.019 |
| 1s3s <sup>1</sup> S <sub>0</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 3.4088E+00    | 2.598E-05 | 2.982E+09              | 3.3947E+00    | 2.385E-05 | 2.738E+09              | 0.083 |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 3.5276E+00    | 1.899E-05 | 2.036E+09              | 3.5127E+00    | 1.903E-05 | 2.040E+09              | 0.014 |
| 1s3d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 3.5291E+00    | 8.666E-06 | 9.282E+08              | 3.5142E+00    | 8.452E-06 | 9.053E+08              | 0.033 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 3.5644E+00    | 8.974E-06 | 9.422E+08              | 3.5492E+00    | 9.129E-06 | 9.585E+08              | 0.026 |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 3.5659E+00    | 2.321E-06 | 2.435E+08              | 3.5507E+00    | 2.101E-06 | 2.204E+08              | 0.049 |
| 1s4s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 7.3299E+00    | 8.891E-05 | 2.208E+09              | 7.2988E+00    | 8.993E-05 | 2.233E+09              | 0.018 |
| 1s4s <sup>1</sup> S <sub>0</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 7.3694E+00    | 6.004E-05 | 1.475E+09              | 7.3385E+00    | 5.614E-05 | 1.378E+09              | 0.065 |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 7.6027E+00    | 4.717E-05 | 1.089E+09              | 7.5707E+00    | 4.709E-05 | 1.086E+09              | 0.005 |
| 1s4d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 7.6055E+00    | 2.106E-05 | 4.857E+08              | 7.5734E+00    | 2.095E-05 | 4.831E+08              | 0.015 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 7.6748E+00    | 2.282E-05 | 5.168E+08              | 7.6422E+00    | 2.304E-05 | 5.219E+08              | 0.009 |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 7.6778E+00    | 5.714E-06 | 1.293E+08              | 7.6453E+00    | 5.373E-06 | 1.216E+08              | 0.022 |
| 1s5s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.5705E+01    | 1.967E-04 | 1.064E+09              | 1.5637E+01    | 1.998E-04 | 1.080E+09              | 0.010 |
| 1s5s <sup>1</sup> S <sub>0</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.5796E+01    | 1.300E-04 | 6.949E+08              | 1.5728E+01    | 1.247E-04 | 6.669E+08              | 0.032 |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.6345E+01    | 1.087E-04 | 5.426E+08              | 1.6276E+01    | 1.083E-04 | 5.410E+08              | 0.002 |
| 1s5d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.6352E+01    | 4.805E-05 | 2.397E+08              | 1.6283E+01    | 4.822E-05 | 2.406E+08              | 0.006 |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.6516E+01    | 5.357E-05 | 2.620E+08              | 1.6446E+01    | 5.404E-05 | 2.643E+08              | 0.003 |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.6523E+01    | 1.324E-05 | 6.468E+07              | 1.6453E+01    | 1.267E-05 | 6.194E+07              | 0.008 |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.6605E+01    | 1.575E-05 | 7.622E+07              | 1.6532E+01    | 1.579E-05 | 7.646E+07              | 0.004 |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.6607E+01    | 1.787E-06 | 8.644E+06              | 1.6534E+01    | 1.793E-06 | 8.675E+06              | 0.006 |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.6658E+01    | 1.251E-09 | 6.016E+03              |               |           |                        | 0.062 |
| 1s6s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.0924E+01    | 6.099E-04 | 4.858E+08              | 4.0701E+01    | 6.286E-04 | 5.019E+08              | 0.005 |
| 1s6s <sup>1</sup> S <sub>0</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.1279E+01    | 4.030E-04 | 3.155E+08              | 4.1000E+01    | 3.906E-04 | 3.073E+08              | 0.010 |
| 1s6d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.3482E+01    | 3.650E-04 | 2.575E+08              | 4.3306E+01    | 3.626E-04 | 2.557E+08              | 0.000 |
| 1s6d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.3508E+01    | 1.610E-04 | 1.134E+08              | 4.3299E+01    | 1.611E-04 | 1.136E+08              | 0.002 |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.4184E+01    | 1.862E-04 | 1.273E+08              | 4.4000E+01    | 1.879E-04 | 1.284E+08              | 0.001 |
| 1s6d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.4215E+01    | 4.585E-05 | 3.129E+07              | 4.4010E+01    | 4.550E-05 | 3.107E+07              | 0.002 |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.4555E+01    | 1.252E-04 | 8.413E+07              | 4.4353E+01    | 1.252E-04 | 8.424E+07              | 0.001 |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.4564E+01    | 1.411E-05 | 9.479E+06              | 4.4353E+01    | 1.421E-05 | 9.558E+06              | 0.001 |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.4778E+01    | 9.656E-09 | 6.424E+03              |               |           |                        | 0.020 |

(continued on next page)

Table 4 (continued)

| Lower   | Upper   | GRASP2K       |           |                  | FAC           |           |                  | dT    |
|---|---|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|   |   | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) |       |
| 1s7s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.1072E+03    | 2.944E-07 | 3.203E+02        | 1.0773E+03    | 3.188E-07 | 3.634E+02        | 0.006 |
| 1s7s <sup>1</sup> S <sub>0</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.2957E+03    | 1.189E-07 | 9.449E+01        | 1.2249E+03    | 1.375E-07 | 1.212E+02        | 0.126 |
| 1s2s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.3252E+00    | 5.552E-06 | 7.029E+09        | 1.3196E+00    | 4.696E-06 | 5.945E+09        | 0.006 |
| 1s3s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 3.3878E+00    | 3.820E-05 | 7.401E+09        | 3.3737E+00    | 3.769E-05 | 7.300E+09        | 0.030 |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 3.5275E+00    | 8.231E-06 | 1.471E+09        | 3.5127E+00    | 8.300E-06 | 1.483E+09        | 0.022 |
| 1s3d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 3.5290E+00    | 8.464E-06 | 1.511E+09        | 3.5142E+00    | 8.198E-06 | 1.463E+09        | 0.028 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 3.5643E+00    | 1.509E-06 | 2.641E+08        | 3.5493E+00    | 1.491E-06 | 2.609E+08        | 0.001 |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 3.5657E+00    | 5.413E-06 | 9.465E+08        | 3.5507E+00    | 5.166E-06 | 9.033E+08        | 0.024 |
| 1s4s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 7.3294E+00    | 8.823E-05 | 3.652E+09        | 7.2989E+00    | 8.841E-05 | 3.658E+09        | 0.022 |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 7.6021E+00    | 2.061E-05 | 7.929E+08        | 7.5708E+00    | 2.062E-05 | 7.933E+08        | 0.010 |
| 1s4d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 7.6050E+00    | 2.052E-05 | 7.888E+08        | 7.5736E+00    | 2.029E-05 | 7.799E+08        | 0.011 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 7.6743E+00    | 3.729E-06 | 1.408E+08        | 7.6424E+00    | 3.765E-06 | 1.421E+08        | 0.009 |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 7.6772E+00    | 1.328E-05 | 5.009E+08        | 7.6454E+00    | 1.298E-05 | 4.895E+08        | 0.009 |
| 1s5s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.5703E+01    | 1.954E-04 | 1.762E+09        | 1.5638E+01    | 1.965E-04 | 1.771E+09        | 0.012 |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.6343E+01    | 4.762E-05 | 3.964E+08        | 1.6277E+01    | 4.755E-05 | 3.957E+08        | 0.004 |
| 1s5d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.6349E+01    | 4.677E-05 | 3.891E+08        | 1.6283E+01    | 4.670E-05 | 3.883E+08        | 0.004 |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.6513E+01    | 8.732E-06 | 7.120E+07        | 1.6446E+01    | 8.833E-06 | 7.199E+07        | 0.004 |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.6521E+01    | 3.074E-05 | 2.504E+08        | 1.6453E+01    | 3.038E-05 | 2.474E+08        | 0.003 |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.6605E+01    | 1.059E-05 | 8.544E+07        | 1.6535E+01    | 1.055E-05 | 8.509E+07        | 0.005 |
| 1s6s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 4.0910E+01    | 6.049E-04 | 8.036E+08        | 4.0705E+01    | 6.166E-04 | 8.204E+08        | 0.005 |
| 1s6d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 4.3465E+01    | 1.599E-04 | 1.882E+08        | 4.3310E+01    | 1.611E-04 | 1.893E+08        | 0.001 |
| 1s6d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 4.3492E+01    | 1.564E-04 | 1.839E+08        | 4.3303E+01    | 1.580E-04 | 1.858E+08        | 0.001 |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 4.4167E+01    | 3.032E-05 | 3.456E+07        | 4.4004E+01    | 3.073E-05 | 3.498E+07        | 0.001 |
| 1s6d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 4.4198E+01    | 1.063E-04 | 1.210E+08        | 4.4015E+01    | 1.044E-04 | 1.188E+08        | 0.001 |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 4.4547E+01    | 8.358E-05 | 9.356E+07        | 4.4358E+01    | 8.369E-05 | 9.377E+07        | 0.001 |
| 1s7s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.0966E+03    | 3.011E-07 | 5.566E+02        | 1.0799E+03    | 3.104E-07 | 5.869E+02        | 0.012 |
| 1s7d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.1420E+05    | 1.309E-13 | 2.231E-08        |               |           |                  | 0.944 |
| 1s2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.3362E+00    | 1.852E-05 | 2.307E+10        | 1.3307E+00    | 1.812E-05 | 2.256E+10        | 0.019 |
| 1s2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.3946E+00    | 7.635E-06 | 8.728E+09        | 1.3888E+00    | 7.793E-06 | 8.907E+09        | 0.061 |
| 1s2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.4001E+00    | 1.156E-05 | 1.311E+10        | 1.3943E+00    | 1.090E-05 | 1.237E+10        | 0.054 |
| 1s3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.4073E+00    | 3.665E-05 | 7.020E+09        | 3.3933E+00    | 3.370E-05 | 6.452E+09        | 0.076 |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.5191E+00    | 1.673E-05 | 3.003E+09        | 3.5046E+00    | 1.472E-05 | 2.642E+09        | 0.087 |
| 1s3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.5290E+00    | 2.143E-05 | 3.826E+09        | 3.5146E+00    | 2.066E-05 | 3.687E+09        | 0.042 |
| 1s4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.3666E+00    | 5.772E-05 | 2.365E+09        | 7.3362E+00    | 5.662E-05 | 2.319E+09        | 0.010 |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.5857E+00    | 2.671E-05 | 1.032E+09        | 7.5543E+00    | 2.524E-05 | 9.753E+08        | 0.018 |
| 1s4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.6047E+00    | 3.529E-05 | 1.357E+09        | 7.5735E+00    | 3.553E-05 | 1.365E+09        | 0.001 |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.6752E+00    | 5.944E-07 | 2.244E+07        | 7.6436E+00    | 6.387E-07 | 2.410E+07        | 0.038 |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.6767E+00    | 1.327E-06 | 5.007E+07        | 7.6451E+00    | 1.227E-06 | 4.628E+07        | 0.037 |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.7125E+00    | 1.103E-05 | 4.124E+08        | 7.6807E+00    | 1.104E-05 | 4.127E+08        | 0.012 |
| 1s5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.5788E+01    | 1.070E-04 | 9.547E+08        | 1.5725E+01    | 1.067E-04 | 9.520E+08        | 0.009 |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.6303E+01    | 5.105E-05 | 4.271E+08        | 1.6237E+01    | 4.929E-05 | 4.121E+08        | 0.003 |
| 1s5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.6348E+01    | 6.835E-05 | 5.686E+08        | 1.6282E+01    | 6.968E-05 | 5.795E+08        | 0.009 |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.6515E+01    | 2.442E-06 | 1.991E+07        | 1.6450E+01    | 2.714E-06 | 2.211E+07        | 0.003 |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.6519E+01    | 5.460E-06 | 4.449E+07        | 1.6453E+01    | 5.203E-06 | 4.237E+07        | 0.003 |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.6604E+01    | 4.732E-05 | 3.817E+08        | 1.6538E+01    | 4.695E-05 | 3.785E+08        | 0.000 |
| 1s6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.1241E+01    | 2.976E-04 | 3.891E+08        | 4.1082E+01    | 2.898E-04 | 3.786E+08        | 0.001 |
| 1s6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.3302E+01    | 1.543E-04 | 1.829E+08        | 4.3133E+01    | 1.489E-04 | 1.764E+08        | 0.002 |
| 1s6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.3483E+01    | 2.090E-04 | 2.457E+08        | 4.3294E+01    | 2.181E-04 | 2.565E+08        | 0.001 |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.4172E+01    | 1.082E-05 | 1.233E+07        | 4.4022E+01    | 1.212E-05 | 1.379E+07        | 0.002 |
| 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.4186E+01    | 2.423E-05 | 2.759E+07        | 4.4022E+01    | 2.300E-05 | 2.617E+07        | 0.002 |
| 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.4540E+01    | 2.117E-04 | 2.373E+08        | 4.4376E+01    | 2.118E-04 | 2.371E+08        | 0.002 |
| 1s7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.2731E+03    | 1.853E-07 | 2.541E+02        | 1.2808E+03    | 1.800E-07 | 2.420E+02        | 0.047 |
| 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.6436E+04    | 4.209E-11 | 3.465E-04        |               |           |                  | 0.021 |
| 1s2s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.3248E+00    | 1.758E-05 | 9.543E+09        | 1.3192E+00    | 1.588E-05 | 8.622E+09        | 0.002 |
| 1s3s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 3.3852E+00    | 9.868E-05 | 8.205E+09        | 3.3710E+00    | 9.907E-05 | 8.237E+09        | 0.026 |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 3.5248E+00    | 9.707E-06 | 7.445E+08        | 3.5099E+00    | 9.973E-06 | 7.649E+08        | 0.021 |
| 1s3d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 3.5263E+00    | 1.642E-06 | 1.258E+08        | 3.5113E+00    | 1.619E-06 | 1.240E+08        | 0.023 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 3.5615E+00    | 3.721E-05 | 2.795E+09        | 3.5464E+00    | 3.778E-05 | 2.838E+09        | 0.022 |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 3.5629E+00    | 6.409E-06 | 4.811E+08        | 3.5478E+00    | 6.234E-06 | 4.679E+08        | 0.024 |
| 1s4s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 7.3175E+00    | 2.171E-04 | 3.863E+09        | 7.2866E+00    | 2.196E-04 | 3.908E+09        | 0.021 |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 7.5894E+00    | 2.398E-05 | 3.967E+08        | 7.5575E+00    | 2.428E-05 | 4.016E+08        | 0.009 |
| 1s4d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 7.5922E+00    | 3.931E-06 | 6.498E+07        | 7.5603E+00    | 3.920E-06 | 6.479E+07        | 0.007 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 7.6613E+00    | 9.279E-05 | 1.506E+09        | 7.6289E+00    | 9.340E-05 | 1.516E+09        | 0.009 |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 7.6642E+00    | 1.550E-05 | 2.515E+08        | 7.6319E+00    | 1.533E-05 | 2.487E+08        | 0.010 |
| 1s5s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.5649E+01    | 4.656E-04 | 1.812E+09        | 1.5581E+01    | 4.708E-04 | 1.832E+09        | 0.011 |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.6284E+01    | 5.459E-05 | 1.962E+08        | 1.6216E+01    | 5.492E-05 | 1.973E+08        | 0.003 |
| 1s5d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.6290E+01    | 8.844E-06 | 3.176E+07        | 1.6222E+01    | 8.848E-06 | 3.176E+07        | 0.002 |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.6453E+01    | 2.142E-04 | 7.541E+08        | 1.6384E+01    | 2.148E-04 | 7.562E+08        | 0.003 |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.6460E+01    | 3.535E-05 | 1.243E+08        | 1.6391E+01    | 3.519E-05 | 1.237E+08        | 0.004 |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.6542E+01    | 1.538E-06 | 5.355E+06        | 1.6470E+01    | 1.547E-06 | 5.389E+06        | 0.004 |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.6544E+01    | 1.868E-07 | 6.503E+05        | 1.6472E+01    | 1.859E-07 | 6.476E+05        | 0.006 |

(continued on next page)

Table 4 (continued)

| Lower                             | Upper                             | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|-----------------------------------|-----------------------------------|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|                                   |                                   | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s 5g <sup>3</sup> G <sub>5</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 1.6593E+01    | 2.071E-05 | 7.169E+07              | 1.6521E+01    | 2.073E-05 | 7.178E+07              | 0.003 |
| 1s 5g <sup>1</sup> G <sub>4</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 1.6595E+01    | 1.270E-06 | 4.394E+06              | 1.6522E+01    | 1.261E-06 | 4.366E+06              | 0.005 |
| 1s 6s <sup>3</sup> S <sub>1</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 4.0543E+01    | 1.383E-03 | 8.018E+08              | 4.0325E+01    | 1.412E-03 | 8.208E+08              | 0.005 |
| 1s 6d <sup>3</sup> D <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 4.3051E+01    | 1.778E-04 | 9.140E+07              | 4.2880E+01    | 1.798E-04 | 9.239E+07              | 0.001 |
| 1s 6d <sup>3</sup> D <sub>1</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 4.3077E+01    | 2.870E-05 | 1.474E+07              | 4.2874E+01    | 2.939E-05 | 1.510E+07              | 0.001 |
| 1s 6d <sup>3</sup> D <sub>3</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 4.3740E+01    | 4.374E-04 | 3.587E+08              | 4.3560E+01    | 7.214E-04 | 3.592E+08              | 0.001 |
| 1s 6d <sup>1</sup> D <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 4.3770E+01    | 1.184E-04 | 5.887E+07              | 4.3571E+01    | 1.168E-04 | 5.813E+07              | 0.001 |
| 1s 6g <sup>3</sup> G <sub>4</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 4.4103E+01    | 1.214E-05 | 5.945E+06              | 4.3907E+01    | 1.220E-05 | 5.980E+06              | 0.001 |
| 1s 6g <sup>3</sup> G <sub>3</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 4.4112E+01    | 1.464E-06 | 7.171E+05              | 4.3907E+01    | 1.464E-06 | 7.176E+05              | 0.001 |
| 1s 6g <sup>3</sup> G <sub>5</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 4.4315E+01    | 1.637E-04 | 7.941E+07              | 4.4116E+01    | 1.636E-04 | 7.946E+07              | 0.001 |
| 1s 6g <sup>1</sup> G <sub>4</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 4.4321E+01    | 9.975E-06 | 4.839E+06              | 4.4116E+01    | 9.920E-06 | 4.815E+06              | 0.001 |
| 1s 7s <sup>3</sup> S <sub>1</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 8.8243E+02    | 1.362E-06 | 1.667E+03              | 8.6393E+02    | 1.431E-06 | 1.811E+03              | 0.002 |
| 1s 7d <sup>3</sup> D <sub>2</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 4.3459E+03    | 2.721E-09 | 1.373E-01              |               |           |                        | 0.004 |
| 1s 7d <sup>3</sup> D <sub>1</sub> | 1s 7d <sup>3</sup> D <sub>3</sub> | 4.5178E+03    | 3.927E-10 | 1.833E-02              |               |           |                        | 0.021 |
| 1s 2p <sup>3</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 1.3358E+00    | 5.669E-04 | 3.027E-11              | 1.3303E+00    | 5.764E-04 | 3.077E+11              | 0.000 |
| 1s 2p <sup>3</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 1.3942E+00    | 1.500E-04 | 7.354E+10              | 1.3883E+00    | 1.493E-04 | 7.322E+10              | 0.014 |
| 1s 2p <sup>1</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 1.3997E+00    | 3.473E-05 | 1.689E+10              | 1.3939E+00    | 3.421E-05 | 1.663E+10              | 0.036 |
| 1s 3p <sup>3</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 3.4047E+00    | 1.597E-05 | 1.313E+09              | 3.3906E+00    | 1.883E-05 | 1.547E+09              | 0.110 |
| 1s 3p <sup>3</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 3.5164E+00    | 9.649E-06 | 7.436E+08              | 3.5016E+00    | 1.109E-05 | 8.551E+08              | 0.073 |
| 1s 3p <sup>1</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 3.5263E+00    | 2.608E-06 | 1.999E+08              | 3.5116E+00    | 2.267E-06 | 1.737E+08              | 0.007 |
| 1s 4p <sup>3</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 7.3546E+00    | 6.464E-05 | 1.139E+09              | 7.3233E+00    | 6.291E-05 | 1.108E+09              | 0.012 |
| 1s 4p <sup>3</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 7.5729E+00    | 7.761E-06 | 1.290E+08              | 7.5406E+00    | 7.141E-06 | 1.186E+08              | 0.023 |
| 1s 4p <sup>1</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 7.5920E+00    | 1.634E-06 | 2.702E+07              | 7.5597E+00    | 1.856E-06 | 3.069E+07              | 0.016 |
| 1s 4f <sup>3</sup> F <sub>3</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 7.6621E+00    | 4.344E-05 | 7.051E+08              | 7.6295E+00    | 4.280E-05 | 6.948E+08              | 0.011 |
| 1s 4f <sup>3</sup> F <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 7.6636E+00    | 7.207E-06 | 1.169E+08              | 7.6310E+00    | 7.140E-06 | 1.158E+08              | 0.011 |
| 1s 4f <sup>3</sup> F <sub>4</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 7.6982E+00    | 7.258E-06 | 1.167E+08              | 7.6653E+00    | 7.235E-06 | 1.163E+08              | 0.004 |
| 1s 4f <sup>1</sup> F <sub>3</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 7.6993E+00    | 8.713E-07 | 1.401E+07              | 7.6665E+00    | 8.328E-07 | 1.338E+07              | 0.003 |
| 1s 5p <sup>3</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 1.5734E+01    | 4.148E-04 | 1.597E+09              | 1.5665E+01    | 4.152E-04 | 1.598E+09              | 0.004 |
| 1s 5p <sup>3</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 1.6245E+01    | 8.271E-05 | 2.987E+08              | 1.6174E+01    | 8.226E-05 | 2.971E+08              | 0.002 |
| 1s 5p <sup>1</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 1.6289E+01    | 1.901E-05 | 6.828E+07              | 1.6219E+01    | 1.921E-05 | 6.900E+07              | 0.008 |
| 1s 5f <sup>3</sup> F <sub>3</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 1.6455E+01    | 1.515E-04 | 5.333E+08              | 1.6385E+01    | 1.511E-04 | 5.319E+08              | 0.001 |
| 1s 5f <sup>3</sup> F <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 1.6459E+01    | 2.517E-05 | 8.855E+07              | 1.6388E+01    | 2.523E-05 | 8.877E+07              | 0.001 |
| 1s 5f <sup>3</sup> F <sub>4</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 1.6540E+01    | 2.593E-05 | 9.030E+07              | 1.6469E+01    | 2.592E-05 | 9.031E+07              | 0.000 |
| 1s 5f <sup>1</sup> F <sub>3</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 1.6543E+01    | 3.118E-06 | 1.086E+07              | 1.6472E+01    | 2.991E-06 | 1.041E+07              | 0.000 |
| 1s 6p <sup>3</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 4.0868E+01    | 1.936E-03 | 1.105E+09              | 4.0680E+01    | 1.929E-03 | 1.101E+09              | 0.001 |
| 1s 6p <sup>3</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 4.2891E+01    | 4.845E-04 | 2.510E+08              | 4.2690E+01    | 4.909E-04 | 2.545E+08              | 0.001 |
| 1s 6p <sup>1</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 4.3069E+01    | 1.141E-04 | 5.864E+07              | 4.2848E+01    | 1.182E-04 | 6.086E+07              | 0.000 |
| 1s 6f <sup>3</sup> F <sub>3</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 4.3744E+01    | 6.234E-04 | 3.104E+08              | 4.3561E+01    | 6.229E-04 | 3.101E+08              | 0.000 |
| 1s 6f <sup>3</sup> F <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 4.3758E+01    | 1.037E-04 | 5.161E+07              | 4.3560E+01    | 1.039E-04 | 5.177E+07              | 0.000 |
| 1s 6f <sup>3</sup> F <sub>4</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 4.4094E+01    | 1.088E-04 | 5.331E+07              | 4.3907E+01    | 1.091E-04 | 5.351E+07              | 0.000 |
| 1s 6f <sup>1</sup> F <sub>3</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 4.4105E+01    | 1.310E-05 | 6.419E+06              | 4.3907E+01    | 1.307E-05 | 6.406E+06              | 0.000 |
| 1s 6h <sup>3</sup> H <sub>3</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 4.4306E+01    | 4.016E-05 | 1.949E+07              | 4.4116E+01    | 4.014E-05 | 1.949E+07              | 0.001 |
| 1s 6h <sup>3</sup> H <sub>4</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 4.4312E+01    | 2.427E-06 | 1.178E+06              | 4.4116E+01    | 2.436E-06 | 1.182E+06              | 0.001 |
| 1s 6h <sup>1</sup> H <sub>3</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 4.4452E+01    | 5.514E-12 | 2.659E+00              |               |           |                        | 0.017 |
| 1s 7p <sup>3</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 9.9322E+02    | 7.907E-07 | 7.638E+02              | 9.7893E+02    | 8.183E-07 | 8.067E+02              | 0.104 |
| 1s 7p <sup>3</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 3.5436E+03    | 4.295E-09 | 3.259E-01              | 3.3920E+03    | 4.895E-09 | 4.019E-01              | 0.273 |
| 1s 7p <sup>1</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>3</sub> | 4.5177E+03    | 4.880E-10 | 2.279E-02              |               |           |                        | 0.371 |
| 1s 2p <sup>3</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 1.3358E+00    | 1.757E-04 | 1.314E+11              | 1.3303E+00    | 1.782E-04 | 1.332E+11              | 0.010 |
| 1s 2p <sup>3</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 1.3367E+00    | 2.481E-04 | 1.852E+11              | 1.3311E+00    | 2.514E-04 | 1.876E+11              | 0.002 |
| 1s 2p <sup>1</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 1.3942E+00    | 3.754E-05 | 2.577E+10              | 1.3883E+00    | 3.730E-05 | 2.559E+10              | 0.012 |
| 1s 2p <sup>1</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 1.3997E+00    | 7.771E-05 | 5.292E+10              | 1.3939E+00    | 7.705E-05 | 5.245E+10              | 0.006 |
| 1s 3p <sup>3</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 3.4047E+00    | 4.739E-06 | 5.454E+08              | 3.3906E+00    | 5.997E-06 | 6.900E+08              | 0.127 |
| 1s 3p <sup>3</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 3.4061E+00    | 6.996E-06 | 8.044E+08              | 3.3920E+00    | 8.272E-06 | 9.510E+08              | 0.112 |
| 1s 3p <sup>1</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 3.5163E+00    | 2.405E-06 | 2.595E+08              | 3.5016E+00    | 2.771E-06 | 2.990E+08              | 0.079 |
| 1s 3p <sup>1</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 3.5262E+00    | 5.409E-06 | 5.803E+08              | 3.5116E+00    | 5.984E-06 | 6.419E+08              | 0.060 |
| 1s 4p <sup>3</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 7.3543E+00    | 1.993E-05 | 4.916E+08              | 7.3233E+00    | 1.884E-05 | 4.647E+08              | 0.016 |
| 1s 4p <sup>3</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 7.3571E+00    | 2.804E-05 | 6.912E+08              | 7.3259E+00    | 2.725E-05 | 6.717E+08              | 0.013 |
| 1s 4p <sup>1</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 7.5727E+00    | 1.956E-06 | 4.550E+07              | 7.5406E+00    | 1.789E-06 | 4.163E+07              | 0.025 |
| 1s 4p <sup>1</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 7.5917E+00    | 3.790E-06 | 8.772E+07              | 7.5597E+00    | 3.599E-06 | 8.193E+07              | 0.018 |
| 1s 4f <sup>3</sup> F <sub>3</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 7.6619E+00    | 7.214E-06 | 1.639E+08              | 7.6295E+00    | 7.104E-06 | 1.614E+08              | 0.010 |
| 1s 4f <sup>3</sup> F <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 7.6634E+00    | 2.888E-05 | 6.561E+08              | 7.6310E+00    | 2.850E-05 | 6.474E+08              | 0.010 |
| 1s 4f <sup>3</sup> F <sub>4</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 7.6979E+00    | 5.832E-07 | 1.313E+07              | 7.6653E+00    | 5.781E-07 | 1.301E+07              | 0.001 |
| 1s 4f <sup>1</sup> F <sub>3</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 7.6990E+00    | 5.275E-06 | 1.187E+08              | 7.6665E+00    | 5.227E-06 | 1.176E+08              | 0.004 |
| 1s 5p <sup>3</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 1.5732E+01    | 1.269E-04 | 6.840E+08              | 1.5665E+01    | 1.261E-04 | 6.801E+08              | 0.003 |
| 1s 5p <sup>3</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 1.5739E+01    | 1.803E-04 | 9.713E+08              | 1.5671E+01    | 1.804E-04 | 9.720E+08              | 0.004 |
| 1s 5p <sup>1</sup> P <sub>0</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 1.6243E+01    | 2.078E-05 | 1.051E+08              | 1.6174E+01    | 2.059E-05 | 1.041E+08              | 0.002 |
| 1s 5p <sup>1</sup> P <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 1.6288E+01    | 4.275E-05 | 2.150E+08              | 1.6219E+01    | 4.240E-05 | 2.132E+08              | 0.003 |
| 1s 5f <sup>3</sup> F <sub>3</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 1.6454E+01    | 2.516E-05 | 1.240E+08              | 1.6385E+01    | 2.509E-05 | 1.236E+08              | 0.001 |
| 1s 5f <sup>3</sup> F <sub>2</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 1.6457E+01    | 1.008E-04 | 4.967E+08              | 1.6388E+01    | 1.006E-04 | 4.955E+08              | 0.001 |
| 1s 5f <sup>3</sup> F <sub>4</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 1.6539E+01    | 2.071E-06 | 1.010E+07              | 1.6469E+01    | 2.072E-06 | 1.010E+07              | 0.001 |
| 1s 5f <sup>1</sup> F <sub>3</sub> | 1s 7f <sup>3</sup> F <sub>2</sub> | 1.6542E+01    | 1.883E-05 | 9.182E+07              | 1.6472E+01    | 1.872E-05 | 9.128E+07              | 0.000 |

(continued on next page)

Table 4 (continued)

| Lower  | Upper  | GRASP2K       |           |                      | FAC           |           |                      | dT    |
|--|--|---------------|-----------|----------------------|---------------|-----------|----------------------|-------|
|  |  | $\lambda$ (Å) | gf        | A (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | A (s <sup>-1</sup> ) |       |
| 1s 6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.0860E+01    | 5.906E-04 | 4.719E+08            | 4.0680E+01    | 6.038E-04 | 4.826E+08            | 0.001 |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.0884E+01    | 8.426E-04 | 6.725E+08            | 4.0618E+01    | 8.498E-04 | 6.814E+08            | 0.001 |
| 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.2882E+01    | 1.216E-04 | 8.820E+07            | 4.2690E+01    | 1.225E-04 | 8.897E+07            | 0.001 |
| 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3060E+01    | 2.556E-04 | 1.839E+08            | 4.2848E+01    | 2.487E-04 | 1.792E+08            | 0.001 |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3735E+01    | 1.035E-04 | 7.216E+07            | 4.3561E+01    | 1.039E-04 | 7.247E+07            | 0.000 |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3749E+01    | 4.148E-04 | 2.891E+08            | 4.3561E+01    | 4.154E-04 | 2.896E+08            | 0.000 |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4085E+01    | 8.672E-06 | 5.953E+06            | 4.3907E+01    | 8.726E-06 | 5.987E+06            | 0.000 |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4096E+01    | 7.898E-05 | 5.418E+07            | 4.3907E+01    | 7.843E-05 | 5.381E+07            | 0.000 |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4302E+01    | 3.039E-05 | 2.066E+07            | 4.4116E+01    | 3.041E-05 | 2.067E+07            | 0.001 |
| 1s 7p <sup>3</sup> P <sub>4</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 9.8851E+02    | 2.450E-07 | 3.345E+02            | 9.7899E+02    | 2.541E-07 | 3.507E+02            | 0.101 |
| 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 9.9743E+02    | 3.397E-07 | 4.556E+02            | 9.5689E+02    | 3.834E-07 | 5.539E+02            | 0.104 |
| 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.8444E+03    | 1.135E-09 | 1.247E-01            | 3.3927E+03    | 1.221E-09 | 1.403E-01            | 0.269 |
| 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4219E+03    | 1.166E-09 | 7.956E-02            | 4.1543E+03    | 1.350E-09 | 1.035E-01            | 0.323 |
| 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 2.0860E+05    | 1.383E-14 | 4.240E-10            |               |           |                      | 0.119 |
| 1s <sup>2</sup> S <sub>0</sub>                 | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.1390E-01    | 1.285E-04 | 1.738E+12            | 3.1267E-01    | 1.498E-04 | 2.027E+12            | 0.002 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.3248E+00    | 5.060E-06 | 3.847E+09            | 1.3192E+00    | 4.425E-06 | 3.363E+09            | 0.012 |
| 1s 2s <sup>1</sup> S <sub>0</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.3369E+00    | 6.434E-06 | 4.802E+09            | 1.3314E+00    | 6.727E-06 | 5.019E+09            | 0.002 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.3851E+00    | 2.803E-05 | 3.263E+09            | 3.3710E+00    | 2.747E-05 | 3.197E+09            | 0.019 |
| 1s 3s <sup>1</sup> S <sub>0</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.4060E+00    | 4.485E-05 | 5.158E+09            | 3.3920E+00    | 4.243E-05 | 4.878E+09            | 0.081 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.5247E+00    | 2.531E-06 | 2.717E+08            | 3.5098E+00    | 2.588E-06 | 2.779E+08            | 0.006 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.5261E+00    | 5.861E-06 | 6.288E+08            | 3.5113E+00    | 5.640E-06 | 6.051E+08            | 0.033 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.5614E+00    | 6.094E-06 | 6.409E+08            | 3.5463E+00    | 6.116E-06 | 6.433E+08            | 0.027 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.5628E+00    | 2.633E-05 | 2.767E+09            | 3.5477E+00    | 2.540E-05 | 2.669E+09            | 0.033 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.3170E+00    | 6.124E-05 | 1.526E+09            | 7.2864E+00    | 6.084E-05 | 1.515E+09            | 0.018 |
| 1s 4s <sup>1</sup> S <sub>0</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.3564E+00    | 9.856E-05 | 2.430E+09            | 7.3260E+00    | 9.436E-05 | 2.325E+09            | 0.064 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.5888E+00    | 6.059E-06 | 1.403E+08            | 7.5573E+00    | 6.203E-06 | 1.436E+08            | 0.003 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.5916E+00    | 1.403E-05 | 3.247E+08            | 7.5601E+00    | 1.369E-05 | 3.169E+08            | 0.015 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.6607E+00    | 1.525E-05 | 3.466E+08            | 7.6287E+00    | 1.511E-05 | 3.435E+08            | 0.010 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.6636E+00    | 6.371E-05 | 1.447E+09            | 7.6317E+00    | 6.287E-05 | 1.427E+09            | 0.014 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.5646E+01    | 1.309E-04 | 7.133E+08            | 1.5580E+01    | 1.303E-04 | 7.100E+08            | 0.010 |
| 1s 5s <sup>1</sup> S <sub>0</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.5737E+01    | 2.061E-04 | 1.110E+09            | 1.5671E+01    | 2.021E-04 | 1.088E+09            | 0.033 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6281E+01    | 1.358E-05 | 6.833E+07            | 1.6215E+01    | 1.394E-05 | 7.013E+07            | 0.001 |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6288E+01    | 3.146E-05 | 1.582E+08            | 1.6221E+01    | 3.092E-05 | 1.554E+08            | 0.006 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6451E+01    | 3.517E-05 | 1.734E+08            | 1.6383E+01    | 3.475E-05 | 1.712E+08            | 0.004 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6458E+01    | 1.450E-04 | 7.144E+08            | 1.6390E+01    | 1.447E-04 | 7.124E+08            | 0.005 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6539E+01    | 1.475E-07 | 7.192E+05            | 1.6469E+01    | 1.668E-07 | 8.136E+05            | 0.010 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6541E+01    | 1.101E-06 | 5.368E+06            | 1.6471E+01    | 1.083E-06 | 5.283E+06            | 0.005 |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6592E+01    | 1.578E-05 | 7.645E+07            | 1.6521E+01    | 1.569E-05 | 7.608E+07            | 0.004 |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.0526E+01    | 3.877E-04 | 3.150E+08            | 4.0319E+01    | 3.915E-04 | 3.186E+08            | 0.005 |
| 1s 6s <sup>1</sup> S <sub>0</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.0874E+01    | 6.098E-04 | 4.870E+08            | 4.0613E+01    | 6.046E-04 | 4.848E+08            | 0.010 |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.3033E+01    | 4.383E-05 | 3.157E+07            | 4.2873E+01    | 4.367E-05 | 3.143E+07            | 0.000 |
| 1s 6d <sup>3</sup> D <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.3059E+01    | 1.018E-04 | 7.325E+07            | 4.2867E+01    | 9.979E-05 | 7.183E+07            | 0.002 |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.3721E+01    | 1.180E-04 | 8.234E+07            | 4.3553E+01    | 1.166E-04 | 8.133E+07            | 0.001 |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.3751E+01    | 4.848E-04 | 3.379E+08            | 4.3564E+01    | 4.878E-04 | 3.400E+08            | 0.001 |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.4084E+01    | 1.166E-06 | 8.003E+05            | 4.3900E+01    | 1.267E-06 | 8.701E+05            | 0.003 |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.4092E+01    | 8.625E-06 | 5.918E+06            | 4.3900E+01    | 8.518E-06 | 5.846E+06            | 0.001 |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.4302E+01    | 1.239E-04 | 8.420E+07            | 4.4109E+01    | 1.240E-04 | 8.433E+07            | 0.001 |
| 1s 7s <sup>3</sup> S <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 8.7478E+02    | 3.916E-07 | 6.827E+02            | 8.6126E+02    | 4.005E-07 | 7.142E+02            | 0.006 |
| 1s 7s <sup>1</sup> S <sub>0</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 9.8833E+02    | 4.178E-07 | 5.706E+02            | 9.5307E+02    | 4.657E-07 | 6.782E+02            | 0.090 |
| 1s 7d <sup>3</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.1666E+03    | 7.586E-10 | 5.829E-02            |               |           |                      | 0.042 |
| 1s 7d <sup>3</sup> D <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 4.3244E+03    | 1.574E-09 | 1.123E-01            |               |           |                      | 0.014 |
| 1s 7d <sup>3</sup> D <sub>3</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.0098E+05    | 1.418E-13 | 1.855E-08            |               |           |                      | 0.727 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3940E+00    | 1.003E-03 | 3.825E+11            | 1.3881E+00    | 1.037E-03 | 3.957E+11            | 0.013 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 3.5150E+00    | 5.714E-05 | 3.428E+09            | 3.5002E+00    | 6.732E-05 | 4.038E+09            | 0.079 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 7.5664E+00    | 6.079E-05 | 7.869E+08            | 7.5341E+00    | 5.644E-05 | 7.306E+08            | 0.021 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 7.6554E+00    | 7.647E-06 | 9.670E+07            | 7.6229E+00    | 7.602E-06 | 9.614E+07            | 0.010 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 7.6569E+00    | 6.110E-07 | 7.724E+06            | 7.6244E+00    | 6.060E-07 | 7.660E+06            | 0.012 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 7.6914E+00    | 6.132E-05 | 7.682E+08            | 7.6587E+00    | 6.131E-05 | 7.682E+08            | 0.004 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 7.6926E+00    | 5.597E-06 | 7.009E+07            | 7.6598E+00    | 5.600E-06 | 7.013E+07            | 0.004 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6215E+01    | 5.823E-04 | 1.642E+09            | 1.6144E+01    | 5.789E-04 | 1.632E+09            | 0.002 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6424E+01    | 2.639E-05 | 7.251E+07            | 1.6354E+01    | 2.644E-05 | 7.266E+07            | 0.001 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6428E+01    | 2.088E-06 | 5.735E+06            | 1.6358E+01    | 2.090E-06 | 5.741E+06            | 0.001 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6509E+01    | 2.165E-04 | 5.887E+08            | 1.6439E+01    | 2.163E-04 | 5.883E+08            | 0.000 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6512E+01    | 1.977E-05 | 5.373E+07            | 1.6441E+01    | 1.975E-05 | 5.369E+07            | 0.000 |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.2681E+01    | 3.276E-03 | 1.333E+09            | 4.2483E+01    | 3.308E-03 | 1.346E+09            | 0.001 |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.3526E+01    | 1.066E-04 | 4.170E+07            | 4.3345E+01    | 1.073E-04 | 4.197E+07            | 0.000 |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.3541E+01    | 8.390E-06 | 3.280E+06            | 4.3345E+01    | 8.576E-06 | 3.354E+06            | 0.000 |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.3873E+01    | 8.912E-04 | 3.432E+08            | 4.3688E+01    | 8.920E-04 | 3.434E+08            | 0.000 |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.3884E+01    | 8.141E-05 | 3.133E+07            | 4.3689E+01    | 8.098E-05 | 3.118E+07            | 0.000 |
| 1s 6h <sup>3</sup> H <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.4083E+01    | 2.238E-06 | 8.534E+05            | 4.3895E+01    | 2.247E-06 | 8.571E+05            | 0.001 |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.4089E+01    | 1.604E-07 | 6.116E+04            |               |           |                      | 0.001 |

(continued on next page)

Table 4 (continued)

| Lower  | Upper  | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|--|--|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|  |  | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s 6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.4223E+01    | 4.928E-05 | 1.868E+07              | 4.4034E+01    | 4.929E-05 | 1.868E+07              | 0.000 |
| 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.4228E+01    | 1.903E-06 | 7.210E+05              | 4.4034E+01    | 1.895E-06 | 7.184E+05              | 0.000 |
| 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 2.5222E+03    | 8.144E-08 | 9.488E+00              | 2.4461E+03    | 8.879E-08 | 1.090E+01              | 0.215 |
| 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 8.7508E+03    | 1.956E-10 | 1.893E-03              | 8.7713E+03    | 1.926E-10 | 1.840E-03              | 0.012 |
| 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 9.1339E+03    | 1.364E-11 | 1.211E-04              |               |           |                        | 0.004 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 3.5233E+00    | 1.943E-03 | 1.160E+11              | 3.5085E+00    | 1.957E-03 | 1.168E+11              | 0.001 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 3.5600E+00    | 2.000E-04 | 1.170E+10              | 3.5449E+00    | 1.996E-04 | 1.167E+10              | 0.002 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 3.5614E+00    | 1.781E-05 | 1.041E+09              | 3.5464E+00    | 1.724E-05 | 1.007E+09              | 0.006 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 7.5825E+00    | 3.212E-04 | 4.141E+09              | 7.5510E+00    | 3.252E-04 | 4.191E+09              | 0.002 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 7.6543E+00    | 3.711E-05 | 4.695E+08              | 7.6223E+00    | 3.748E-05 | 4.741E+08              | 0.003 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 7.6572E+00    | 3.439E-06 | 4.347E+07              | 7.6253E+00    | 3.353E-06 | 4.237E+07              | 0.011 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 1.6252E+01    | 1.272E-04 | 3.569E+08              | 1.6186E+01    | 1.258E-04 | 3.529E+08              | 0.002 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 1.6421E+01    | 1.005E-05 | 2.763E+07              | 1.6353E+01    | 9.930E-06 | 2.728E+07              | 0.003 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 1.6428E+01    | 9.544E-07 | 2.621E+06              | 1.6361E+01    | 9.268E-07 | 2.544E+06              | 0.013 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 1.6509E+01    | 1.030E-04 | 2.801E+08              | 1.6439E+01    | 1.029E-04 | 2.799E+08              | 0.001 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 1.6511E+01    | 9.340E-06 | 2.539E+07              | 1.6441E+01    | 9.352E-06 | 2.542E+07              | 0.001 |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 1.6560E+01    | 9.418E-06 | 2.545E+07              | 1.6490E+01    | 9.404E-06 | 2.541E+07              | 0.001 |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 1.6562E+01    | 6.755E-07 | 1.825E+06              | 1.6491E+01    | 6.402E-07 | 1.730E+06              | 0.000 |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.2832E+01    | 4.032E-03 | 1.629E+09              | 4.2672E+01    | 4.028E-03 | 1.625E+09              | 0.000 |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.3514E+01    | 4.098E-04 | 1.604E+08              | 4.3345E+01    | 4.110E-04 | 1.607E+08              | 0.000 |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.3543E+01    | 3.925E-05 | 1.534E+07              | 4.3356E+01    | 4.179E-05 | 1.633E+07              | 0.001 |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.3873E+01    | 6.859E-04 | 2.641E+08              | 4.3688E+01    | 6.861E-04 | 2.641E+08              | 0.000 |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.3882E+01    | 6.214E-05 | 2.392E+07              | 4.3688E+01    | 6.237E-05 | 2.401E+07              | 0.000 |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.4082E+01    | 6.352E-05 | 2.423E+07              | 4.3896E+01    | 6.369E-05 | 2.429E+07              | 0.000 |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 4.4089E+01    | 4.557E-06 | 1.737E+06              | 4.3896E+01    | 4.548E-06 | 1.734E+06              | 0.000 |
| 1s 7d <sup>3</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 2.8662E+03    | 4.119E-08 | 3.716E+00              | 2.9148E+03    | 3.861E-08 | 3.339E+00              | 0.001 |
| 1s 7d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 8.4183E+03    | 1.657E-10 | 1.733E-03              | 8.7854E+03    | 1.443E-10 | 1.374E-03              | 0.001 |
| 1s 7d <sup>1</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>4</sub>              | 9.1839E+03    | 1.227E-11 | 1.078E-04              |               |           |                        | 0.142 |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 1.3246E+00    | 1.973E-11 | 1.072E+04              |               |           |                        | 0.848 |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 3.3838E+00    | 3.349E-09 | 2.787E+05              |               |           |                        | 0.424 |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 3.5233E+00    | 2.174E-04 | 1.669E+10              | 3.5085E+00    | 2.189E-04 | 1.680E+10              | 0.002 |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 3.5248E+00    | 1.293E-03 | 9.919E+10              | 3.5099E+00    | 1.304E-03 | 1.000E+11              | 0.002 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 3.5600E+00    | 2.399E-05 | 1.804E+09              | 3.5449E+00    | 2.396E-05 | 1.801E+09              | 0.003 |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 3.5614E+00    | 1.430E-04 | 1.074E+10              | 3.5464E+00    | 1.423E-04 | 1.069E+10              | 0.002 |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 7.3110E+00    | 5.849E-10 | 1.043E+04              |               |           |                        | 0.588 |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 7.5824E+00    | 3.602E-05 | 5.970E+08              | 7.5510E+00    | 3.653E-05 | 6.054E+08              | 0.002 |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 7.5852E+00    | 2.142E-04 | 3.547E+09              | 7.5538E+00    | 2.168E-04 | 3.590E+09              | 0.004 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 7.6541E+00    | 4.463E-06 | 7.260E+07              | 7.6223E+00    | 4.498E-06 | 7.314E+07              | 0.001 |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 7.6571E+00    | 2.646E-05 | 4.300E+08              | 7.6253E+00    | 2.660E-05 | 4.323E+08              | 0.003 |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 1.5619E+01    | 3.106E-10 | 1.213E+03              |               |           |                        | 0.374 |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 1.6252E+01    | 1.432E-05 | 5.167E+07              | 1.6186E+01    | 1.412E-05 | 5.095E+07              | 0.002 |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 1.6258E+01    | 8.465E-05 | 3.052E+08              | 1.6192E+01    | 8.387E-05 | 3.022E+08              | 0.004 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 1.6420E+01    | 1.213E-06 | 4.288E+06              | 1.6353E+01    | 1.192E-06 | 4.211E+06              | 0.003 |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 1.6428E+01    | 7.124E-06 | 2.515E+07              | 1.6361E+01    | 7.012E-06 | 2.475E+07              | 0.003 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 1.6509E+01    | 9.333E-06 | 3.263E+07              | 1.6439E+01    | 9.323E-06 | 3.259E+07              | 0.001 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 1.6511E+01    | 7.814E-05 | 2.732E+08              | 1.6441E+01    | 7.792E-05 | 2.723E+08              | 0.001 |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 1.6560E+01    | 4.513E-07 | 1.568E+06              | 1.6490E+01    | 4.478E-07 | 1.556E+06              | 0.001 |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 1.6561E+01    | 7.471E-06 | 2.595E+07              | 1.6491E+01    | 7.418E-06 | 2.577E+07              | 0.001 |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 4.0344E+01    | 7.208E-09 | 4.220E+03              |               |           |                        | 0.052 |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 4.2827E+01    | 4.534E-04 | 2.355E+08              | 4.2672E+01    | 4.574E-04 | 2.373E+08              | 0.000 |
| 1s 6d <sup>3</sup> D <sub>1</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 4.2853E+01    | 2.691E-03 | 1.397E+09              | 4.2665E+01    | 2.693E-03 | 1.397E+09              | 0.000 |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 4.3508E+01    | 4.934E-05 | 2.484E+07              | 4.3345E+01    | 4.933E-05 | 2.480E+07              | 0.000 |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 4.3538E+01    | 2.913E-04 | 1.465E+08              | 4.3356E+01    | 2.873E-04 | 1.444E+08              | 0.000 |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 4.3868E+01    | 6.210E-05 | 3.075E+07              | 4.3688E+01    | 6.237E-05 | 3.087E+07              | 0.000 |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 4.3876E+01    | 5.195E-04 | 2.571E+08              | 4.3688E+01    | 5.197E-04 | 2.573E+08              | 0.000 |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 4.4077E+01    | 3.033E-06 | 1.488E+06              | 4.3896E+01    | 3.033E-06 | 1.487E+06              | 0.001 |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 4.4084E+01    | 5.031E-05 | 2.467E+07              | 4.3896E+01    | 5.004E-05 | 2.453E+07              | 0.000 |
| 1s 7s <sup>3</sup> S <sub>1</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 7.9695E+02    | 3.661E-12 | 5.493E-03              |               |           |                        | 0.386 |
| 1s 7d <sup>3</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 2.8438E+03    | 4.743E-09 | 5.589E-01              | 2.9148E+03    | 4.385E-09 | 4.876E-01              | 0.015 |
| 1s 7d <sup>3</sup> D <sub>1</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 2.9164E+03    | 2.608E-08 | 2.922E+00              | 2.8963E+03    | 2.630E-08 | 2.962E+00              | 0.002 |
| 1s 7d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 8.2277E+03    | 2.137E-11 | 3.008E-04              |               |           |                        | 0.039 |
| 1s 7d <sup>1</sup> D <sub>2</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 8.9575E+03    | 9.678E-11 | 1.160E-03              | 9.0724E+03    | 9.158E-11 | 1.051E-03              | 0.002 |
| 1s 7g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>3</sub>              | 3.6344E+05    | 1.613E-15 | 1.163E-11              |               |           |                        | 0.864 |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.3356E+00    | 1.408E-06 | 7.519E+08              | 1.3301E+00    | 1.248E-06 | 6.667E+08              | 0.241 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.3940E+00    | 1.120E-04 | 5.494E+10              | 1.3881E+00    | 1.151E-04 | 5.645E+10              | 0.014 |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.3995E+00    | 6.566E-04 | 3.195E+11              | 1.3937E+00    | 6.826E-04 | 3.320E+11              | 0.007 |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.4034E+00    | 1.180E-08 | 9.704E+05              | 3.3893E+00    | 6.892E-08 | 5.669E+06              | 0.526 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.5149E+00    | 6.355E-06 | 4.902E+08              | 3.5002E+00    | 7.469E-06 | 5.759E+08              | 0.079 |
| 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.5248E+00    | 4.161E-05 | 3.192E+09              | 3.5102E+00    | 4.445E-05 | 3.408E+09              | 0.049 |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.3482E+00    | 1.302E-07 | 2.298E+06              | 7.3172E+00    | 5.346E-08 | 9.435E+05              | 0.117 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.5662E+00    | 6.809E-06 | 1.133E+08              | 7.5341E+00    | 6.257E-06 | 1.041E+08              | 0.022 |

(continued on next page)

Table 4 (continued)

| Lower  | Upper  | GRASP2K       |           |                  | FAC           |           |                  | dT    |
|--|--|---------------|-----------|------------------|---------------|-----------|------------------|-------|
|  |  | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | gf        | $A$ ( $s^{-1}$ ) |       |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.5852E+00    | 3.726E-05 | 6.171E+08        | 7.5532E+00    | 3.730E-05 | 6.177E+08        | 0.008 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.6552E+00    | 9.269E-07 | 1.507E+07        | 7.6229E+00    | 9.527E-07 | 1.549E+07        | 0.010 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.6567E+00    | 5.558E-06 | 9.034E+07        | 7.6244E+00    | 5.487E-06 | 8.918E+07        | 0.011 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.6912E+00    | 5.600E-06 | 9.020E+07        | 7.6586E+00    | 5.566E-06 | 8.966E+07        | 0.005 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.6923E+00    | 4.638E-05 | 7.469E+08        | 7.6598E+00    | 4.641E-05 | 7.473E+08        | 0.004 |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.5704E+01    | 7.014E-07 | 2.710E+06        | 1.5637E+01    | 5.464E-07 | 2.111E+06        | 0.020 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6214E+01    | 6.503E-05 | 2.357E+08        | 1.6144E+01    | 6.420E-05 | 2.327E+08        | 0.002 |
| 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6258E+01    | 3.793E-04 | 1.367E+09        | 1.6189E+01    | 3.824E-04 | 1.378E+09        | 0.004 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6423E+01    | 3.189E-06 | 1.127E+07        | 1.6354E+01    | 3.307E-06 | 1.168E+07        | 0.001 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6427E+01    | 1.919E-05 | 6.775E+07        | 1.6358E+01    | 1.910E-05 | 6.744E+07        | 0.001 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6508E+01    | 1.977E-05 | 6.914E+07        | 1.6439E+01    | 1.963E-05 | 6.866E+07        | 0.000 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6511E+01    | 1.638E-04 | 5.726E+08        | 1.6441E+01    | 1.637E-04 | 5.723E+08        | 0.000 |
| 1s 6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.0672E+01    | 3.065E-06 | 1.766E+06        | 4.0492E+01    | 5.449E-06 | 3.139E+06        | 0.004 |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.2675E+01    | 3.654E-04 | 1.912E+08        | 4.2483E+01    | 3.670E-04 | 1.921E+08        | 0.001 |
| 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.2851E+01    | 2.180E-03 | 1.131E+09        | 4.2639E+01    | 2.177E-03 | 1.131E+09        | 0.001 |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3519E+01    | 1.285E-05 | 6.468E+06        | 4.3345E+01    | 1.287E-05 | 6.472E+06        | 0.000 |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3534E+01    | 7.753E-05 | 3.898E+07        | 4.3345E+01    | 7.707E-05 | 3.875E+07        | 0.000 |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3866E+01    | 8.135E-05 | 4.029E+07        | 4.3688E+01    | 8.097E-05 | 4.008E+07        | 0.000 |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3877E+01    | 6.744E-04 | 3.338E+08        | 4.3688E+01    | 6.760E-04 | 3.346E+08        | 0.000 |
| 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.4076E+01    | 1.054E-07 | 5.168E+04        |               |           |                  | 0.001 |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.4082E+01    | 1.770E-06 | 8.681E+05        | 4.3895E+01    | 1.763E-06 | 8.646E+05        | 0.001 |
| 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.4221E+01    | 3.978E-05 | 1.938E+07        | 4.4034E+01    | 3.981E-05 | 1.939E+07        | 0.000 |
| 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 8.8911E+02    | 1.783E-09 | 2.149E+00        | 8.8057E+02    | 2.686E-09 | 3.273E+00        | 0.046 |
| 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.4995E+03    | 9.333E-09 | 1.424E+00        | 2.4456E+03    | 9.858E-09 | 1.557E+00        | 0.214 |
| 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.9477E+03    | 3.391E-08 | 3.719E+00        | 2.8179E+03    | 3.864E-08 | 4.598E+00        | 0.254 |
| 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 8.4824E+03    | 2.588E-11 | 3.428E-04        |               |           |                  | 0.007 |
| 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 8.8420E+03    | 1.378E-10 | 1.679E-03        | 8.7598E+03    | 1.389E-10 | 1.710E-03        | 0.012 |
| 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.7665E+05    | 4.698E-15 | 5.850E-11        |               |           |                  | 0.132 |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 3.5591E+00    | 2.642E-03 | 1.265E+11        | 3.5441E+00    | 2.685E-03 | 1.285E+11        | 0.001 |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 7.6503E+00    | 4.732E-04 | 4.903E+09        | 7.6183E+00    | 4.810E-04 | 4.983E+09        | 0.003 |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 1.6403E+01    | 1.449E-04 | 3.266E+08        | 1.6335E+01    | 1.433E-04 | 3.230E+08        | 0.003 |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 1.6491E+01    | 9.575E-06 | 2.135E+07        | 1.6420E+01    | 9.612E-06 | 2.143E+07        | 0.001 |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 1.6493E+01    | 4.578E-07 | 1.021E+06        | 1.6423E+01    | 4.587E-07 | 1.022E+06        | 0.002 |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 1.6542E+01    | 1.322E-04 | 2.929E+08        | 1.6471E+01    | 1.320E-04 | 2.927E+08        | 0.001 |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 1.6543E+01    | 7.667E-06 | 1.699E+07        | 1.6473E+01    | 7.651E-06 | 1.695E+07        | 0.001 |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 4.3385E+01    | 5.440E-03 | 1.753E+09        | 4.3218E+01    | 5.448E-03 | 1.753E+09        | 0.000 |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 4.3743E+01    | 6.292E-05 | 1.994E+07        | 4.3559E+01    | 6.329E-05 | 2.005E+07        | 0.000 |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 4.3751E+01    | 3.000E-06 | 9.504E+05        | 4.3559E+01    | 3.014E-06 | 9.551E+05        | 0.001 |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 4.3950E+01    | 8.795E-04 | 2.761E+08        | 4.3765E+01    | 8.804E-04 | 2.763E+08        | 0.000 |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 4.3957E+01    | 5.098E-05 | 1.600E+07        | 4.3765E+01    | 5.079E-05 | 1.594E+07        | 0.000 |
| 1s 7d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 5.3499E+03    | 8.610E-09 | 1.824E-01        | 5.4978E+03    | 7.830E-09 | 1.557E-01        | 0.002 |
| 1s 7g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 1.4677E+04    | 2.497E-11 | 7.029E-05        | 1.4692E+04    | 2.466E-11 | 6.870E-05        | 0.006 |
| 1s 7g <sup>3</sup> G <sub>3</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 1.5295E+04    | 1.053E-12 | 2.729E-06        |               |           |                  | 0.076 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 7.6514E+00    | 4.645E-03 | 4.811E+10        | 7.6190E+00    | 4.671E-03 | 4.838E+10        | 0.000 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 7.6874E+00    | 2.681E-04 | 2.751E+09        | 7.6547E+00    | 2.682E-04 | 2.752E+09        | 0.000 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 7.6885E+00    | 1.250E-05 | 1.282E+08        | 7.6558E+00    | 1.173E-05 | 1.203E+08        | 0.000 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.6406E+01    | 5.665E-04 | 1.276E+09        | 1.6336E+01    | 5.720E-04 | 1.288E+09        | 0.000 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.6491E+01    | 3.505E-05 | 7.816E+07        | 1.6420E+01    | 3.535E-05 | 7.882E+07        | 0.000 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.6493E+01    | 1.647E-06 | 3.671E+06        | 1.6423E+01    | 1.560E-06 | 3.478E+06        | 0.000 |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.3397E+01    | 5.768E-03 | 1.857E+09        | 4.3218E+01    | 5.771E-03 | 1.857E+09        | 0.000 |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.3742E+01    | 3.291E-04 | 1.043E+08        | 4.3559E+01    | 3.298E-04 | 1.045E+08        | 0.000 |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.3753E+01    | 1.547E-05 | 4.902E+06        | 4.3560E+01    | 1.605E-05 | 5.087E+06        | 0.000 |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.3951E+01    | 5.094E-04 | 1.599E+08        | 4.3765E+01    | 5.095E-04 | 1.599E+08        | 0.000 |
| 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.3956E+01    | 2.930E-05 | 9.194E+06        | 4.3765E+01    | 2.939E-05 | 9.227E+06        | 0.000 |
| 1s 6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.4090E+01    | 2.964E-05 | 9.245E+06        | 4.3903E+01    | 2.968E-05 | 9.258E+06        | 0.000 |
| 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.4094E+01    | 1.416E-06 | 4.417E+05        | 4.3903E+01    | 1.413E-06 | 4.408E+05        | 0.000 |
| 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 5.4734E+03    | 4.836E-09 | 9.789E-02        | 5.5022E+03    | 4.700E-09 | 9.334E-02        | 0.005 |
| 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.4614E+04    | 1.456E-11 | 4.135E-05        | 1.4763E+04    | 1.399E-11 | 3.860E-05        | 0.019 |
| 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.5429E+04    | 5.832E-13 | 1.485E-06        |               |           |                  | 0.016 |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.3938E+00    | 1.355E-12 | 5.171E+02        |               |           |                  | 0.965 |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 3.5141E+00    | 1.656E-13 | 9.938E+00        |               |           |                  | 0.818 |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 7.5624E+00    | 4.126E-10 | 5.348E+03        |               |           |                  | 0.039 |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 7.6513E+00    | 2.804E-04 | 3.550E+09        | 7.6190E+00    | 2.819E-04 | 3.569E+09        | 0.000 |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 7.6528E+00    | 3.518E-03 | 4.452E+10        | 7.6205E+00    | 3.536E-03 | 4.474E+10        | 0.000 |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 7.6873E+00    | 1.920E-05 | 2.408E+08        | 7.6547E+00    | 1.916E-05 | 2.403E+08        | 0.000 |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 7.6884E+00    | 2.123E-04 | 2.662E+09        | 7.6558E+00    | 2.117E-04 | 2.654E+09        | 0.000 |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6196E+01    | 6.804E-11 | 1.922E+02        |               |           |                  | 0.031 |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6405E+01    | 3.416E-05 | 9.407E+07        | 1.6336E+01    | 3.453E-05 | 9.509E+07        | 0.000 |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6409E+01    | 4.298E-04 | 1.183E+09        | 1.6340E+01    | 4.329E-04 | 1.191E+09        | 0.000 |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6490E+01    | 2.507E-06 | 6.833E+06        | 1.6420E+01    | 2.525E-06 | 6.881E+06        | 0.001 |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6493E+01    | 2.778E-05 | 7.568E+07        | 1.6423E+01    | 2.788E-05 | 7.597E+07        | 0.000 |

(continued on next page)

Table 4 (continued)

| Lower   | Upper   | GRASP2K       |           |                        | FAC           |           |                        | dT    |
|---|---|---------------|-----------|------------------------|---------------|-----------|------------------------|-------|
|   |   | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | gf        | $A$ (s <sup>-1</sup> ) |       |
| 1s6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.2554E+01    | 1.171E-09 | 4.791E+02              |               |           |                        | 0.003 |
| 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.3394E+01    | 3.484E-04 | 1.371E+08              | 4.3218E+01    | 3.501E-04 | 1.377E+08              | 0.000 |
| 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.3408E+01    | 4.367E-03 | 1.718E+09              | 4.3218E+01    | 4.372E-03 | 1.720E+09              | 0.000 |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.3738E+01    | 2.358E-05 | 9.134E+06              | 4.3559E+01    | 2.356E-05 | 9.125E+06              | 0.000 |
| 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.3749E+01    | 2.604E-04 | 1.008E+08              | 4.3560E+01    | 2.588E-04 | 1.002E+08              | 0.000 |
| 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.3947E+01    | 2.929E-05 | 1.124E+07              | 4.3765E+01    | 2.939E-05 | 1.127E+07              | 0.000 |
| 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.3953E+01    | 4.113E-04 | 1.578E+08              | 4.3765E+01    | 4.115E-04 | 1.578E+08              | 0.000 |
| 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.4086E+01    | 9.436E-07 | 3.598E+05              | 4.3903E+01    | 9.422E-07 | 3.592E+05              | 0.000 |
| 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.4091E+01    | 2.461E-05 | 9.384E+06              | 4.3903E+01    | 2.449E-05 | 9.340E+06              | 0.000 |
| 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 2.1428E+03    | 1.866E-14 | 3.013E-06              |               |           |                        | 0.042 |
| 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 5.4206E+03    | 3.007E-10 | 7.586E-03              | 5.5022E+03    | 2.852E-10 | 6.922E-03              | 0.007 |
| 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 5.5652E+03    | 3.484E-09 | 8.338E-02              | 5.5003E+03    | 3.564E-09 | 8.658E-02              | 0.006 |
| 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.4244E+04    | 1.127E-12 | 4.117E-06              |               |           |                        | 0.019 |
| 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.5017E+04    | 1.062E-11 | 3.491E-05              | 1.4782E+04    | 1.093E-11 | 3.677E-05              | 0.022 |
| 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 5.6215E+05    | 2.508E-16 | 5.883E-13              |               |           |                        | 0.445 |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 3.5224E+00    | 5.663E-08 | 3.382E+06              |               |           |                        | 0.083 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 3.5591E+00    | 1.610E-04 | 9.419E+09              | 3.5441E+00    | 1.627E-04 | 9.520E+09              | 0.002 |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 3.5605E+00    | 1.996E-03 | 1.167E+11              | 3.5455E+00    | 2.031E-03 | 1.187E+11              | 0.002 |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 7.5785E+00    | 1.751E-08 | 2.260E+05              |               |           |                        | 0.121 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 7.6502E+00    | 2.879E-05 | 3.646E+08              | 7.6183E+00    | 2.915E-05 | 3.691E+08              | 0.002 |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 7.6531E+00    | 3.580E-04 | 4.530E+09              | 7.6213E+00    | 3.640E-04 | 4.605E+09              | 0.004 |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 1.6234E+01    | 8.108E-09 | 2.280E+04              |               |           |                        | 0.102 |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 1.6402E+01    | 8.842E-06 | 2.436E+07              | 1.6335E+01    | 8.687E-06 | 2.392E+07              | 0.002 |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 1.6409E+01    | 1.093E-04 | 3.008E+08              | 1.6342E+01    | 1.084E-04 | 2.984E+08              | 0.004 |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 1.6490E+01    | 6.864E-07 | 1.871E+06              | 1.6420E+01    | 7.222E-07 | 1.968E+06              | 0.003 |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 1.6492E+01    | 7.595E-06 | 2.069E+07              | 1.6423E+01    | 7.575E-06 | 2.064E+07              | 0.001 |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 1.6541E+01    | 7.660E-06 | 2.075E+07              | 1.6471E+01    | 7.620E-06 | 2.064E+07              | 0.001 |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 1.6543E+01    | 1.069E-04 | 2.894E+08              | 1.6473E+01    | 1.066E-04 | 2.887E+08              | 0.001 |
| 1s6d <sup>3</sup> D <sub>2</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 4.2703E+01    | 2.860E-07 | 1.162E+05              | 4.2548E+01    | 6.028E-07 | 2.447E+05              | 0.010 |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 4.3381E+01    | 3.312E-04 | 1.304E+08              | 4.3218E+01    | 3.302E-04 | 1.299E+08              | 0.000 |
| 1s6d <sup>1</sup> D <sub>2</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 4.3410E+01    | 4.120E-03 | 1.620E+09              | 4.3228E+01    | 4.124E-03 | 1.621E+09              | 0.000 |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 4.3738E+01    | 4.512E-06 | 1.748E+06              | 4.3559E+01    | 4.522E-06 | 1.751E+06              | 0.001 |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 4.3747E+01    | 4.984E-05 | 1.930E+07              | 4.3559E+01    | 4.973E-05 | 1.926E+07              | 0.000 |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 4.3946E+01    | 5.095E-05 | 1.955E+07              | 4.3765E+01    | 5.079E-05 | 1.948E+07              | 0.000 |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 4.3953E+01    | 7.102E-04 | 2.725E+08              | 4.3765E+01    | 7.111E-04 | 2.728E+08              | 0.000 |
| 1s7d <sup>3</sup> D <sub>2</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 2.3855E+03    | 5.465E-12 | 7.117E-04              | 2.4322E+03    | 1.002E-11 | 1.245E-03              | 0.288 |
| 1s7d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 5.2883E+03    | 5.425E-10 | 1.438E-02              | 5.4978E+03    | 4.745E-10 | 1.153E-02              | 0.023 |
| 1s7d <sup>1</sup> D <sub>2</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 5.5805E+03    | 5.741E-09 | 1.366E-01              | 5.6088E+03    | 5.585E-09 | 1.304E-01              | 0.009 |
| 1s7g <sup>3</sup> G <sub>4</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 1.4223E+04    | 1.969E-12 | 7.213E-06              |               |           |                        | 0.050 |
| 1s7g <sup>3</sup> G <sub>3</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 1.4802E+04    | 1.927E-11 | 6.519E-05              | 1.4691E+04    | 1.938E-11 | 6.599E-05              | 0.001 |
| 1s7g <sup>3</sup> G <sub>5</sub>              | 1s7g <sup>1</sup> G <sub>4</sub>              | 4.5954E+05    | 6.580E-16 | 2.309E-12              |               |           |                        | 0.926 |
| 1s4f <sup>3</sup> F <sub>6</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 7.6847E+00    | 5.821E-03 | 5.058E+10              | 7.6520E+00    | 5.875E-03 | 5.104E+10              | 0.000 |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1.6478E+01    | 7.392E-04 | 1.397E+09              | 1.6408E+01    | 7.475E-04 | 1.412E+09              | 0.000 |
| 1s6f <sup>3</sup> F <sub>6</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 4.3655E+01    | 7.178E-03 | 1.933E+09              | 4.3474E+01    | 7.190E-03 | 1.935E+09              | 0.000 |
| 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 4.3863E+01    | 2.951E-05 | 7.870E+06              | 4.3678E+01    | 2.967E-05 | 7.912E+06              | 0.000 |
| 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 4.3869E+01    | 9.395E-07 | 2.505E+05              | 4.3678E+01    | 9.419E-07 | 2.511E+05              | 0.000 |
| 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 4.4002E+01    | 6.178E-04 | 1.637E+08              | 4.3816E+01    | 6.178E-04 | 1.638E+08              | 0.000 |
| 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 4.4006E+01    | 2.480E-05 | 6.570E+06              | 4.3816E+01    | 2.473E-05 | 6.553E+06              | 0.000 |
| 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 8.7953E+03    | 1.460E-09 | 9.686E-03              | 8.8520E+03    | 1.414E-09 | 9.182E-03              | 0.009 |
| 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 2.2090E+04    | 4.176E-12 | 4.392E-06              | 2.2109E+04    | 4.124E-12 | 4.292E-06              | 0.008 |
| 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 2.2993E+04    | 1.179E-13 | 1.144E-07              |               |           |                        | 0.100 |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7i <sup>3</sup> I <sub>6</sub>              | 1.6478E+01    | 1.124E-02 | 2.123E+10              | 1.6408E+01    | 1.128E-02 | 2.131E+10              | 0.000 |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s7i <sup>3</sup> I <sub>6</sub>              | 1.6529E+01    | 4.191E-04 | 7.871E+08              | 1.6459E+01    | 4.199E-04 | 7.886E+08              | 0.000 |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7i <sup>3</sup> I <sub>6</sub>              | 1.6531E+01    | 1.290E-05 | 2.422E+07              | 1.6460E+01    | 1.190E-05 | 2.234E+07              | 0.000 |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7i <sup>3</sup> I <sub>6</sub>              | 4.3656E+01    | 5.574E-03 | 1.501E+09              | 4.3473E+01    | 5.578E-03 | 1.501E+09              | 0.000 |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s7i <sup>3</sup> I <sub>6</sub>              | 4.3863E+01    | 2.052E-04 | 5.471E+07              | 4.3678E+01    | 2.055E-04 | 5.481E+07              | 0.000 |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s7i <sup>3</sup> I <sub>6</sub>              | 4.3870E+01    | 6.313E-06 | 1.683E+06              | 4.3678E+01    | 6.525E-06 | 1.740E+06              | 0.000 |
| 1s7g <sup>3</sup> G <sub>4</sub>              | 1s7i <sup>3</sup> I <sub>6</sub>              | 8.8113E+03    | 5.733E-10 | 3.789E-03              | 8.8262E+03    | 5.630E-10 | 3.677E-03              | 0.006 |
| 1s7g <sup>3</sup> G <sub>5</sub>              | 1s7i <sup>3</sup> I <sub>6</sub>              | 2.2046E+04    | 1.354E-12 | 1.429E-06              | 2.2108E+04    | 1.328E-12 | 1.383E-06              | 0.019 |
| 1s7g <sup>1</sup> G <sub>4</sub>              | 1s7i <sup>3</sup> I <sub>6</sub>              | 2.3157E+04    | 3.597E-14 | 3.442E-08              |               |           |                        | 0.064 |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7i <sup>3</sup> I <sub>5</sub>              | 3.5586E+00    | 2.773E-12 | 1.328E+02              |               |           |                        | 1.000 |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7i <sup>3</sup> I <sub>5</sub>              | 7.6476E+00    | 9.356E-14 | 9.701E-01              |               |           |                        | 0.538 |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7i <sup>3</sup> I <sub>5</sub>              | 1.6390E+01    | 3.142E-12 | 7.092E+00              |               |           |                        | 0.057 |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7i <sup>3</sup> I <sub>5</sub>              | 1.6478E+01    | 4.307E-04 | 9.619E+08              | 1.6408E+01    | 4.324E-04 | 9.656E+08              | 0.000 |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7i <sup>3</sup> I <sub>5</sub>              | 1.6480E+01    | 9.076E-03 | 2.026E+10              | 1.6410E+01    | 9.108E-03 | 2.033E+10              | 0.000 |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s7i <sup>3</sup> I <sub>5</sub>              | 1.6529E+01    | 2.000E-05 | 4.439E+07              | 1.6459E+01    | 1.999E-05 | 4.438E+07              | 0.000 |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7i <sup>3</sup> I <sub>5</sub>              | 1.6531E+01    | 3.483E-04 | 7.728E+08              | 1.6460E+01    | 3.479E-04 | 7.721E+08              | 0.000 |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7i <sup>3</sup> I <sub>5</sub>              | 4.3297E+01    | 3.945E-12 | 1.276E+00              |               |           |                        | 0.033 |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7i <sup>3</sup> I <sub>5</sub>              | 4.3654E+01    | 2.137E-04 | 6.799E+07              | 4.3473E+01    | 2.145E-04 | 6.825E+07              | 0.000 |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7i <sup>3</sup> I <sub>5</sub>              | 4.3662E+01    | 4.500E-03 | 1.431E+09              | 4.3473E+01    | 4.505E-03 | 1.433E+09              | 0.000 |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s7i <sup>3</sup> I <sub>5</sub>              | 4.3861E+01    | 9.795E-06 | 3.088E+06              | 4.3678E+01    | 9.787E-06 | 3.084E+06              | 0.000 |

(continued on next page)

Table 4 (continued)

| Lower  | Upper  | GRASP2K       |           |                             | FAC           |           |                             | <i>dT</i> |
|--|--|---------------|-----------|-----------------------------|---------------|-----------|-----------------------------|-----------|
|  |  | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) |           |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 4.3867E+01    | 1.704E-04 | 5.371E+07                   | 4.3678E+01    | 1.696E-04 | 5.346E+07                   | 0.000     |
| 1s 7d <sup>3</sup> D <sub>3</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 4.2822E+03    | 5.348E-18 | 1.769E-10                   |               |           |                             | 0.999     |
| 1s 7g <sup>3</sup> G <sub>4</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 8.7156E+03    | 2.271E-11 | 1.813E-04                   | 8.8262E+03    | 2.165E-11 | 1.671E-04                   | 0.016     |
| 1s 7g <sup>3</sup> G <sub>3</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 8.9298E+03    | 4.447E-10 | 3.382E-03                   | 8.8261E+03    | 4.547E-10 | 3.510E-03                   | 0.007     |
| 1s 7g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 2.1457E+04    | 7.011E-14 | 9.234E-08                   |               |           |                             | 0.044     |
| 1s 7g <sup>1</sup> G <sub>4</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 2.2508E+04    | 1.057E-12 | 1.265E-06                   | 2.2108E+04    | 1.096E-12 | 1.349E-06                   | 0.014     |
| 1s 7i <sup>3</sup> I <sub>6</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 8.0263E+05    | 4.303E-17 | 4.051E-14                   |               |           |                             | 0.989     |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 7.6487E+00    | 1.890E-09 | 1.959E+04                   |               |           |                             | 0.012     |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 7.6846E+00    | 2.247E-04 | 2.307E+09                   | 7.6520E+00    | 2.259E-04 | 2.320E+09                   | 0.000     |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 7.6858E+00    | 4.701E-03 | 4.826E+10                   | 7.6532E+00    | 4.743E-03 | 4.868E+10                   | 0.000     |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.6393E+01    | 1.359E-10 | 3.067E+02                   |               |           |                             | 0.012     |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.6478E+01    | 2.850E-05 | 6.365E+07                   | 1.6408E+01    | 2.875E-05 | 6.420E+07                   | 0.000     |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.6481E+01    | 5.977E-04 | 1.334E+09                   | 1.6411E+01    | 6.034E-04 | 1.347E+09                   | 0.000     |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3309E+01    | 1.004E-09 | 3.246E+02                   |               |           |                             | 0.001     |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3652E+01    | 2.771E-04 | 8.817E+07                   | 4.3474E+01    | 2.765E-04 | 8.798E+07                   | 0.000     |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3663E+01    | 5.796E-03 | 1.843E+09                   | 4.3474E+01    | 5.807E-03 | 1.847E+09                   | 0.000     |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3860E+01    | 1.410E-06 | 4.444E+05                   | 4.3678E+01    | 1.412E-06 | 4.452E+05                   | 0.000     |
| 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3866E+01    | 2.451E-05 | 7.724E+06                   | 4.3678E+01    | 2.449E-05 | 7.718E+06                   | 0.000     |
| 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3999E+01    | 2.480E-05 | 7.767E+06                   | 4.3816E+01    | 2.473E-05 | 7.744E+06                   | 0.000     |
| 1s 6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.4004E+01    | 5.188E-04 | 1.625E+08                   | 4.3816E+01    | 5.193E-04 | 1.626E+08                   | 0.000     |
| 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3583E+03    | 1.278E-15 | 4.080E-08                   |               |           |                             | 0.059     |
| 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 8.6829E+03    | 5.859E-11 | 4.712E-04                   | 8.8520E+03    | 5.439E-11 | 4.174E-04                   | 0.007     |
| 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 8.9642E+03    | 1.114E-09 | 8.405E-03                   | 8.8589E+03    | 1.139E-09 | 8.731E-03                   | 0.008     |
| 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.1394E+04    | 2.197E-13 | 2.911E-07                   |               |           |                             | 0.012     |
| 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.2240E+04    | 3.399E-12 | 4.167E-06                   | 2.2109E+04    | 3.404E-12 | 4.187E-06                   | 0.007     |
| 1s 7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 6.7907E+05    | 1.209E-16 | 1.590E-13                   |               |           |                             | 0.542     |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>3</sup> I <sub>7</sub>              | 1.6520E+01    | 1.348E-02 | 2.196E+10                   | 1.6450E+01    | 1.355E-02 | 2.208E+10                   | 0.000     |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>3</sup> I <sub>7</sub>              | 4.3801E+01    | 6.642E-03 | 1.539E+09                   | 4.3617E+01    | 6.653E-03 | 1.541E+09                   | 0.000     |
| 1s 7g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>3</sup> I <sub>7</sub>              | 1.2886E+04    | 2.195E-10 | 5.879E-04                   | 1.2907E+04    | 2.156E-10 | 5.708E-04                   | 0.009     |
| 1s 7i <sup>3</sup> I <sub>6</sub>              | 1s 7i <sup>3</sup> I <sub>7</sub>              | 3.1014E+04    | 7.499E-13 | 3.467E-07                   | 3.1015E+04    | 7.421E-13 | 3.401E-07                   | 0.006     |
| 1s 7i <sup>3</sup> I <sub>5</sub>              | 1s 7i <sup>3</sup> I <sub>7</sub>              | 3.2260E+04    | 1.518E-14 | 6.488E-09                   |               |           |                             | 0.243     |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 1.6469E+01    | 3.770E-09 | 7.132E+03                   |               |           |                             | 0.005     |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 1.6520E+01    | 3.605E-04 | 6.777E+08                   | 1.6450E+01    | 3.615E-04 | 6.796E+08                   | 0.000     |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 1.6522E+01    | 1.132E-02 | 2.128E+10                   | 1.6452E+01    | 1.138E-02 | 2.139E+10                   | 0.000     |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 4.3593E+01    | 1.872E-09 | 5.054E+02                   |               |           |                             | 0.006     |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 4.3799E+01    | 1.776E-04 | 4.751E+07                   | 4.3617E+01    | 1.774E-04 | 4.744E+07                   | 0.000     |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 4.3806E+01    | 5.577E-03 | 1.491E+09                   | 4.3617E+01    | 5.588E-03 | 1.494E+09                   | 0.000     |
| 1s 7g <sup>3</sup> G <sub>4</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 6.8121E+03    | 4.202E-16 | 4.646E-09                   |               |           |                             | 0.315     |
| 1s 7g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 1.2712E+04    | 6.116E-12 | 1.942E-05                   | 1.2907E+04    | 5.751E-12 | 1.756E-05                   | 0.019     |
| 1s 7g <sup>1</sup> G <sub>4</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 1.3074E+04    | 1.765E-10 | 5.300E-04                   | 1.2907E+04    | 1.811E-10 | 5.532E-04                   | 0.008     |
| 1s 7i <sup>3</sup> I <sub>6</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 3.0023E+04    | 2.826E-14 | 1.609E-08                   |               |           |                             | 0.071     |
| 1s 7i <sup>3</sup> I <sub>5</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 3.1190E+04    | 6.317E-13 | 3.332E-07                   | 3.1015E+04    | 6.325E-13 | 3.345E-07                   | 0.006     |
| 1s 7i <sup>3</sup> I <sub>7</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 9.4020E+05    | 2.328E-17 | 1.351E-14                   |               |           | 0.998                       |           |



**Table 5**  
Magnetic dipole transitions  $M1$  calculated with GRASP2K and FAC for all  $n = 1-7$  configurations. For the GRASP2K calculation, the active set is expanded to  $n = 10$  (GRASP3) and only the length form is considered. A comparison between the wavelengths, weighted oscillator strengths and transition probabilities is given.

| Lower  | Upper  | GRASP2K       |           |                  | FAC           |           |                  |
|--|--|---------------|-----------|------------------|---------------|-----------|------------------|
|  |  | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s <sup>2</sup> 1S <sub>0</sub>                | 1s 2s <sup>3</sup> S <sub>1</sub>              | 4.1150E-01    | 2.918E-05 | 3.831E+11        | 4.0980E-01    | 2.867E-05 | 3.763E+11        |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 2.0697E+03    | 2.433E-06 | 3.788E+03        | 2.1628E+03    | 2.322E-06 | 3.283E+03        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 2s <sup>1</sup> S <sub>0</sub>              | 1.4576E+02    | 1.373E-07 | 4.310E+04        | 1.4307E+02    | 1.353E-07 | 4.373E+04        |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.1908E+01    | 2.163E-04 | 2.834E+08        | 3.1815E+01    | 2.161E-04 | 2.824E+08        |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.9274E+01    | 4.310E-05 | 1.118E+08        | 2.9150E+01    | 4.314E-05 | 1.119E+08        |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.9694E+01    | 7.934E-05 | 2.001E+08        | 2.9548E+01    | 7.919E-05 | 1.999E+08        |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.5465E+02    | 6.279E-06 | 1.110E+05        | 3.4797E+02    | 6.377E-06 | 1.161E+05        |
| 1s <sup>2</sup> 1S <sub>0</sub>                | 1s 3s <sup>3</sup> S <sub>1</sub>              | 3.4600E-01    | 8.922E-06 | 1.656E+11        | 3.4464E-01    | 8.819E-06 | 1.637E+11        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 3s <sup>3</sup> S <sub>1</sub>              | 2.1766E+00    | 6.344E-07 | 2.977E+08        | 2.1673E+00    | 6.310E-07 | 2.961E+08        |
| 1s 2s <sup>1</sup> S <sub>0</sub>              | 1s 3s <sup>3</sup> S <sub>1</sub>              | 2.2096E+00    | 3.489E-07 | 1.589E+08        | 2.2006E+00    | 1.177E-07 | 1.454E+08        |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 2.1983E+00    | 1.490E-07 | 6.856E+07        | 2.1892E+00    | 1.782E-07 | 8.199E+07        |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 2.2006E+00    | 7.444E-08 | 3.417E+07        | 2.1914E+00    | 1.063E-07 | 4.884E+07        |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 2.3610E+00    | 5.406E-06 | 2.156E+09        | 2.3509E+00    | 5.520E-06 | 2.202E+09        |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 2.3768E+00    | 1.276E-06 | 5.023E+08        | 2.3669E+00    | 1.177E-06 | 4.633E+08        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 3s <sup>1</sup> S <sub>0</sub>              | 2.1681E+00    | 2.934E-07 | 4.163E+08        | 2.1587E+00    | 3.141E-07 | 4.459E+08        |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 3s <sup>1</sup> S <sub>0</sub>              | 5.5160E+02    | 5.089E-08 | 1.116E+03        | 5.4343E+02    | 5.012E-08 | 1.122E+03        |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 2.1977E+00    | 1.005E-07 | 1.389E+08        | 2.1886E+00    | 5.046E-08 | 6.967E+07        |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 2.3761E+00    | 2.226E-06 | 2.630E+09        | 2.3662E+00    | 2.678E-06 | 2.678E+09        |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 7.8853E+03    | 6.217E-07 | 6.669E+01        | 8.1583E+03    | 5.996E-07 | 5.958E+01        |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 2.1541E+00    | 2.836E-06 | 8.154E+08        | 2.1452E+00    | 2.941E-06 | 8.454E+08        |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 2.3101E+00    | 2.316E-06 | 5.790E+08        | 2.3003E+00    | 2.323E-06 | 5.808E+08        |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 2.3252E+00    | 2.020E-07 | 4.984E+07        | 2.3156E+00    | 1.970E-07 | 4.859E+07        |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.0725E+02    | 6.475E-05 | 7.509E+06        | 1.0689E+02    | 6.471E-05 | 7.491E+06        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 3d <sup>3</sup> D <sub>2</sub>              | 2.1226E+00    | 8.050E-08 | 2.384E+07        | 2.1136E+00    | 8.285E-08 | 2.453E+07        |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 3d <sup>3</sup> D <sub>2</sub>              | 8.5509E+01    | 7.271E-10 | 1.327E+02        | 8.5230E+01    | 7.255E-10 | 1.322E+02        |
| 1s <sup>2</sup> 1S <sub>0</sub>                | 1s 3d <sup>3</sup> D <sub>1</sub>              | 3.4460E-01    | 9.108E-08 | 1.705E+09        | 3.4323E-01    | 9.156E-08 | 1.713E+09        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 3d <sup>3</sup> D <sub>1</sub>              | 2.1220E+00    | 2.165E-08 | 1.069E+07        | 2.1130E+00    | 1.630E-08 | 8.048E+06        |
| 1s 2s <sup>1</sup> S <sub>0</sub>              | 1s 3d <sup>3</sup> D <sub>1</sub>              | 2.1534E+00    | 3.345E-08 | 1.604E+07        | 2.1447E+00    | 3.438E-08 | 1.647E+07        |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 3d <sup>3</sup> D <sub>1</sub>              | 8.4639E+01    | 6.335E-10 | 1.966E+02        | 8.4368E+01    | 6.521E-10 | 2.019E+02        |
| 1s 3s <sup>1</sup> S <sub>0</sub>              | 1s 3d <sup>3</sup> D <sub>1</sub>              | 9.9981E+01    | 7.121E-11 | 1.584E+01        | 9.9873E+01    | 7.246E-11 | 1.601E+01        |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 3d <sup>3</sup> D <sub>1</sub>              | 8.3264E+03    | 1.110E-06 | 3.561E+01        | 8.3383E+03    | 1.107E-06 | 3.511E+01        |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 2.1504E+00    | 5.477E-07 | 2.633E+08        | 2.1415E+00    | 5.343E-07 | 2.568E+08        |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 2.1527E+00    | 1.076E-06 | 5.162E+08        | 2.1436E+00    | 1.127E-06 | 5.408E+08        |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.3058E+00    | 4.193E-07 | 1.754E+08        | 2.2961E+00    | 3.571E-07 | 1.493E+08        |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.3209E+00    | 1.288E-06 | 5.315E+08        | 2.3113E+00    | 1.266E-06 | 5.227E+08        |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 9.8786E+01    | 1.299E-05 | 2.960E+06        | 9.8358E+01    | 1.298E-05 | 2.959E+06        |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.0004E+02    | 2.400E-05 | 5.332E+06        | 9.9559E+01    | 2.397E-05 | 5.331E+06        |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.2519E+03    | 1.718E-06 | 2.437E+03        | 1.2319E+03    | 1.743E-06 | 2.532E+03        |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 3d <sup>3</sup> D <sub>3</sub>              | 3.4166E+02    | 3.300E-05 | 2.694E+05        | 3.4098E+02    | 3.294E-05 | 2.677E+05        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 3d <sup>1</sup> D <sub>2</sub>              | 2.1090E+00    | 5.714E-11 | 1.714E+04        | 2.1000E+00    | 1.086E-12 | 3.258E+02        |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 3d <sup>1</sup> D <sub>2</sub>              | 6.7876E+01    | 1.745E-10 | 5.052E+01        | 6.7664E+01    | 1.801E-10 | 5.205E+01        |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 3d <sup>1</sup> D <sub>2</sub>              | 3.2917E+02    | 2.437E-06 | 3.000E+04        | 3.2831E+02    | 2.433E-06 | 2.985E+04        |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 3d <sup>1</sup> D <sub>2</sub>              | 3.4272E+02    | 2.090E-05 | 2.374E+05        | 3.4177E+02    | 2.084E-05 | 2.360E+05        |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 3d <sup>1</sup> D <sub>2</sub>              | 8.9990E+03    | 6.377E-07 | 1.050E+01        |               |           |                  |
| 1s <sup>2</sup> 1S <sub>0</sub>                | 1s 4s <sup>3</sup> S <sub>1</sub>              | 3.2800E-01    | 3.766E-06 | 7.780E+10        | 3.2669E-01    | 3.731E-06 | 7.706E+10        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 4s <sup>3</sup> S <sub>1</sub>              | 1.6177E+00    | 2.937E-07 | 2.495E+08        | 1.6108E+00    | 2.937E-07 | 2.495E+08        |
| 1s 2s <sup>1</sup> S <sub>0</sub>              | 1s 4s <sup>3</sup> S <sub>1</sub>              | 1.6358E+00    | 1.581E-07 | 1.313E+08        | 1.6291E+00    | 1.481E-07 | 1.230E+08        |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 4s <sup>3</sup> S <sub>1</sub>              | 6.2995E+00    | 5.467E-08 | 3.063E+06        | 6.2733E+00    | 5.451E-08 | 3.053E+06        |
| 1s 3s <sup>1</sup> S <sub>0</sub>              | 1s 4s <sup>3</sup> S <sub>1</sub>              | 6.3723E+00    | 3.304E-08 | 1.809E+06        | 6.3465E+00    | 2.752E-08 | 1.506E+06        |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 4s <sup>3</sup> S <sub>1</sub>              | 6.8005E+00    | 7.832E-12 | 3.766E+02        | 6.7717E+00    | 2.642E-11 | 1.270E+03        |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 4s <sup>3</sup> S <sub>1</sub>              | 6.8061E+00    | 5.861E-11 | 2.813E+03        |               |           |                  |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 4s <sup>3</sup> S <sub>1</sub>              | 6.9440E+00    | 7.996E-12 | 3.687E+02        |               |           |                  |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.6323E+00    | 6.280E-08 | 5.241E+07        | 1.6255E+00    | 7.524E-08 | 6.277E+07        |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.6336E+00    | 3.333E-08 | 2.777E+07        | 1.6268E+00    | 4.319E-08 | 3.598E+07        |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.7203E+00    | 1.671E-06 | 1.255E+09        | 1.7131E+00    | 1.700E-06 | 1.277E+09        |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.7287E+00    | 3.958E-07 | 2.945E+08        | 1.7215E+00    | 3.662E-07 | 2.724E+08        |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 6.3396E+00    | 1.616E-08 | 8.938E+05        | 6.3138E+00    | 1.862E-08 | 1.029E+06        |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 6.3447E+00    | 6.591E-09 | 3.640E+05        | 6.3187E+00    | 1.409E-08 | 7.784E+05        |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 6.7379E+00    | 1.885E-06 | 9.233E+07        | 6.7101E+00    | 1.933E-06 | 9.466E+07        |
| 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 6.7743E+00    | 4.274E-07 | 2.071E+07        | 6.7469E+00    | 4.002E-07 | 1.938E+07        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 4s <sup>1</sup> S <sub>0</sub>              | 1.6158E+00    | 1.404E-07 | 3.587E+08        | 1.6089E+00    | 1.466E-07 | 3.746E+08        |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 4s <sup>1</sup> S <sub>0</sub>              | 6.2706E+00    | 2.269E-08 | 3.850E+06        | 6.2442E+00    | 2.713E-08 | 4.602E+06        |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 4s <sup>1</sup> S <sub>0</sub>              | 6.7723E+00    | 8.192E-12 | 1.191E+03        | 6.7433E+00    | 9.047E-12 | 1.319E+03        |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 4s <sup>1</sup> S <sub>0</sub>              | 1.3658E+03    | 2.282E-08 | 8.159E+01        | 1.3474E+03    | 2.246E-08 | 8.184E+01        |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.6322E+00    | 4.224E-08 | 1.058E+08        | 1.6254E+00    | 2.329E-08 | 5.831E+07        |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.7285E+00    | 6.899E-07 | 1.540E+09        | 1.7214E+00    | 7.028E-07 | 1.568E+09        |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 6.3375E+00    | 1.172E-08 | 1.946E+06        | 6.3118E+00    | 5.619E-09 | 5.619E+05        |
| 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 6.7720E+00    | 7.666E-07 | 1.115E+08        | 6.7446E+00    | 7.828E-07 | 1.138E+08        |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.9682E+04    | 2.467E-07 | 4.247E+00        | 2.0312E+04    | 2.386E-07 | 3.825E+00        |

(continued on next page)

Table 5 (continued)

| Lower  | Upper  | GRASP2K       |           |                             | FAC           |           |                             |
|--|--|---------------|-----------|-----------------------------|---------------|-----------|-----------------------------|
|  |  | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6219E+00    | 8.188E-07 | 4.153E+08                   | 1.6152E+00    | 8.517E-07 | 4.318E+08                   |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.7088E+00    | 9.864E-07 | 4.507E+08                   | 1.7016E+00    | 9.961E-07 | 4.550E+08                   |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.7170E+00    | 9.347E-08 | 4.230E+07                   | 1.7100E+00    | 8.866E-08 | 4.010E+07                   |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 6.1858E+00    | 1.301E-06 | 4.535E+07                   | 6.1607E+00    | 1.338E-06 | 4.665E+07                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 6.5644E+00    | 2.489E-07 | 7.705E+06                   | 6.5375E+00    | 2.511E-07 | 7.773E+06                   |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 6.5991E+00    | 1.418E-08 | 4.343E+05                   | 6.5723E+00    | 1.571E-08 | 4.812E+05                   |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 2.5504E+02    | 2.729E-05 | 5.597E+05                   | 2.5410E+02    | 2.728E-05 | 5.589E+05                   |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 4d <sup>3</sup> D <sub>2</sub>              | 1.6050E+00    | 2.666E-08 | 1.380E+07                   | 1.5981E+00    | 2.759E-08 | 1.429E+07                   |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 4d <sup>3</sup> D <sub>2</sub>              | 6.1111E+00    | 2.618E-09 | 9.352E+04                   | 6.0854E+00    | 2.952E-09 | 1.054E+05                   |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 4d <sup>3</sup> D <sub>2</sub>              | 6.5814E+00    | 9.907E-08 | 3.051E+06                   | 6.5534E+00    | 9.901E-08 | 3.049E+06                   |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 4d <sup>3</sup> D <sub>2</sub>              | 6.5866E+00    | 7.839E-09 | 2.410E+05                   | 6.5585E+00    | 1.134E-08 | 3.487E+05                   |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 4d <sup>3</sup> D <sub>2</sub>              | 6.7107E+00    | 3.091E-07 | 9.158E+06                   | 6.6818E+00    | 3.090E-07 | 9.155E+06                   |
| 1s 3d <sup>1</sup> D <sub>3</sub>              | 1s 4d <sup>3</sup> D <sub>2</sub>              | 6.7157E+00    | 2.412E-08 | 7.136E+05                   | 6.6868E+00    | 2.277E-08 | 6.736E+05                   |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 4d <sup>3</sup> D <sub>2</sub>              | 2.0428E+02    | 2.882E-10 | 9.211E+00                   | 2.0324E+02    | 2.883E-10 | 9.234E+00                   |
| 1s <sup>2</sup> S <sub>0</sub>                 | 1s 4d <sup>3</sup> D <sub>1</sub>              | 3.2750E-01    | 5.115E-08 | 1.060E+09                   | 3.2616E-01    | 5.140E-08 | 1.065E+09                   |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 4d <sup>3</sup> D <sub>1</sub>              | 1.6048E+00    | 7.191E-09 | 6.208E+06                   | 1.5980E+00    | 5.396E-09 | 4.658E+06                   |
| 1s 2s <sup>1</sup> S <sub>0</sub>              | 1s 4d <sup>3</sup> D <sub>1</sub>              | 1.6227E+00    | 1.101E-08 | 9.298E+06                   | 1.6161E+00    | 1.127E-08 | 9.515E+06                   |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 4d <sup>3</sup> D <sub>1</sub>              | 6.1092E+00    | 1.076E-09 | 6.410E+04                   | 6.0836E+00    | 5.912E-10 | 3.521E+04                   |
| 1s 3s <sup>1</sup> S <sub>0</sub>              | 1s 4d <sup>3</sup> D <sub>1</sub>              | 6.1777E+00    | 1.224E-09 | 7.130E+04                   | 6.1525E+00    | 1.246E-09 | 7.260E+04                   |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 4d <sup>3</sup> D <sub>1</sub>              | 6.5793E+00    | 1.479E-08 | 7.599E+05                   | 6.5513E+00    | 1.065E-08 | 5.475E+05                   |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 4d <sup>3</sup> D <sub>1</sub>              | 6.5845E+00    | 5.503E-08 | 2.822E+06                   | 6.5564E+00    | 5.496E-08 | 2.818E+06                   |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 4d <sup>3</sup> D <sub>1</sub>              | 6.7135E+00    | 1.969E-07 | 9.715E+06                   | 6.6847E+00    | 1.995E-07 | 9.846E+06                   |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 4d <sup>3</sup> D <sub>1</sub>              | 2.0227E+02    | 4.243E-10 | 2.306E+01                   | 2.0125E+02    | 4.340E-10 | 2.362E+01                   |
| 1s 4s <sup>1</sup> S <sub>0</sub>              | 1s 4d <sup>3</sup> D <sub>1</sub>              | 2.3744E+02    | 2.003E-11 | 7.899E-01                   | 2.3659E+02    | 2.025E-11 | 7.976E-01                   |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 4d <sup>3</sup> D <sub>1</sub>              | 2.0536E+04    | 4.486E-07 | 2.365E+00                   | 2.0610E+04    | 4.464E-07 | 2.317E+00                   |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.6210E+00    | 1.525E-07 | 1.290E+08                   | 1.6143E+00    | 1.504E-07 | 1.272E+08                   |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.6223E+00    | 3.076E-07 | 2.598E+08                   | 1.6155E+00    | 3.230E-07 | 2.728E+08                   |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.7078E+00    | 1.729E-07 | 1.318E+08                   | 1.7006E+00    | 1.452E-07 | 1.107E+08                   |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.7161E+00    | 5.523E-07 | 4.170E+08                   | 1.7090E+00    | 5.447E-07 | 4.112E+08                   |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 6.1732E+00    | 2.703E-07 | 1.577E+07                   | 6.1480E+00    | 2.570E-07 | 1.499E+07                   |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 6.1780E+00    | 5.068E-07 | 2.952E+07                   | 6.1526E+00    | 5.255E-07 | 3.060E+07                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 6.5502E+00    | 5.703E-08 | 2.955E+06                   | 6.5232E+00    | 4.794E-08 | 2.483E+06                   |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 6.5847E+00    | 1.399E-07 | 7.175E+06                   | 6.5579E+00    | 1.361E-07 | 6.978E+06                   |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.3520E+02    | 5.486E-06 | 2.205E+05                   | 2.3412E+02    | 5.485E-06 | 2.206E+05                   |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.3804E+02    | 1.015E-05 | 3.983E+05                   | 2.3685E+02    | 1.014E-05 | 3.986E+05                   |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.0236E+03    | 7.020E-07 | 1.707E+02                   | 2.9782E+03    | 7.124E-07 | 1.770E+02                   |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 4d <sup>3</sup> D <sub>3</sub>              | 6.5283E+00    | 1.218E-07 | 2.724E+06                   | 6.5006E+00    | 1.221E-07 | 2.731E+06                   |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 4d <sup>3</sup> D <sub>3</sub>              | 6.6555E+00    | 4.750E-07 | 1.022E+07                   | 6.6270E+00    | 4.735E-07 | 1.018E+07                   |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 4d <sup>3</sup> D <sub>3</sub>              | 6.6604E+00    | 2.024E-08 | 4.348E+05                   | 6.6320E+00    | 2.330E-08 | 5.005E+05                   |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 4d <sup>3</sup> D <sub>3</sub>              | 8.0890E+02    | 1.403E-05 | 2.043E+04                   | 8.0816E+02    | 1.399E-05 | 2.032E+04                   |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.7043E+00    | 2.513E-08 | 8.245E+06                   | 1.6971E+00    | 2.356E-08 | 7.728E+06                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 6.4989E+00    | 1.254E-08 | 2.829E+05                   | 6.4721E+00    | 1.209E-08 | 2.729E+05                   |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 6.5059E+02    | 1.536E-11 | 3.458E-02                   | 6.4694E+02    | 1.460E-11 | 3.297E-02                   |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6178E+00    | 3.126E-11 | 1.593E+04                   | 1.6111E+00    | 1.478E-11 | 7.535E+03                   |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.7042E+00    | 1.963E-09 | 9.016E+05                   | 1.6971E+00    | 1.712E-09 | 7.863E+05                   |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.7124E+00    | 1.619E-08 | 7.364E+06                   | 1.7054E+00    | 1.552E-08 | 7.060E+06                   |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 6.1266E+00    | 2.174E-11 | 7.726E+02                   | 6.1016E+00    | 1.249E-11 | 4.437E+02                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 6.4978E+00    | 1.077E-09 | 3.402E+04                   | 6.4710E+00    | 8.534E-10 | 2.696E+04                   |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 6.5317E+00    | 8.213E-09 | 2.568E+05                   | 6.5052E+00    | 7.853E-09 | 2.454E+05                   |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.8236E+02    | 4.207E-12 | 1.688E-01                   | 1.8158E+02    | 4.868E-12 | 1.953E-01                   |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 6.3989E+02    | 1.075E-11 | 3.504E-02                   | 6.3631E+02    | 1.094E-11 | 3.574E-02                   |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 8.1166E+02    | 1.204E-12 | 2.438E-03                   | 8.0920E+02    | 1.035E-12 | 2.090E-03                   |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.8916E+04    | 3.280E-07 | 2.889E-01                   | 3.8737E+04    | 3.272E-07 | 2.884E-01                   |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 4d <sup>1</sup> D <sub>2</sub>              | 1.6017E+00    | 2.260E-11 | 1.175E+04                   | 1.5948E+00    | 8.840E-13 | 4.597E+02                   |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 4d <sup>1</sup> D <sub>2</sub>              | 6.0634E+00    | 1.398E-11 | 5.074E+02                   |               |           |                             |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 4d <sup>1</sup> D <sub>2</sub>              | 6.5262E+00    | 9.491E-09 | 2.973E+05                   | 6.4985E+00    | 8.647E-09 | 2.708E+05                   |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 4d <sup>1</sup> D <sub>2</sub>              | 6.5313E+00    | 7.615E-08 | 2.382E+06                   | 6.5035E+00    | 7.788E-08 | 2.435E+06                   |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 4d <sup>1</sup> D <sub>2</sub>              | 6.6532E+00    | 2.818E-08 | 8.493E+05                   | 6.6247E+00    | 2.465E-08 | 7.431E+05                   |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 4d <sup>1</sup> D <sub>2</sub>              | 6.6582E+00    | 3.320E-07 | 9.989E+06                   | 6.6297E+00    | 3.309E-07 | 9.959E+06                   |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 4d <sup>1</sup> D <sub>2</sub>              | 1.6177E+02    | 1.007E-10 | 5.133E+00                   | 1.6105E+02    | 1.039E-10 | 5.302E+00                   |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 4d <sup>1</sup> D <sub>2</sub>              | 7.7722E+02    | 1.036E-06 | 2.289E+03                   | 7.7592E+02    | 1.033E-06 | 2.271E+03                   |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 4d <sup>1</sup> D <sub>2</sub>              | 8.0779E+02    | 8.860E-06 | 1.811E+04                   | 8.0628E+02    | 8.829E-06 | 1.796E+04                   |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 4d <sup>1</sup> D <sub>2</sub>              | 1.9845E+04    | 2.845E-07 | 9.638E-01                   |               |           |                             |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6355E+03    | 9.461E-06 | 2.621E+03                   | 1.6325E+03    | 9.436E-06 | 2.602E+03                   |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.7025E+00    | 1.542E-12 | 5.069E+02                   | 1.6953E+00    | 1.104E-13 | 3.631E+01                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 6.4724E+00    | 5.423E-13 | 1.234E+01                   | 6.4457E+00    | 5.663E-14 | 1.287E+00                   |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.6135E+02    | 3.233E-12 | 1.447E-02                   |               |           |                             |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.5861E+03    | 3.618E-07 | 1.371E+02                   | 1.5830E+03    | 3.609E-07 | 1.360E+02                   |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6535E+03    | 6.987E-06 | 2.435E+03                   | 1.6504E+03    | 6.969E-06 | 2.417E+03                   |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.2510E+04    | 1.734E-07 | 5.991E-02                   |               |           |                             |
| 1s <sup>2</sup> S <sub>0</sub>                 | 1s 5s <sup>3</sup> S <sub>1</sub>              | 3.2040E-01    | 1.922E-06 | 4.161E+10                   | 3.1907E-01    | 1.905E-06 | 4.127E+10                   |

(continued on next page)

Table 5 (continued)

| Lower          | Upper          | GRASP2K       |           |                  | FAC           |           |                  |
|----------------|----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                |                | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s2s $^3S_1$   | 1s5s $^3S_1$   | 1.4473E+00    | 1.544E-07 | 1.639E+08        | 1.4412E+00    | 1.548E-07 | 1.643E+08        |
| 1s2s $^1S_0$   | 1s5s $^3S_1$   | 1.4618E+00    | 8.255E-08 | 8.589E+07        | 1.4559E+00    | 7.804E-08 | 8.117E+07        |
| 1s3s $^3S_1$   | 1s5s $^3S_1$   | 4.3197E+00    | 3.183E-08 | 3.792E+06        | 4.3017E+00    | 3.191E-08 | 3.802E+06        |
| 1s3s $^1S_0$   | 1s5s $^3S_1$   | 4.3538E+00    | 1.834E-08 | 2.152E+06        | 4.3360E+00    | 1.605E-08 | 1.882E+06        |
| 1s3d $^3D_2$   | 1s5s $^3S_1$   | 4.5495E+00    | 1.900E-12 | 2.041E+02        | 4.5304E+00    | 7.521E-12 | 8.078E+02        |
| 1s3d $^3D_1$   | 1s5s $^3S_1$   | 4.5520E+00    | 1.815E-11 | 1.948E+03        |               |           |                  |
| 1s3d $^1D_2$   | 1s5s $^3S_1$   | 4.6133E+00    | 2.661E-12 | 2.780E+02        |               |           |                  |
| 1s4s $^3S_1$   | 1s5s $^3S_1$   | 1.3745E+01    | 8.945E-09 | 1.053E+05        | 1.3688E+01    | 8.938E-09 | 1.051E+05        |
| 1s4s $^1S_0$   | 1s5s $^3S_1$   | 1.3885E+01    | 6.095E-09 | 7.030E+04        | 1.3828E+01    | 4.509E-09 | 5.198E+04        |
| 1s4d $^3D_2$   | 1s5s $^3S_1$   | 1.4736E+01    | 2.859E-12 | 2.927E+01        | 1.4676E+01    | 1.277E-11 | 1.308E+02        |
| 1s4d $^3D_1$   | 1s5s $^3S_1$   | 1.4747E+01    | 3.595E-11 | 3.675E+02        | 1.4686E+01    | 2.338E-12 | 2.389E+01        |
| 1s4d $^1D_2$   | 1s5s $^3S_1$   | 1.5021E+01    | 4.998E-12 | 4.925E+01        |               |           |                  |
| 1s2p $^3P_0^0$ | 1s5p $^3P_0^0$ | 1.4598E+00    | 3.325E-08 | 3.469E+07        | 1.4537E+00    | 3.812E-08 | 3.977E+07        |
| 1s2p $^3P_0^1$ | 1s5p $^3P_0^1$ | 1.4608E+00    | 1.660E-08 | 1.729E+07        | 1.4547E+00    | 2.159E-08 | 2.249E+07        |
| 1s2p $^3P_0^2$ | 1s5p $^3P_0^2$ | 1.5297E+00    | 7.583E-07 | 7.205E+08        | 1.5233E+00    | 7.714E-07 | 7.329E+08        |
| 1s2p $^1P_1^0$ | 1s5p $^3P_0^1$ | 1.5364E+00    | 1.790E-07 | 1.686E+08        | 1.5300E+00    | 1.667E-07 | 1.570E+08        |
| 1s3p $^3P_0^0$ | 1s5p $^3P_0^1$ | 4.3450E+00    | 9.303E-09 | 1.096E+06        | 4.3271E+00    | 1.018E-08 | 1.198E+06        |
| 1s3p $^3P_0^1$ | 1s5p $^3P_0^1$ | 4.3474E+00    | 3.783E-09 | 4.450E+05        | 4.3294E+00    | 7.068E-09 | 8.313E+05        |
| 1s3p $^3P_0^2$ | 1s5p $^3P_0^2$ | 4.5285E+00    | 6.596E-07 | 7.151E+07        | 4.5097E+00    | 6.741E-07 | 7.307E+07        |
| 1s3p $^1P_1^0$ | 1s5p $^3P_0^1$ | 4.5449E+00    | 1.499E-07 | 1.613E+07        | 4.5263E+00    | 1.410E-07 | 1.517E+07        |
| 1s4p $^3P_0^1$ | 1s5p $^3P_0^1$ | 1.3810E+01    | 3.141E-09 | 3.662E+04        | 1.3752E+01    | 3.286E-09 | 3.831E+04        |
| 1s4p $^3P_0^2$ | 1s5p $^3P_0^1$ | 1.3820E+01    | 8.034E-10 | 9.353E+03        | 1.3761E+01    | 3.266E-09 | 3.803E+04        |
| 1s4p $^3P_0^3$ | 1s5p $^3P_0^1$ | 1.4601E+01    | 8.508E-07 | 8.874E+06        | 1.4539E+01    | 8.744E-07 | 9.120E+06        |
| 1s4p $^1P_1^0$ | 1s5p $^3P_0^1$ | 1.4672E+01    | 1.898E-07 | 1.961E+06        | 1.4610E+01    | 1.785E-07 | 1.843E+06        |
| 1s4f $^3F_2^0$ | 1s5p $^3P_0^1$ | 1.4942E+01    | 2.377E-13 | 2.367E+00        |               |           |                  |
| 1s2s $^3S_1$   | 1s5s $^1S_0$   | 1.4466E+00    | 7.497E-08 | 2.390E+08        | 1.4404E+00    | 7.736E-08 | 2.466E+08        |
| 1s3s $^3S_1$   | 1s5s $^1S_0$   | 4.3129E+00    | 1.408E-08 | 5.050E+06        | 4.2949E+00    | 1.592E-08 | 5.711E+06        |
| 1s3d $^3D_1$   | 1s5s $^1S_0$   | 4.5444E+00    | 2.226E-12 | 7.191E+02        | 4.5252E+00    | 2.275E-12 | 7.347E+02        |
| 1s4s $^3S_1$   | 1s5s $^1S_0$   | 1.3676E+01    | 3.196E-09 | 1.140E+05        | 1.3618E+01    | 4.447E-09 | 1.585E+05        |
| 1s4d $^3D_1$   | 1s5s $^1S_0$   | 1.4668E+01    | 4.200E-12 | 1.302E+02        | 1.4607E+01    | 4.661E-12 | 1.445E+02        |
| 1s5s $^3S_1$   | 1s5s $^1S_0$   | 2.7268E+03    | 1.197E-08 | 1.074E+01        | 2.6934E+03    | 1.177E-08 | 1.073E+01        |
| 1s2p $^3P_0^0$ | 1s5p $^3P_0^0$ | 1.4597E+00    | 2.071E-08 | 6.482E+07        | 1.4537E+00    | 1.212E-08 | 3.793E+07        |
| 1s2p $^1P_1^0$ | 1s5p $^3P_0^0$ | 1.5363E+00    | 3.127E-07 | 8.836E+08        | 1.5300E+00    | 3.196E-07 | 9.030E+08        |
| 1s3p $^3P_0^0$ | 1s5p $^3P_0^0$ | 4.3445E+00    | 5.943E-09 | 2.100E+06        | 4.3267E+00    | 2.377E-09 | 8.397E+05        |
| 1s3p $^1P_1^0$ | 1s5p $^3P_0^0$ | 4.5444E+00    | 2.684E-07 | 8.670E+07        | 4.5258E+00    | 2.745E-07 | 8.864E+07        |
| 1s4p $^3P_0^1$ | 1s5p $^3P_0^0$ | 1.3805E+01    | 2.173E-09 | 7.604E+04        | 1.3747E+01    | 2.595E-10 | 9.084E+03        |
| 1s4p $^1P_1^0$ | 1s5p $^3P_0^0$ | 1.4666E+01    | 3.440E-07 | 1.067E+07        | 1.4605E+01    | 3.519E-07 | 1.091E+07        |
| 1s5p $^3P_0^0$ | 1s5p $^3P_0^0$ | 3.9500E+04    | 1.224E-07 | 5.231E-01        | 4.0718E+04    | 1.185E-07 | 4.729E-01        |
| 1s2p $^3P_0^1$ | 1s5p $^3P_0^2$ | 1.4555E+00    | 3.625E-07 | 2.283E+08        | 1.4495E+00    | 3.760E-07 | 2.367E+08        |
| 1s2p $^3P_0^2$ | 1s5p $^3P_0^2$ | 1.5251E+00    | 5.039E-07 | 2.890E+08        | 1.5187E+00    | 5.187E-07 | 2.912E+08        |
| 1s2p $^1P_1^0$ | 1s5p $^3P_0^2$ | 1.5317E+00    | 4.698E-08 | 2.672E+07        | 1.5253E+00    | 4.591E-08 | 2.610E+07        |
| 1s3p $^3P_0^0$ | 1s5p $^3P_0^2$ | 4.3076E+00    | 4.374E-07 | 3.145E+07        | 4.2899E+00    | 4.510E-07 | 3.242E+07        |
| 1s3p $^3P_0^1$ | 1s5p $^3P_0^2$ | 4.4878E+00    | 1.396E-07 | 9.247E+06        | 4.4692E+00    | 1.403E-07 | 9.293E+06        |
| 1s3p $^1P_1^0$ | 1s5p $^3P_0^2$ | 4.5039E+00    | 9.365E-09 | 6.158E+05        | 4.4855E+00    | 1.008E-08 | 6.628E+05        |
| 1s4p $^3P_0^1$ | 1s5p $^3P_0^2$ | 1.3439E+01    | 6.586E-07 | 4.865E+06        | 1.3383E+01    | 6.762E-07 | 4.994E+06        |
| 1s4p $^3P_0^2$ | 1s5p $^3P_0^2$ | 1.4186E+01    | 4.513E-08 | 2.991E+05        | 1.4127E+01    | 4.470E-08 | 2.963E+05        |
| 1s4p $^1P_1^0$ | 1s5p $^3P_0^2$ | 1.4253E+01    | 1.024E-09 | 6.726E+03        | 1.4194E+01    | 1.700E-09 | 1.116E+04        |
| 1s4f $^3F_3^0$ | 1s5p $^3P_0^2$ | 1.4503E+01    | 1.154E-12 | 7.318E+00        |               |           |                  |
| 1s4f $^3F_2^0$ | 1s5p $^3P_0^2$ | 1.4508E+01    | 3.204E-13 | 2.031E+00        |               |           |                  |
| 1s4f $^1F_3^0$ | 1s5p $^3P_0^2$ | 1.4636E+01    | 4.259E-14 | 2.652E-01        |               |           |                  |
| 1s5p $^3P_0^1$ | 1s5p $^3P_0^2$ | 4.9993E+02    | 1.394E-05 | 7.439E+04        | 4.9817E+02    | 1.393E-05 | 7.425E+04        |
| 1s2s $^3S_1$   | 1s5d $^3D_2$   | 1.4421E+00    | 1.207E-08 | 7.745E+06        | 1.4360E+00    | 1.251E-08 | 8.030E+06        |
| 1s3s $^3S_1$   | 1s5d $^3D_2$   | 4.2737E+00    | 1.741E-09 | 1.272E+05        | 4.2558E+00    | 1.922E-09 | 1.403E+05        |
| 1s3d $^3D_2$   | 1s5d $^3D_2$   | 4.4985E+00    | 4.750E-08 | 3.132E+06        | 4.4794E+00    | 4.750E-08 | 3.131E+06        |
| 1s3d $^3D_1$   | 1s5d $^3D_2$   | 4.5010E+00    | 4.030E-09 | 2.654E+05        | 4.4818E+00    | 5.426E-09 | 3.573E+05        |
| 1s3d $^3D_3$   | 1s5d $^3D_2$   | 4.5585E+00    | 1.063E-07 | 6.826E+06        | 4.5391E+00    | 1.063E-07 | 6.830E+06        |
| 1s3d $^1D_2$   | 1s5d $^3D_2$   | 4.5609E+00    | 8.379E-09 | 5.374E+05        | 4.5414E+00    | 7.951E-09 | 5.099E+05        |
| 1s4s $^3S_1$   | 1s5d $^3D_2$   | 1.3290E+01    | 1.420E-10 | 1.073E+03        | 1.3233E+01    | 1.983E-10 | 1.498E+03        |
| 1s4d $^3D_2$   | 1s5d $^3D_2$   | 1.4214E+01    | 2.217E-08 | 1.464E+05        | 1.4154E+01    | 2.214E-08 | 1.462E+05        |
| 1s4d $^3D_1$   | 1s5d $^3D_2$   | 1.4224E+01    | 1.417E-09 | 9.343E+03        | 1.4164E+01    | 2.610E-09 | 1.720E+04        |
| 1s4d $^3D_3$   | 1s5d $^3D_2$   | 1.4468E+01    | 1.506E-07 | 9.600E+05        | 1.4407E+01    | 1.507E-07 | 9.606E+05        |
| 1s4d $^1D_2$   | 1s5d $^3D_2$   | 1.4479E+01    | 1.171E-08 | 7.449E+04        | 1.4417E+01    | 1.098E-08 | 6.991E+04        |
| 1s5s $^3S_1$   | 1s5d $^3D_2$   | 4.0118E+02    | 1.290E-10 | 1.070E+00        | 3.9828E+02    | 1.291E-10 | 1.076E+00        |
| 1s2p $^3P_0^0$ | 1s5p $^1P_1^0$ | 1.4551E+00    | 6.636E-08 | 6.969E+07        | 1.4491E+00    | 6.566E-08 | 6.893E+07        |
| 1s2p $^3P_0^1$ | 1s5p $^1P_1^0$ | 1.4562E+00    | 1.354E-07 | 1.420E+08        | 1.4501E+00    | 1.420E-07 | 1.489E+08        |
| 1s2p $^3P_0^2$ | 1s5p $^1P_1^0$ | 1.5247E+00    | 8.556E-08 | 8.183E+07        | 1.5183E+00    | 7.479E-08 | 6.962E+07        |
| 1s2p $^1P_1^0$ | 1s5p $^1P_1^0$ | 1.5313E+00    | 2.795E-07 | 2.651E+08        | 1.5249E+00    | 2.779E-07 | 2.635E+08        |
| 1s3p $^3P_0^0$ | 1s5p $^1P_1^0$ | 4.3044E+00    | 8.940E-08 | 1.073E+07        | 4.2867E+00    | 8.521E-08 | 1.022E+07        |
| 1s3p $^3P_0^1$ | 1s5p $^1P_1^0$ | 4.3068E+00    | 1.695E-07 | 2.032E+07        | 4.2890E+00    | 1.758E-07 | 2.107E+07        |
| 1s3p $^3P_0^2$ | 1s5p $^1P_1^0$ | 4.4844E+00    | 2.833E-08 | 3.132E+06        | 4.4658E+00    | 2.453E-08 | 2.656E+06        |
| 1s3p $^1P_1^0$ | 1s5p $^1P_1^0$ | 4.5006E+00    | 7.769E-08 | 8.528E+06        | 4.4821E+00    | 7.651E-08 | 8.396E+06        |

(continued on next page)

Table 5 (continued)

| Lower  | Upper  | GRASP2K       |           |                  | FAC           |           |                  |
|--|--|---------------|-----------|------------------|---------------|-----------|------------------|
|  |  | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.3409E+01    | 1.400E-07 | 1.732E+06        | 1.3352E+01    | 1.323E-07 | 1.636E+06        |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.3418E+01    | 2.593E-07 | 3.202E+06        | 1.3361E+01    | 2.678E-07 | 3.307E+06        |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.4153E+01    | 1.282E-08 | 1.423E+05        | 1.4093E+01    | 1.104E-08 | 1.226E+05        |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.4219E+01    | 2.450E-08 | 2.695E+05        | 1.4160E+01    | 2.407E-08 | 2.647E+05        |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.4473E+01    | 1.066E-12 | 1.131E+01        |               |           |                  |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.6126E+02    | 2.804E-06 | 2.931E+04        | 4.5925E+02    | 2.803E-06 | 2.930E+04        |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.6671E+02    | 5.192E-06 | 5.300E+04        | 4.6449E+02    | 5.187E-06 | 5.301E+04        |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 5.9640E+03    | 3.535E-07 | 2.210E+01        | 5.8780E+03    | 3.589E-07 | 2.290E+01        |
| 1s <sup>2</sup> 1S <sub>0</sub>                | 1s 5d <sup>3</sup> D <sub>1</sub>              | 3.2010E-01    | 2.906E-08 | 6.303E+08        | 3.1882E-01    | 2.923E-08 | 6.341E+08        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4421E+00    | 3.269E-09 | 3.496E+06        | 1.4359E+00    | 2.440E-09 | 2.609E+06        |
| 1s 2s <sup>1</sup> S <sub>0</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4565E+00    | 4.982E-09 | 5.221E+06        | 1.4505E+00    | 5.091E-09 | 5.335E+06        |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.2732E+00    | 6.295E-10 | 7.664E+04        | 4.2553E+00    | 3.832E-10 | 4.666E+04        |
| 1s 3s <sup>1</sup> S <sub>0</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.3066E+00    | 7.848E-10 | 9.408E+04        | 4.2889E+00    | 7.962E-10 | 9.543E+04        |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.4980E+00    | 6.754E-09 | 7.423E+05        | 4.4789E+00    | 5.140E-09 | 5.648E+05        |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.5005E+00    | 2.642E-08 | 2.900E+06        | 4.4813E+00    | 2.637E-08 | 2.895E+06        |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.5603E+00    | 6.789E-08 | 7.258E+06        | 4.5409E+00    | 6.881E-08 | 7.357E+06        |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.3285E+01    | 1.345E-10 | 1.694E+03        | 1.3229E+01    | 4.034E-11 | 5.082E+02        |
| 1s 4s <sup>1</sup> S <sub>0</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.3416E+01    | 8.406E-11 | 1.038E+03        | 1.3360E+01    | 8.608E-11 | 1.063E+03        |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4209E+01    | 3.779E-09 | 4.162E+04        | 1.4150E+01    | 2.284E-09 | 2.515E+04        |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4219E+01    | 1.231E-08 | 1.354E+05        | 1.4159E+01    | 1.228E-08 | 1.350E+05        |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4474E+01    | 9.593E-08 | 1.018E+06        | 1.4412E+01    | 9.728E-08 | 1.032E+06        |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 3.9728E+02    | 2.647E-10 | 3.728E+00        | 3.9446E+02    | 2.698E-10 | 3.823E+00        |
| 1s 5s <sup>1</sup> S <sub>0</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.6504E+02    | 6.464E-12 | 6.646E-02        | 4.6214E+02    | 6.512E-12 | 6.722E-02        |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.0886E+04    | 2.249E-07 | 2.991E-01        | 4.1075E+04    | 2.236E-07 | 2.922E-01        |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 4.4858E+00    | 3.427E-08 | 1.623E+06        | 4.4668E+00    | 3.435E-08 | 1.627E+06        |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 4.5454E+00    | 2.279E-07 | 1.051E+07        | 4.5261E+00    | 2.277E-07 | 1.050E+07        |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 4.5477E+00    | 1.002E-08 | 4.616E+05        | 4.5284E+00    | 1.125E-08 | 5.183E+05        |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4088E+01    | 8.337E-08 | 4.003E+05        | 1.4029E+01    | 8.359E-08 | 4.013E+05        |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4337E+01    | 1.068E-07 | 4.952E+05        | 1.4277E+01    | 1.064E-07 | 4.936E+05        |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4348E+01    | 4.050E-09 | 1.875E+04        | 1.4287E+01    | 5.092E-09 | 2.357E+04        |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.5807E+03    | 7.199E-06 | 2.745E+03        | 1.5799E+03    | 7.177E-06 | 2.716E+03        |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.5232E+00    | 1.777E-08 | 7.298E+06        | 1.5168E+00    | 1.651E-08 | 6.783E+06        |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4720E+00    | 2.760E-09 | 1.315E+05        | 4.4534E+00    | 2.752E-09 | 1.311E+05        |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4030E+01    | 1.450E-09 | 7.019E+03        | 1.3970E+01    | 1.413E-09 | 6.842E+03        |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4339E+01    | 1.073E-08 | 4.974E+04        | 1.4278E+01    | 4.705E-08 | 2.180E+05        |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4344E+01    | 2.972E-08 | 1.376E+05        | 1.4283E+01    | 2.334E-09 | 1.081E+04        |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4466E+01    | 4.502E-08 | 2.050E+05        | 1.4404E+01    | 4.477E-08 | 2.039E+05        |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4470E+01    | 1.697E-09 | 7.722E+03        | 1.4408E+01    | 1.639E-09 | 7.462E+03        |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.2712E+03    | 9.159E-12 | 5.401E-03        | 1.2579E+03    | 8.880E-12 | 5.302E-03        |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4538E+00    | 2.242E-11 | 1.415E+04        | 1.4478E+00    | 1.093E-11 | 6.903E+03        |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.5232E+00    | 1.262E-09 | 7.255E+05        | 1.5168E+00    | 1.202E-09 | 6.912E+05        |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.5298E+00    | 1.114E-08 | 6.351E+06        | 1.5234E+00    | 1.084E-08 | 6.179E+06        |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.2928E+00    | 5.686E-12 | 4.116E+02        | 4.2750E+00    | 3.642E-12 | 2.636E+02        |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4718E+00    | 2.443E-10 | 1.630E+04        | 4.4531E+00    | 1.918E-10 | 1.279E+04        |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4878E+00    | 1.807E-09 | 1.197E+05        | 4.4693E+00    | 1.767E-09 | 1.170E+05        |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3296E+01    | 3.412E-12 | 2.575E+01        |               |           |                  |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4027E+01    | 1.361E-10 | 9.228E+02        | 1.3967E+01    | 1.003E-10 | 6.806E+02        |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4093E+01    | 9.657E-10 | 6.487E+03        | 1.4033E+01    | 9.194E-10 | 6.175E+03        |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4336E+01    | 3.412E-08 | 2.215E+05        | 1.4275E+01    | 2.392E-09 | 1.552E+04        |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4342E+01    | 6.360E-08 | 4.125E+05        | 1.4281E+01    | 3.295E-08 | 2.137E+05        |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.4467E+01    | 3.281E-08 | 2.091E+05        | 1.4405E+01    | 3.308E-08 | 2.109E+05        |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.5713E+02    | 3.711E-12 | 3.882E-02        | 3.5518E+02    | 4.170E-12 | 4.372E-02        |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.2503E+03    | 9.975E-12 | 8.513E-03        | 1.2374E+03    | 9.996E-12 | 8.635E-03        |
| 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.5820E+03    | 3.550E-13 | 1.892E-04        | 1.5673E+03    | 3.191E-13 | 1.718E-04        |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.6009E+04    | 1.688E-07 | 3.897E-02        | 7.5649E+04    | 1.670E-07 | 3.861E-02        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4408E+00    | 1.086E-11 | 6.980E+03        | 1.4346E+00    | 5.345E-13 | 3.435E+02        |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 4.2617E+00    | 6.144E-12 | 4.513E+02        |               |           |                  |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 4.4852E+00    | 2.704E-09 | 1.793E+05        | 4.4662E+00    | 2.441E-09 | 1.619E+05        |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 4.4876E+00    | 2.134E-08 | 1.413E+06        | 4.4686E+00    | 2.183E-08 | 1.446E+06        |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 4.5449E+00    | 1.323E-08 | 8.542E+05        | 4.5255E+00    | 1.184E-08 | 7.652E+05        |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 4.5472E+00    | 1.594E-07 | 1.028E+07        | 4.5278E+00    | 1.591E-07 | 1.026E+07        |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.3174E+01    | 5.744E-12 | 4.415E+01        |               |           |                  |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4082E+01    | 6.400E-09 | 4.306E+04        | 1.4023E+01    | 5.870E-09 | 3.948E+04        |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4092E+01    | 5.236E-08 | 3.517E+05        | 1.4033E+01    | 5.341E-08 | 3.587E+05        |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4332E+01    | 6.968E-09 | 4.525E+04        | 1.4271E+01    | 5.701E-09 | 3.703E+04        |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4342E+01    | 7.473E-08 | 4.847E+05        | 1.4282E+01    | 7.441E-08 | 4.825E+05        |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 3.1728E+02    | 5.803E-11 | 7.691E-01        | 3.1538E+02    | 5.834E-11 | 7.758E-01        |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.5170E+03    | 5.320E-07 | 3.084E+02        | 1.5150E+03    | 5.304E-07 | 3.056E+02        |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.5755E+03    | 4.542E-06 | 2.441E+03        | 1.5730E+03    | 4.524E-06 | 2.418E+03        |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 5d <sup>1</sup> D <sub>2</sub>              | 3.7649E+04    | 1.489E-07 | 1.401E-01        |               |           |                  |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.4275E+01    | 1.498E-08 | 5.450E+04        | 1.4214E+01    | 1.496E-08 | 5.443E+04        |

(continued on next page)

Table 5 (continued)

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |           |                  |
|-----------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                 |                 | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 4f $^3F_4^0$ | 1s 5f $^3F_4^0$ | 1.4401E+01    | 1.395E-07 | 4.986E+05        | 1.4339E+01    | 1.440E-07 | 5.146E+05        |
| 1s 4f $^1F_4^0$ | 1s 5f $^3F_4^0$ | 1.4404E+01    | 4.779E-09 | 1.707E+04        | 1.4343E+01    | 4.148E-09 | 1.481E+04        |
| 1s 5f $^3F_3^0$ | 1s 5f $^3F_4^0$ | 3.1889E+03    | 4.861E-06 | 3.543E+02        | 3.1838E+03    | 4.848E-06 | 3.514E+02        |
| 1s 3d $^3D_3$   | 1s 5g $^3G_4$   | 4.5387E+00    | 6.705E-09 | 2.412E+05        | 4.5195E+00    | 6.765E-09 | 2.433E+05        |
| 1s 4d $^3D_3$   | 1s 5g $^3G_4$   | 1.4271E+01    | 2.645E-09 | 9.626E+03        | 1.4212E+01    | 2.645E-09 | 9.624E+03        |
| 1s 5d $^3D_3$   | 1s 5g $^3G_4$   | 3.0779E+03    | 3.885E-13 | 3.040E-05        | 3.1417E+03    | 4.330E-13 | 3.223E-05        |
| 1s 3d $^3D_2$   | 1s 5g $^3G_3$   | 4.4791E+00    | 4.386E-13 | 2.083E+01        |               |           |                  |
| 1s 3d $^3D_3$   | 1s 5g $^3G_3$   | 4.5386E+00    | 2.962E-10 | 1.370E+04        | 4.5194E+00    | 2.508E-10 | 1.160E+04        |
| 1s 3d $^1D_2$   | 1s 5g $^3G_3$   | 4.5409E+00    | 5.076E-09 | 2.346E+05        | 4.5217E+00    | 5.023E-09 | 2.321E+05        |
| 1s 4d $^3D_2$   | 1s 5g $^3G_3$   | 1.4022E+01    | 1.928E-13 | 9.345E-01        |               |           |                  |
| 1s 4d $^3D_3$   | 1s 5g $^3G_3$   | 1.4269E+01    | 1.108E-10 | 5.186E+02        | 1.4210E+01    | 9.782E-11 | 4.576E+02        |
| 1s 4d $^1D_2$   | 1s 5g $^3G_3$   | 1.4280E+01    | 1.987E-09 | 9.285E+03        | 1.4221E+01    | 1.961E-09 | 9.165E+03        |
| 1s 5d $^3D_2$   | 1s 5g $^3G_3$   | 1.0362E+03    | 4.213E-15 | 3.739E-06        | 1.0430E+03    | 4.189E-15 | 3.638E-06        |
| 1s 5d $^3D_3$   | 1s 5g $^3G_3$   | 3.0082E+03    | 1.694E-16 | 1.784E-08        |               |           |                  |
| 1s 5d $^1D_2$   | 1s 5g $^3G_3$   | 3.2694E+03    | 2.036E-13 | 1.815E-05        | 3.3474E+03    | 1.574E-13 | 1.327E-05        |
| 1s 5g $^3G_4$   | 1s 5g $^3G_3$   | 1.3281E+05    | 1.209E-07 | 6.534E-03        | 1.3215E+05    | 1.213E-07 | 6.564E-03        |
| 1s 2p $^3P_0^0$ | 1s 5f $^1F_3^0$ | 1.5225E+00    | 1.031E-12 | 4.240E+02        | 1.5161E+00    | 6.722E-14 | 2.763E+01        |
| 1s 3p $^3P_0^0$ | 1s 5f $^1F_3^0$ | 4.4656E+00    | 1.185E-13 | 5.664E+00        | 4.4470E+00    | 1.124E-14 | 5.370E-01        |
| 1s 4p $^3P_0^0$ | 1s 5f $^1F_3^0$ | 1.3966E+01    | 2.140E-13 | 1.045E+00        |               |           |                  |
| 1s 4f $^3F_3^0$ | 1s 5f $^1F_3^0$ | 1.4273E+01    | 6.420E-10 | 3.003E+03        | 1.4212E+01    | 5.692E-10 | 2.662E+03        |
| 1s 4f $^3F_2^0$ | 1s 5f $^1F_3^0$ | 1.4278E+01    | 1.100E-08 | 5.141E+04        | 1.4218E+01    | 1.112E-08 | 5.201E+04        |
| 1s 4f $^3F_4^0$ | 1s 5f $^1F_3^0$ | 1.4398E+01    | 5.942E-09 | 2.731E+04        | 1.4337E+01    | 4.059E-09 | 1.866E+04        |
| 1s 4f $^1F_3^0$ | 1s 5f $^1F_3^0$ | 1.4402E+01    | 1.154E-07 | 5.300E+05        | 1.4341E+01    | 1.111E-07 | 5.104E+05        |
| 1s 5p $^3P_0^0$ | 1s 5f $^1F_3^0$ | 9.0084E+02    | 2.726E-12 | 3.201E-03        |               |           |                  |
| 1s 5f $^3F_3^0$ | 1s 5f $^1F_3^0$ | 3.0918E+03    | 1.860E-07 | 1.854E+01        | 3.0864E+03    | 1.854E-07 | 1.839E+01        |
| 1s 5f $^3F_2^0$ | 1s 5f $^1F_3^0$ | 3.2229E+03    | 3.589E-06 | 3.293E+02        | 3.2177E+03    | 3.579E-06 | 3.266E+02        |
| 1s 5f $^3F_4^0$ | 1s 5f $^1F_3^0$ | 1.0160E+05    | 8.920E-08 | 8.235E-03        |               |           |                  |
| 1s 5g $^3G_4$   | 1s 5g $^3G_5$   | 5.3554E+03    | 3.669E-06 | 7.758E+01        | 5.3442E+03    | 3.661E-06 | 7.707E+01        |
| 1s 3d $^3D_3$   | 1s 5g $^1G_4$   | 4.5348E+00    | 1.337E-13 | 4.817E+00        | 4.5156E+00    | 2.425E-14 | 8.741E-01        |
| 1s 4d $^3D_3$   | 1s 5g $^1G_4$   | 1.4232E+01    | 1.748E-14 | 6.398E-02        | 1.4173E+01    | 9.478E-15 | 3.467E-02        |
| 1s 5d $^3D_3$   | 1s 5g $^1G_4$   | 1.9321E+03    | 3.849E-15 | 7.643E-07        |               |           |                  |
| 1s 5g $^3G_4$   | 1s 5g $^1G_4$   | 5.1900E+03    | 8.607E-08 | 2.368E+00        | 5.1787E+03    | 8.589E-08 | 2.353E+00        |
| 1s 5g $^3G_3$   | 1s 5g $^1G_4$   | 5.4011E+03    | 2.914E-06 | 7.403E+01        | 5.3899E+03    | 2.907E-06 | 7.354E+01        |
| 1s 5g $^3G_5$   | 1s 5g $^1G_4$   | 1.6804E+05    | 7.357E-08 | 1.931E-03        |               |           |                  |
| 1s $^2S_0$      | 1s 6s $^3S_1$   | 3.1640E-01    | 1.107E-06 | 2.457E+10        | 3.1511E-01    | 1.098E-06 | 2.438E+10        |
| 1s 2s $^3S_1$   | 1s 6s $^3S_1$   | 1.3696E+00    | 9.015E-08 | 1.069E+08        | 1.3638E+00    | 9.066E-08 | 1.074E+08        |
| 1s 2s $^1S_0$   | 1s 6s $^3S_1$   | 1.3825E+00    | 4.807E-08 | 5.592E+07        | 1.3769E+00    | 4.572E-08 | 5.317E+07        |
| 1s 3s $^3S_1$   | 1s 6s $^3S_1$   | 3.6936E+00    | 1.931E-08 | 3.147E+06        | 3.6786E+00    | 1.938E-08 | 3.157E+06        |
| 1s 3s $^1S_0$   | 1s 6s $^3S_1$   | 3.7185E+00    | 1.086E-08 | 1.747E+06        | 3.7036E+00    | 9.751E-09 | 1.567E+06        |
| 1s 3d $^3D_2$   | 1s 6s $^3S_1$   | 3.8604E+00    | 5.613E-13 | 8.374E+01        |               |           |                  |
| 1s 3d $^3D_1$   | 1s 6s $^3S_1$   | 3.8622E+00    | 8.232E-12 | 1.227E+03        |               |           |                  |
| 1s 3d $^1D_2$   | 1s 6s $^3S_1$   | 3.9062E+00    | 1.282E-12 | 1.868E+02        |               |           |                  |
| 1s 4s $^3S_1$   | 1s 6s $^3S_1$   | 8.9291E+00    | 6.023E-09 | 1.680E+05        | 8.8936E+00    | 6.051E-09 | 1.686E+05        |
| 1s 4s $^1S_0$   | 1s 6s $^3S_1$   | 8.9879E+00    | 3.778E-09 | 1.040E+05        | 8.9527E+00    | 3.044E-09 | 8.374E+04        |
| 1s 4d $^3D_2$   | 1s 6s $^3S_1$   | 9.3373E+00    | 1.297E-12 | 3.306E+01        | 9.3006E+00    | 4.837E-12 | 1.232E+02        |
| 1s 4d $^3D_1$   | 1s 6s $^3S_1$   | 9.3415E+00    | 1.313E-11 | 3.344E+02        | 9.3048E+00    | 1.214E-12 | 3.092E+01        |
| 1s 4d $^1D_2$   | 1s 6s $^3S_1$   | 9.4508E+00    | 1.784E-12 | 4.442E+01        |               |           |                  |
| 1s 5s $^3S_1$   | 1s 6s $^3S_1$   | 2.5485E+01    | 2.125E-09 | 7.273E+03        | 2.5393E+01    | 2.131E-09 | 7.285E+03        |
| 1s 5s $^1S_0$   | 1s 6s $^3S_1$   | 2.5726E+01    | 1.670E-09 | 5.611E+03        | 2.5635E+01    | 1.075E-09 | 3.606E+03        |
| 1s 5d $^3D_2$   | 1s 6s $^3S_1$   | 2.7214E+01    | 7.250E-13 | 2.176E+00        | 2.7122E+01    | 5.172E-12 | 1.550E+01        |
| 1s 5d $^3D_1$   | 1s 6s $^3S_1$   | 2.7232E+01    | 2.052E-11 | 6.152E+01        | 2.7140E+01    | 1.190E-12 | 3.562E+00        |
| 1s 5d $^1D_2$   | 1s 6s $^3S_1$   | 2.7711E+01    | 3.013E-12 | 8.724E+00        |               |           |                  |
| 1s 2p $^3P_0^0$ | 1s 6p $^3P_0^0$ | 1.3810E+00    | 2.067E-08 | 2.410E+07        | 1.3752E+00    | 2.129E-08 | 2.482E+07        |
| 1s 2p $^3P_1^0$ | 1s 6p $^3P_0^0$ | 1.3819E+00    | 8.740E-09 | 1.018E+07        | 1.3761E+00    | 1.295E-08 | 1.508E+07        |
| 1s 2p $^3P_2^0$ | 1s 6p $^3P_0^0$ | 1.4434E+00    | 4.128E-07 | 4.405E+08        | 1.4374E+00    | 4.168E-07 | 4.448E+08        |
| 1s 2p $^1P_1^0$ | 1s 6p $^3P_1^0$ | 1.4493E+00    | 9.654E-08 | 1.022E+08        | 1.4433E+00    | 9.341E-08 | 9.885E+07        |
| 1s 3p $^3P_0^0$ | 1s 6p $^3P_0^0$ | 3.7142E+00    | 6.133E-09 | 9.884E+05        | 3.6989E+00    | 5.685E-09 | 9.160E+05        |
| 1s 3p $^3P_1^0$ | 1s 6p $^3P_0^0$ | 3.7159E+00    | 2.025E-09 | 3.261E+05        | 3.7005E+00    | 4.431E-09 | 7.134E+05        |
| 1s 3p $^3P_2^0$ | 1s 6p $^3P_0^0$ | 3.8474E+00    | 3.258E-07 | 4.893E+07        | 3.8314E+00    | 3.312E-07 | 4.974E+07        |
| 1s 3p $^1P_1^0$ | 1s 6p $^3P_1^0$ | 3.8593E+00    | 7.372E-08 | 1.101E+07        | 3.8434E+00    | 7.108E-08 | 1.060E+07        |
| 1s 4p $^3P_0^0$ | 1s 6p $^3P_0^0$ | 8.9685E+00    | 2.399E-09 | 6.631E+04        | 8.9310E+00    | 1.888E-09 | 5.218E+04        |
| 1s 4p $^3P_1^0$ | 1s 6p $^3P_0^0$ | 8.9726E+00    | 4.830E-10 | 1.334E+04        | 8.9350E+00    | 2.091E-09 | 5.775E+04        |
| 1s 4p $^3P_2^0$ | 1s 6p $^3P_0^0$ | 9.2954E+00    | 3.183E-07 | 8.190E+06        | 9.2564E+00    | 3.253E-07 | 8.369E+06        |
| 1s 4p $^1P_1^0$ | 1s 6p $^3P_1^0$ | 9.3241E+00    | 7.090E-08 | 1.813E+06        | 9.2853E+00    | 6.788E-08 | 1.735E+06        |
| 1s 4f $^3F_2^0$ | 1s 6p $^3P_0^0$ | 9.4324E+00    | 7.883E-14 | 1.970E+00        |               |           |                  |
| 1s 5p $^3P_0^0$ | 1s 6p $^3P_0^0$ | 2.5582E+01    | 1.080E-09 | 3.667E+03        | 2.5476E+01    | 6.650E-10 | 2.258E+03        |
| 1s 5p $^3P_1^0$ | 1s 6p $^3P_0^0$ | 2.5599E+01    | 6.529E-11 | 2.215E+02        | 2.5492E+01    | 1.370E-09 | 4.650E+03        |
| 1s 5p $^3P_2^0$ | 1s 6p $^3P_0^0$ | 2.6962E+01    | 4.537E-07 | 1.388E+06        | 2.6849E+01    | 4.659E-07 | 1.424E+06        |
| 1s 5p $^1P_1^0$ | 1s 6p $^3P_0^0$ | 2.7084E+01    | 1.005E-07 | 3.045E+05        | 2.6972E+01    | 9.510E-08 | 2.881E+05        |
| 1s 5f $^3F_2^0$ | 1s 6p $^3P_1^0$ | 2.7556E+01    | 2.189E-13 | 6.408E-01        |               |           |                  |
| 1s 2s $^3S_1$   | 1s 6s $^1S_0$   | 1.3692E+00    | 4.431E-08 | 1.577E+08        | 1.3635E+00    | 4.532E-08 | 1.612E+08        |

(continued on next page)

Table 5 (continued)

| Lower                             | Upper                             | GRASP2K       |           |                  | FAC           |           |                  |
|-----------------------------------|-----------------------------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                                   |                                   | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 3s <sup>3</sup> S <sub>1</sub> | 1s 6s <sup>1</sup> S <sub>0</sub> | 3.6908E+00    | 8.788E-09 | 4.303E+06        | 3.6761E+00    | 9.684E-09 | 4.739E+06        |
| 1s 3d <sup>3</sup> D <sub>1</sub> | 1s 6s <sup>1</sup> S <sub>0</sub> | 3.8591E+00    | 9.086E-13 | 4.070E+02        |               |           |                  |
| 1s 4s <sup>3</sup> S <sub>1</sub> | 1s 6s <sup>1</sup> S <sub>0</sub> | 8.9125E+00    | 2.416E-09 | 2.029E+05        | 8.8795E+00    | 3.021E-09 | 2.534E+05        |
| 1s 4d <sup>3</sup> D <sub>1</sub> | 1s 6s <sup>1</sup> S <sub>0</sub> | 9.3233E+00    | 1.668E-12 | 1.280E+02        | 9.2893E+00    | 1.732E-12 | 1.327E+02        |
| 1s 5s <sup>3</sup> S <sub>1</sub> | 1s 6s <sup>1</sup> S <sub>0</sub> | 2.5350E+01    | 6.194E-10 | 6.429E+03        | 2.5278E+01    | 1.061E-09 | 1.098E+04        |
| 1s 5d <sup>3</sup> D <sub>1</sub> | 1s 6s <sup>1</sup> S <sub>0</sub> | 2.7078E+01    | 1.807E-12 | 1.644E+01        | 2.7009E+01    | 1.992E-12 | 1.806E+01        |
| 1s 6s <sup>3</sup> S <sub>1</sub> | 1s 6s <sup>1</sup> S <sub>0</sub> | 4.7691E+03    | 7.013E-09 | 2.057E+00        | 5.5745E+03    | 5.830E-09 | 1.240E+00        |
| 1s 2p <sup>3</sup> P <sub>0</sub> | 1s 6p <sup>3</sup> P <sub>0</sub> | 1.3809E+00    | 1.094E-08 | 3.828E+07        | 1.3753E+00    | 7.037E-09 | 2.460E+07        |
| 1s 2p <sup>1</sup> P <sub>0</sub> | 1s 6p <sup>3</sup> P <sub>0</sub> | 1.4493E+00    | 1.695E-07 | 5.381E+08        | 1.4434E+00    | 1.740E-07 | 5.525E+08        |
| 1s 3p <sup>3</sup> P <sub>0</sub> | 1s 6p <sup>3</sup> P <sub>0</sub> | 3.7140E+00    | 3.120E-09 | 1.509E+06        | 3.6994E+00    | 1.511E-09 | 7.306E+05        |
| 1s 3p <sup>1</sup> P <sub>0</sub> | 1s 6p <sup>3</sup> P <sub>0</sub> | 3.8591E+00    | 1.323E-07 | 5.925E+07        | 3.8440E+00    | 1.357E-07 | 6.077E+07        |
| 1s 4p <sup>3</sup> P <sub>0</sub> | 1s 6p <sup>3</sup> P <sub>0</sub> | 8.9674E+00    | 1.092E-09 | 9.058E+04        | 8.9341E+00    | 3.075E-10 | 2.548E+04        |
| 1s 4p <sup>1</sup> P <sub>0</sub> | 1s 6p <sup>3</sup> P <sub>0</sub> | 9.3228E+00    | 1.285E-07 | 9.865E+06        | 9.2885E+00    | 1.318E-07 | 1.010E+07        |
| 1s 5p <sup>3</sup> P <sub>0</sub> | 1s 6p <sup>3</sup> P <sub>0</sub> | 2.5573E+01    | 4.594E-10 | 4.685E+03        |               |           |                  |
| 1s 5p <sup>1</sup> P <sub>0</sub> | 1s 6p <sup>3</sup> P <sub>0</sub> | 2.7074E+01    | 1.828E-07 | 1.663E+06        | 2.7000E+01    | 1.870E-07 | 1.697E+06        |
| 1s 6p <sup>3</sup> P <sub>0</sub> | 1s 6p <sup>3</sup> P <sub>0</sub> | 6.9398E+04    | 6.942E-08 | 9.614E-02        |               |           |                  |
| 1s 2p <sup>3</sup> P <sub>1</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 1.3788E+00    | 1.951E-07 | 1.369E+08        | 1.3731E+00    | 2.017E-07 | 1.415E+08        |
| 1s 2p <sup>3</sup> P <sub>2</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 1.4410E+00    | 2.930E-07 | 1.883E+08        | 1.4350E+00    | 2.925E-07 | 1.878E+08        |
| 1s 2p <sup>1</sup> P <sub>1</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 1.4469E+00    | 2.548E-08 | 1.624E+07        | 1.4409E+00    | 2.662E-08 | 1.696E+07        |
| 1s 3p <sup>3</sup> P <sub>1</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 3.6983E+00    | 2.115E-07 | 2.063E+07        | 3.6831E+00    | 2.178E-07 | 2.123E+07        |
| 1s 3p <sup>3</sup> P <sub>2</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 3.8304E+00    | 8.438E-08 | 7.672E+06        | 3.8145E+00    | 8.336E-08 | 7.578E+06        |
| 1s 3p <sup>1</sup> P <sub>1</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 3.8422E+00    | 5.285E-09 | 4.776E+05        | 3.8264E+00    | 6.273E-09 | 5.667E+05        |
| 1s 4p <sup>3</sup> P <sub>1</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 8.8767E+00    | 2.421E-07 | 4.098E+06        | 8.8397E+00    | 2.488E-07 | 4.212E+06        |
| 1s 4p <sup>3</sup> P <sub>2</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 9.1968E+00    | 3.073E-08 | 4.846E+05        | 9.1583E+00    | 2.935E-08 | 4.630E+05        |
| 1s 4p <sup>1</sup> P <sub>1</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 9.2248E+00    | 8.915E-10 | 1.398E+04        | 9.1865E+00    | 1.536E-09 | 2.408E+04        |
| 1s 4f <sup>3</sup> F <sub>3</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 9.3286E+00    | 6.451E-14 | 9.889E-01        |               |           |                  |
| 1s 4f <sup>3</sup> F <sub>2</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 9.3309E+00    | 3.163E-14 | 4.846E-01        |               |           |                  |
| 1s 4f <sup>1</sup> F <sub>3</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 9.3838E+00    | 1.153E-14 | 1.747E-01        |               |           |                  |
| 1s 5p <sup>3</sup> P <sub>0</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 2.4849E+01    | 3.725E-07 | 8.048E+05        | 2.4746E+01    | 3.819E-07 | 8.251E+05        |
| 1s 5p <sup>3</sup> P <sub>1</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 2.6148E+01    | 1.229E-08 | 2.397E+04        | 2.6040E+01    | 1.110E-08 | 2.166E+04        |
| 1s 5p <sup>1</sup> P <sub>0</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 2.6264E+01    | 4.017E-13 | 7.770E-01        | 2.6156E+01    | 1.763E-10 | 3.409E+02        |
| 1s 5f <sup>3</sup> F <sub>3</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 2.6698E+01    | 1.051E-12 | 1.966E+00        |               |           |                  |
| 1s 5f <sup>3</sup> F <sub>2</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 2.6707E+01    | 3.579E-13 | 6.695E-01        |               |           |                  |
| 1s 5f <sup>1</sup> F <sub>3</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 2.6930E+01    | 4.012E-14 | 7.380E-02        |               |           |                  |
| 1s 6p <sup>3</sup> P <sub>0</sub> | 1s 6p <sup>3</sup> P <sub>2</sub> | 8.6654E+02    | 8.046E-06 | 1.429E+04        | 8.6410E+02    | 8.128E-06 | 1.440E+04        |
| 1s 2s <sup>3</sup> S <sub>1</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 1.3669E+00    | 6.514E-09 | 4.651E+06        | 1.3610E+00    | 6.766E-09 | 4.831E+06        |
| 1s 3s <sup>3</sup> S <sub>1</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 3.6741E+00    | 1.083E-09 | 1.070E+05        | 3.6587E+00    | 1.183E-09 | 1.169E+05        |
| 1s 3d <sup>3</sup> D <sub>2</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 3.8391E+00    | 2.622E-08 | 2.373E+06        | 3.8228E+00    | 2.617E-08 | 2.369E+06        |
| 1s 3d <sup>3</sup> D <sub>1</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 3.8409E+00    | 2.274E-09 | 2.057E+05        | 3.8245E+00    | 3.045E-09 | 2.753E+05        |
| 1s 3d <sup>3</sup> D <sub>3</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 3.8827E+00    | 5.188E-08 | 4.591E+06        | 3.8661E+00    | 5.171E-08 | 4.576E+06        |
| 1s 3d <sup>1</sup> D <sub>2</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 3.8844E+00    | 4.104E-09 | 3.629E+05        | 3.8678E+00    | 4.089E-09 | 3.615E+05        |
| 1s 4s <sup>3</sup> S <sub>1</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 8.8160E+00    | 1.556E-10 | 2.671E+03        | 8.7783E+00    | 1.935E-10 | 3.322E+03        |
| 1s 4d <sup>3</sup> D <sub>2</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 9.2136E+00    | 1.330E-08 | 2.090E+05        | 9.1745E+00    | 1.325E-08 | 2.082E+05        |
| 1s 4d <sup>3</sup> D <sub>1</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 9.2178E+00    | 9.779E-10 | 1.535E+04        | 9.1786E+00    | 1.599E-09 | 2.511E+04        |
| 1s 4d <sup>3</sup> D <sub>3</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 9.3198E+00    | 5.775E-08 | 8.870E+05        | 9.2799E+00    | 5.767E-08 | 8.859E+05        |
| 1s 4d <sup>1</sup> D <sub>2</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 9.3242E+00    | 4.505E-09 | 6.913E+04        | 9.2843E+00    | 4.384E-09 | 6.727E+04        |
| 1s 5s <sup>3</sup> S <sub>1</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 2.4585E+01    | 7.247E-12 | 1.600E+01        | 2.4475E+01    | 1.833E-11 | 4.048E+01        |
| 1s 5d <sup>3</sup> D <sub>2</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 2.6190E+01    | 5.971E-09 | 1.161E+04        | 2.6077E+01    | 5.919E-09 | 1.151E+04        |
| 1s 5d <sup>3</sup> D <sub>1</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 2.6207E+01    | 2.824E-10 | 5.485E+02        | 2.6094E+01    | 7.777E-10 | 1.510E+03        |
| 1s 5d <sup>3</sup> D <sub>3</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 2.6631E+01    | 7.999E-08 | 1.505E+05        | 2.6515E+01    | 8.000E-08 | 1.505E+05        |
| 1s 5d <sup>1</sup> D <sub>2</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 2.6650E+01    | 6.203E-09 | 1.165E+04        | 2.6534E+01    | 5.909E-09 | 1.110E+04        |
| 1s 5g <sup>3</sup> G <sub>3</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 2.6869E+01    | 6.611E-17 | 1.222E-04        |               |           |                  |
| 1s 6s <sup>3</sup> S <sub>1</sub> | 1s 6d <sup>3</sup> D <sub>2</sub> | 6.9582E+02    | 6.652E-11 | 1.833E-01        | 6.7673E+02    | 4.523E-12 | 1.306E-02        |
| 1s 2p <sup>3</sup> P <sub>1</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 1.3786E+00    | 3.538E-08 | 4.139E+07        | 1.3729E+00    | 3.559E-08 | 4.163E+07        |
| 1s 2p <sup>3</sup> P <sub>0</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 1.3795E+00    | 7.258E-08 | 8.481E+07        | 1.3738E+00    | 7.541E-08 | 8.809E+07        |
| 1s 2p <sup>3</sup> P <sub>2</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 1.4408E+00    | 4.726E-08 | 5.062E+07        | 1.4348E+00    | 4.441E-08 | 4.756E+07        |
| 1s 2p <sup>1</sup> P <sub>0</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 1.4467E+00    | 1.592E-07 | 1.691E+08        | 1.4407E+00    | 1.576E-07 | 1.674E+08        |
| 1s 3p <sup>3</sup> P <sub>0</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 3.6970E+00    | 4.301E-08 | 6.997E+06        | 3.6819E+00    | 4.116E-08 | 6.693E+06        |
| 1s 3p <sup>3</sup> P <sub>1</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 3.6987E+00    | 8.169E-08 | 1.328E+07        | 3.6836E+00    | 8.426E-08 | 1.368E+07        |
| 1s 3p <sup>3</sup> P <sub>2</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 3.8290E+00    | 1.541E-08 | 2.336E+06        | 3.8133E+00    | 1.521E-08 | 2.307E+06        |
| 1s 3p <sup>1</sup> P <sub>0</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 3.8407E+00    | 4.522E-08 | 6.817E+06        | 3.8251E+00    | 4.434E-08 | 6.680E+06        |
| 1s 4p <sup>3</sup> P <sub>0</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 8.8691E+00    | 5.110E-08 | 1.444E+06        | 8.8329E+00    | 4.835E-08 | 1.366E+06        |
| 1s 4p <sup>3</sup> P <sub>1</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 8.8731E+00    | 9.506E-08 | 2.685E+06        | 8.8368E+00    | 9.774E-08 | 2.759E+06        |
| 1s 4p <sup>3</sup> P <sub>2</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 9.1886E+00    | 6.437E-09 | 1.695E+05        | 9.1511E+00    | 7.060E-09 | 1.858E+05        |
| 1s 4p <sup>1</sup> P <sub>0</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 9.2166E+00    | 1.567E-08 | 4.102E+05        | 9.1793E+00    | 1.527E-08 | 3.997E+05        |
| 1s 4f <sup>3</sup> F <sub>2</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 9.3225E+00    | 8.951E-14 | 2.290E+00        |               |           |                  |
| 1s 5p <sup>3</sup> P <sub>0</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 2.4789E+01    | 7.996E-08 | 2.893E+05        | 2.4694E+01    | 7.555E-08 | 2.731E+05        |
| 1s 5p <sup>3</sup> P <sub>1</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 2.4805E+01    | 1.475E-07 | 5.332E+05        | 2.4708E+01    | 1.515E-07 | 5.473E+05        |
| 1s 5p <sup>3</sup> P <sub>2</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 2.6083E+01    | 3.633E-09 | 1.187E+04        | 2.5981E+01    | 4.572E-09 | 1.493E+04        |
| 1s 5p <sup>1</sup> P <sub>0</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 2.6197E+01    | 5.654E-09 | 1.832E+04        | 2.6097E+01    | 5.441E-09 | 1.761E+04        |
| 1s 5f <sup>3</sup> F <sub>2</sub> | 1s 6p <sup>1</sup> P <sub>0</sub> | 2.6638E+01    | 9.179E-13 | 2.876E+00        |               |           |                  |

(continued on next page)

Table 5 (continued)

| Lower          | Upper          | GRASP2K       |           |                  | FAC           |           |                  |
|----------------|----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                |                | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s6p $^3P_0^o$ | 1s6p $^1P_1^o$ | 7.9973E+02    | 1.620E-06 | 5.631E+03        | 8.0416E+02    | 1.584E-06 | 5.402E+03        |
| 1s6p $^3P_1^o$ | 1s6p $^1P_1^o$ | 8.0906E+02    | 3.000E-06 | 1.019E+04        | 7.8043E+02    | 3.001E-06 | 1.086E+04        |
| 1s6p $^3P_2^o$ | 1s6p $^1P_1^o$ | 1.0374E+04    | 2.022E-07 | 4.177E+00        | 1.1592E+04    | 1.745E-07 | 2.864E+00        |
| 1s2 $^1S_0$    | 1s6d $^3D_1$   | 3.1620E-01    | 1.772E-08 | 3.939E+08        | 3.1497E-01    | 1.829E-08 | 4.066E+08        |
| 1s2s $^3S_1$   | 1s6d $^3D_1$   | 1.3668E+00    | 1.773E-09 | 2.110E+06        | 1.3611E+00    | 1.353E-09 | 1.610E+06        |
| 1s2s $^1S_0$   | 1s6d $^3D_1$   | 1.3798E+00    | 2.691E-09 | 3.142E+06        | 1.3741E+00    | 2.709E-09 | 3.163E+06        |
| 1s3s $^3S_1$   | 1s6d $^3D_1$   | 3.6740E+00    | 3.764E-10 | 6.199E+04        | 3.6587E+00    | 2.428E-10 | 3.998E+04        |
| 1s3s $^1S_0$   | 1s6d $^3D_1$   | 3.6986E+00    | 4.789E-10 | 7.785E+04        | 3.6835E+00    | 4.807E-10 | 7.811E+04        |
| 1s3d $^3D_2$   | 1s6d $^3D_1$   | 3.8389E+00    | 3.667E-09 | 5.532E+05        | 3.8228E+00    | 2.842E-09 | 4.287E+05        |
| 1s3d $^3D_1$   | 1s6d $^3D_1$   | 3.8407E+00    | 1.459E-08 | 2.199E+06        | 3.8246E+00    | 1.456E-08 | 2.194E+06        |
| 1s3d $^1D_2$   | 1s6d $^3D_1$   | 3.8842E+00    | 3.313E-08 | 4.882E+06        | 3.8678E+00    | 3.359E-08 | 4.950E+06        |
| 1s4s $^3S_1$   | 1s6d $^3D_1$   | 8.8149E+00    | 9.426E-11 | 2.697E+03        | 8.7785E+00    | 4.075E-11 | 1.165E+03        |
| 1s4s $^1S_0$   | 1s6d $^3D_1$   | 8.8722E+00    | 8.005E-11 | 2.261E+03        | 8.8361E+00    | 7.985E-11 | 2.254E+03        |
| 1s4d $^3D_2$   | 1s6d $^3D_1$   | 9.2124E+00    | 2.076E-09 | 5.438E+04        | 9.1748E+00    | 1.393E-09 | 3.648E+04        |
| 1s4d $^3D_1$   | 1s6d $^3D_1$   | 9.2166E+00    | 7.395E-09 | 1.936E+05        | 9.1789E+00    | 7.377E-09 | 1.930E+05        |
| 1s4d $^1D_2$   | 1s6d $^3D_1$   | 9.3230E+00    | 3.684E-08 | 9.425E+05        | 9.2846E+00    | 3.736E-08 | 9.555E+05        |
| 1s5s $^3S_1$   | 1s6d $^3D_1$   | 2.4577E+01    | 3.235E-11 | 1.191E+02        |               |           |                  |
| 1s5s $^1S_0$   | 1s6d $^3D_1$   | 2.4800E+01    | 7.939E-12 | 2.870E+01        | 2.4701E+01    | 8.057E-12 | 2.911E+01        |
| 1s5d $^3D_2$   | 1s6d $^3D_1$   | 2.6180E+01    | 1.194E-09 | 3.875E+03        | 2.6079E+01    | 5.867E-10 | 1.901E+03        |
| 1s5d $^3D_1$   | 1s6d $^3D_1$   | 2.6197E+01    | 3.318E-09 | 1.075E+04        | 2.6096E+01    | 3.305E-09 | 1.069E+04        |
| 1s5d $^1D_2$   | 1s6d $^3D_1$   | 2.6640E+01    | 5.090E-08 | 1.595E+05        | 2.6536E+01    | 5.161E-08 | 1.616E+05        |
| 1s6s $^3S_1$   | 1s6d $^3D_1$   | 6.8911E+02    | 1.701E-10 | 7.963E-01        | 6.7829E+02    | 9.027E-13 | 4.325E-03        |
| 1s6s $^1S_0$   | 1s6d $^3D_1$   | 8.0550E+02    | 2.477E-12 | 8.489E-03        | 7.7225E+02    | 1.588E-12 | 5.871E-03        |
| 1s6d $^3D_2$   | 1s6d $^3D_1$   | 7.1428E+04    | 1.286E-07 | 5.604E-02        |               |           |                  |
| 1s3d $^3D_2$   | 1s6d $^3D_3$   | 3.8337E+00    | 1.524E-08 | 9.880E+05        | 3.8174E+00    | 1.528E-08 | 9.910E+05        |
| 1s3d $^3D_3$   | 1s6d $^3D_3$   | 3.8772E+00    | 1.259E-07 | 7.984E+06        | 3.8607E+00    | 1.258E-07 | 7.977E+06        |
| 1s3d $^1D_2$   | 1s6d $^3D_3$   | 3.8789E+00    | 5.579E-09 | 3.533E+05        | 3.8624E+00    | 6.223E-09 | 3.941E+05        |
| 1s4d $^3D_2$   | 1s6d $^3D_3$   | 9.1827E+00    | 2.734E-08 | 3.090E+05        | 9.1440E+00    | 2.741E-08 | 3.097E+05        |
| 1s4d $^3D_3$   | 1s6d $^3D_3$   | 9.2881E+00    | 6.413E-08 | 7.083E+05        | 9.2486E+00    | 6.411E-08 | 7.081E+05        |
| 1s4d $^1D_2$   | 1s6d $^3D_3$   | 9.2925E+00    | 2.601E-09 | 2.870E+04        | 9.2530E+00    | 3.101E-09 | 3.422E+04        |
| 1s5d $^3D_2$   | 1s6d $^3D_3$   | 2.5941E+01    | 5.300E-08 | 7.505E+04        | 2.5832E+01    | 5.314E-08 | 7.524E+04        |
| 1s5d $^3D_3$   | 1s6d $^3D_3$   | 2.6374E+01    | 2.886E-08 | 3.954E+04        | 2.6261E+01    | 2.878E-08 | 3.944E+04        |
| 1s5d $^1D_2$   | 1s6d $^3D_3$   | 2.6393E+01    | 9.368E-10 | 1.281E+03        | 2.6280E+01    | 1.329E-09 | 1.818E+03        |
| 1s5g $^3G_4$   | 1s6d $^3D_3$   | 2.6602E+01    | 1.073E-13 | 1.445E-01        |               |           |                  |
| 1s5g $^3G_3$   | 1s6d $^3D_3$   | 2.6608E+01    | 3.697E-15 | 4.976E-03        |               |           |                  |
| 1s5g $^1G_4$   | 1s6d $^3D_3$   | 2.6739E+01    | 2.636E-18 | 3.513E-06        |               |           |                  |
| 1s6d $^3D_2$   | 1s6d $^3D_3$   | 2.7340E+03    | 4.169E-06 | 5.314E+02        | 2.7456E+03    | 4.164E-06 | 5.219E+02        |
| 1s2p $^3P_0^o$ | 1s6f $^3F_3^o$ | 1.4401E+00    | 1.195E-08 | 5.491E+06        | 1.4340E+00    | 1.080E-08 | 4.965E+06        |
| 1s3p $^3P_0^o$ | 1s6f $^3F_3^o$ | 3.8237E+00    | 9.083E-10 | 5.920E+04        | 3.8077E+00    | 9.348E-10 | 6.092E+04        |
| 1s4p $^3P_0^o$ | 1s6f $^3F_3^o$ | 9.1585E+00    | 7.725E-10 | 8.776E+03        | 9.1192E+00    | 7.636E-10 | 8.676E+03        |
| 1s4f $^3F_3^o$ | 1s6f $^3F_3^o$ | 9.2892E+00    | 1.742E-09 | 1.924E+04        | 9.2496E+00    | 2.338E-08 | 2.582E+05        |
| 1s4f $^3F_2^o$ | 1s6f $^3F_3^o$ | 9.2914E+00    | 6.431E-08 | 7.099E+05        | 9.2518E+00    | 1.172E-09 | 1.294E+04        |
| 1s4f $^3F_4^o$ | 1s6f $^3F_3^o$ | 9.3423E+00    | 1.585E-08 | 1.731E+05        | 9.3023E+00    | 1.577E-08 | 1.722E+05        |
| 1s4f $^1F_3^o$ | 1s6f $^3F_3^o$ | 9.3440E+00    | 5.753E-10 | 6.279E+03        | 9.3039E+00    | 6.071E-10 | 6.627E+03        |
| 1s5p $^3P_2^o$ | 1s6f $^3F_3^o$ | 2.5841E+01    | 2.188E-10 | 3.122E+02        | 2.5726E+01    | 2.180E-10 | 3.112E+02        |
| 1s5f $^3F_3^o$ | 1s6f $^3F_3^o$ | 2.6377E+01    | 2.923E-09 | 4.004E+03        | 2.6263E+01    | 1.627E-08 | 2.228E+04        |
| 1s5f $^3F_2^o$ | 1s6f $^3F_3^o$ | 2.6386E+01    | 5.326E-08 | 7.290E+04        | 2.6272E+01    | 6.180E-10 | 1.119E+03        |
| 1s5f $^3F_4^o$ | 1s6f $^3F_3^o$ | 2.6597E+01    | 2.772E-08 | 3.733E+04        | 2.6482E+01    | 2.755E-08 | 3.712E+04        |
| 1s5f $^1F_3^o$ | 1s6f $^3F_3^o$ | 2.6604E+01    | 1.038E-09 | 1.397E+03        | 2.6488E+01    | 1.044E-09 | 1.406E+03        |
| 1s6p $^3P_2^o$ | 1s6f $^3F_3^o$ | 2.1987E+03    | 5.085E-12 | 1.002E-03        | 2.1353E+03    | 1.018E-12 | 2.110E-04        |
| 1s2p $^3P_0^o$ | 1s6f $^3F_2^o$ | 1.3779E+00    | 1.521E-11 | 1.069E+04        | 1.3722E+00    | 8.594E-12 | 6.038E+03        |
| 1s2p $^3P_2^o$ | 1s6f $^3F_2^o$ | 1.4401E+00    | 7.687E-10 | 4.945E+05        | 1.4340E+00    | 7.719E-10 | 4.965E+05        |
| 1s2p $^1P_0^o$ | 1s6f $^3F_2^o$ | 1.4459E+00    | 7.214E-09 | 4.603E+06        | 1.4400E+00    | 7.095E-09 | 4.526E+06        |
| 1s3p $^3P_0^o$ | 1s6f $^3F_2^o$ | 3.6920E+00    | 2.140E-12 | 2.094E+02        | 3.6768E+00    | 9.298E-13 | 9.098E+01        |
| 1s3p $^3P_2^o$ | 1s6f $^3F_2^o$ | 3.8236E+00    | 8.615E-11 | 7.861E+03        | 3.8077E+00    | 6.677E-11 | 6.092E+03        |
| 1s3p $^1P_0^o$ | 1s6f $^3F_2^o$ | 3.8353E+00    | 6.057E-10 | 5.493E+04        | 3.8195E+00    | 5.957E-10 | 5.401E+04        |
| 1s4p $^3P_0^o$ | 1s6f $^3F_2^o$ | 8.8404E+00    | 1.764E-12 | 3.011E+01        |               |           |                  |
| 1s4p $^3P_2^o$ | 1s6f $^3F_2^o$ | 9.1578E+00    | 7.183E-11 | 1.143E+03        | 9.1192E+00    | 5.527E-11 | 8.792E+02        |
| 1s4p $^1P_0^o$ | 1s6f $^3F_2^o$ | 9.1856E+00    | 5.112E-10 | 8.083E+03        | 9.1472E+00    | 4.920E-10 | 7.779E+03        |
| 1s4f $^3F_3^o$ | 1s6f $^3F_2^o$ | 9.2886E+00    | 6.731E-08 | 1.041E+06        | 9.2496E+00    | 1.186E-09 | 1.833E+04        |
| 1s4f $^3F_2^o$ | 1s6f $^3F_2^o$ | 9.2908E+00    | 6.173E-08 | 9.540E+05        | 9.2518E+00    | 1.637E-08 | 2.530E+05        |
| 1s4f $^1F_3^o$ | 1s6f $^3F_2^o$ | 9.3433E+00    | 1.148E-08 | 1.754E+05        | 9.3039E+00    | 1.167E-08 | 1.783E+05        |
| 1s5p $^3P_0^o$ | 1s6f $^3F_2^o$ | 2.4566E+01    | 8.810E-13 | 1.948E+00        |               |           |                  |
| 1s5p $^3P_2^o$ | 1s6f $^3F_2^o$ | 2.5836E+01    | 2.337E-11 | 4.672E+01        | 2.5726E+01    | 1.599E-11 | 3.195E+01        |
| 1s5p $^1P_0^o$ | 1s6f $^3F_2^o$ | 2.5948E+01    | 1.502E-10 | 2.975E+02        | 2.5839E+01    | 1.421E-10 | 2.815E+02        |
| 1s5f $^3F_3^o$ | 1s6f $^3F_2^o$ | 2.6372E+01    | 5.803E-08 | 1.113E+05        | 2.6263E+01    | 8.311E-10 | 1.593E+03        |
| 1s5f $^3F_2^o$ | 1s6f $^3F_2^o$ | 2.6381E+01    | 4.801E-08 | 9.203E+04        | 2.6272E+01    | 1.140E-08 | 2.184E+04        |
| 1s5f $^1F_3^o$ | 1s6f $^3F_2^o$ | 2.6599E+01    | 2.011E-08 | 3.793E+04        | 2.6489E+01    | 2.040E-08 | 3.845E+04        |
| 1s6p $^3P_0^o$ | 1s6f $^3F_2^o$ | 6.1864E+02    | 2.732E-12 | 9.524E-03        | 6.1520E+02    | 4.924E-15 | 1.721E-05        |
| 1s6p $^3P_2^o$ | 1s6f $^3F_2^o$ | 2.1625E+03    | 7.609E-12 | 2.171E-03        | 2.1357E+03    | 7.272E-14 | 2.109E-05        |
| 1s6p $^1P_0^o$ | 1s6f $^3F_2^o$ | 2.7321E+03    | 7.961E-14 | 1.423E-05        | 2.6181E+03    | 5.329E-13 | 1.028E-04        |

(continued on next page)

Table 5 (continued)

| Lower  | Upper  | GRASP2K       |           |                             | FAC           |           |                             |
|--|--|---------------|-----------|-----------------------------|---------------|-----------|-----------------------------|
|  |  | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3144E+05    | 9.863E-08 | 7.617E-03                   |               |           |                             |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 1.3661E+00    | 5.469E-12 | 3.909E+03                   | 1.3604E+00    | 9.449E-13 | 6.754E+02                   |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 3.6690E+00    | 3.296E-12 | 3.266E+02                   |               |           |                             |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 3.8335E+00    | 1.210E-09 | 1.098E+05                   | 3.8174E+00    | 1.142E-09 | 1.037E+05                   |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 3.8353E+00    | 9.479E-09 | 8.597E+05                   | 3.8191E+00    | 9.644E-09 | 8.746E+05                   |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 3.8770E+00    | 7.265E-09 | 6.447E+05                   | 3.8606E+00    | 6.726E-09 | 5.969E+05                   |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 3.8787E+00    | 8.796E-08 | 7.800E+06                   | 3.8623E+00    | 8.773E-08 | 7.779E+06                   |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 8.7865E+00    | 2.542E-12 | 4.392E+01                   |               |           |                             |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 9.1814E+00    | 2.104E-09 | 3.330E+04                   | 9.1435E+00    | 1.965E-09 | 3.109E+04                   |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 9.1855E+00    | 1.712E-08 | 2.707E+05                   | 9.1476E+00    | 1.742E-08 | 2.753E+05                   |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 9.2868E+00    | 3.981E-09 | 6.158E+04                   | 9.2482E+00    | 3.535E-09 | 5.468E+04                   |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 9.2911E+00    | 4.489E-08 | 6.938E+05                   | 9.2526E+00    | 4.466E-08 | 6.900E+05                   |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 2.4357E+01    | 3.021E-12 | 6.793E+00                   |               |           |                             |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 2.5931E+01    | 4.067E-09 | 8.068E+03                   | 2.5828E+01    | 3.787E-09 | 7.509E+03                   |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 2.5947E+01    | 3.338E-08 | 6.614E+04                   | 2.5844E+01    | 3.395E-08 | 6.723E+04                   |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 2.6363E+01    | 2.106E-09 | 4.043E+03                   | 2.6257E+01    | 1.705E-09 | 3.271E+03                   |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 2.6382E+01    | 2.022E-08 | 3.875E+04                   | 2.6276E+01    | 2.001E-08 | 3.834E+04                   |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 2.6597E+01    | 7.626E-14 | 1.438E-01                   |               |           |                             |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 5.4990E+02    | 3.558E-11 | 1.570E-01                   |               |           |                             |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 2.6222E+03    | 3.081E-07 | 5.978E+01                   | 2.7042E+03    | 2.977E-07 | 5.385E+01                   |
| 1s 6d <sup>3</sup> D <sub>1</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 2.7221E+03    | 2.629E-06 | 4.733E+02                   | 2.6795E+03    | 2.626E-06 | 4.838E+02                   |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 6d <sup>1</sup> D <sub>2</sub>              | 6.4120E+04    | 8.705E-08 | 2.825E-02                   |               |           |                             |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 9.2736E+00    | 3.992E-09 | 3.440E+04                   | 9.2341E+00    | 3.977E-09 | 3.427E+04                   |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 9.3265E+00    | 6.690E-08 | 5.701E+05                   | 9.2866E+00    | 7.168E-08 | 6.107E+05                   |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 9.3281E+00    | 2.991E-09 | 2.548E+04                   | 9.2883E+00    | 2.060E-09 | 1.755E+04                   |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.6252E+01    | 1.288E-08 | 1.385E+04                   | 2.6139E+01    | 1.283E-08 | 1.380E+04                   |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 2.6469E+01    | 4.726E-08 | 4.999E+04                   | 2.6355E+01    | 4.994E-08 | 5.283E+04                   |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 2.6476E+01    | 1.811E-09 | 1.915E+03                   | 2.6362E+01    | 1.444E-09 | 1.527E+03                   |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 5.5078E+03    | 2.817E-06 | 6.883E+01                   | 5.5226E+03    | 2.808E-06 | 6.766E+01                   |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 6g <sup>3</sup> G <sub>4</sub>              | 3.8744E+00    | 5.198E-09 | 2.567E+05                   | 3.8580E+00    | 5.256E-09 | 2.595E+05                   |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 6g <sup>3</sup> G <sub>4</sub>              | 9.2719E+00    | 2.896E-10 | 2.497E+03                   | 9.2332E+00    | 2.894E-10 | 2.494E+03                   |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 6g <sup>3</sup> G <sub>4</sub>              | 2.6244E+01    | 5.638E-10 | 6.067E+02                   | 2.6137E+01    | 5.631E-10 | 6.057E+02                   |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 6g <sup>3</sup> G <sub>4</sub>              | 2.6470E+01    | 2.319E-08 | 2.453E+04                   | 2.6356E+01    | 2.313E-08 | 2.447E+04                   |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 6g <sup>3</sup> G <sub>4</sub>              | 2.6475E+01    | 5.258E-10 | 5.560E+02                   | 2.6361E+01    | 6.612E-10 | 6.992E+02                   |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 6g <sup>3</sup> G <sub>4</sub>              | 2.6601E+01    | 1.013E-08 | 1.061E+04                   | 2.6487E+01    | 1.007E-08 | 1.054E+04                   |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 6g <sup>3</sup> G <sub>4</sub>              | 2.6605E+01    | 2.379E-10 | 2.491E+02                   | 2.6491E+01    | 2.376E-10 | 2.489E+02                   |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 6g <sup>3</sup> G <sub>4</sub>              | 5.3075E+03    | 2.734E-13 | 7.194E-06                   | 5.5194E+03    | 2.107E-13 | 5.082E-06                   |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 3.8309E+00    | 3.305E-13 | 2.146E+01                   |               |           |                             |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 3.8743E+00    | 2.294E-10 | 1.456E+04                   | 3.8580E+00    | 1.946E-10 | 1.235E+04                   |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 3.8760E+00    | 3.937E-09 | 2.497E+05                   | 3.8597E+00    | 3.902E-09 | 2.474E+05                   |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 9.1665E+00    | 1.291E-14 | 1.464E-01                   |               |           |                             |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 9.2715E+00    | 1.119E-11 | 1.241E+02                   | 9.2332E+00    | 1.071E-11 | 1.187E+02                   |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 9.2759E+00    | 2.148E-10 | 2.379E+03                   | 9.2375E+00    | 2.140E-10 | 2.370E+03                   |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.5812E+01    | 5.221E-14 | 7.467E-02                   |               |           |                             |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.6241E+01    | 2.382E-11 | 3.297E+01                   | 2.6137E+01    | 2.088E-11 | 2.888E+01                   |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.6259E+01    | 4.243E-10 | 5.863E+02                   | 2.6155E+01    | 4.177E-10 | 5.769E+02                   |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.6467E+01    | 8.195E-10 | 1.115E+03                   | 2.6356E+01    | 6.700E-10 | 9.112E+02                   |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.6472E+01    | 1.789E-08 | 2.432E+04                   | 2.6361E+01    | 1.785E-08 | 2.427E+04                   |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.6602E+01    | 7.974E-09 | 1.074E+04                   | 2.6491E+01    | 8.002E-09 | 1.077E+04                   |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 1.7904E+03    | 5.103E-15 | 1.517E-06                   | 1.8335E+03    | 6.550E-17 | 1.841E-08                   |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 5.1873E+03    | 1.899E-15 | 6.726E-08                   | 5.5194E+03    | 7.803E-15 | 2.420E-07                   |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 5.6439E+03    | 1.309E-13 | 3.915E-06                   | 5.6946E+03    | 1.512E-13 | 4.406E-06                   |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 6g <sup>3</sup> G <sub>3</sub>              | 2.2908E+05    | 6.999E-08 | 1.271E-03                   |               |           |                             |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4397E+00    | 7.159E-13 | 3.291E+02                   | 1.4336E+00    | 3.610E-15 | 1.659E+00                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.8210E+00    | 4.243E-14 | 2.769E+00                   | 3.8051E+00    | 3.132E-16 | 2.044E-02                   |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 9.1428E+00    | 9.110E-14 | 1.038E+00                   |               |           |                             |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 9.2731E+00    | 1.854E-10 | 2.055E+03                   | 9.2341E+00    | 1.626E-10 | 1.802E+03                   |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 9.2753E+00    | 2.969E-09 | 3.289E+04                   | 9.2363E+00    | 2.951E-09 | 3.269E+04                   |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 9.3260E+00    | 3.495E-09 | 3.829E+04                   | 9.2866E+00    | 2.054E-09 | 2.250E+04                   |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 9.3276E+00    | 5.878E-08 | 6.437E+05                   | 9.2883E+00    | 5.528E-08 | 6.054E+05                   |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.5717E+01    | 9.470E-14 | 1.365E-01                   |               |           |                             |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.6248E+01    | 5.478E-10 | 7.577E+02                   | 2.6139E+01    | 4.968E-10 | 6.870E+02                   |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.6257E+01    | 9.502E-09 | 1.313E+04                   | 2.6148E+01    | 9.514E-09 | 1.314E+04                   |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.6465E+01    | 2.429E-09 | 3.305E+03                   | 2.6355E+01    | 1.434E-09 | 1.950E+03                   |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.6472E+01    | 4.062E-08 | 5.523E+04                   | 2.6362E+01    | 3.850E-08 | 5.234E+04                   |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.5574E+03    | 1.960E-12 | 6.799E-04                   |               |           |                             |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.3394E+03    | 1.078E-07 | 3.603E+00                   | 5.5188E+03    | 1.040E-07 | 3.227E+00                   |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.5655E+03    | 2.080E-06 | 6.399E+01                   | 5.5161E+03    | 2.078E-06 | 6.453E+01                   |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.7466E+05    | 5.173E-08 | 1.616E-03                   |               |           |                             |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 6g <sup>3</sup> G <sub>5</sub>              | 2.6394E+01    | 3.048E-09 | 2.653E+03                   | 2.6281E+01    | 3.041E-09 | 2.647E+03                   |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 6g <sup>3</sup> G <sub>5</sub>              | 2.6525E+01    | 5.550E-08 | 4.783E+04                   | 2.6411E+01    | 5.531E-08 | 4.767E+04                   |

(continued on next page)



Table 5 (continued)

| Lower                   | Upper           | GRASP2K       |           |                  | FAC           |           |                  |
|-------------------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                         |                 | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 5g $^1G_4$           | 1s 6g $^3G_5$   | 2.6529E+01    | 9.023E-10 | 7.774E+02        | 2.6415E+01    | 1.031E-09 | 8.883E+02        |
| 1s 6g $^3G_4$           | 1s 6g $^3G_5$   | 9.2456E+03    | 2.127E-06 | 1.509E+01        | 9.2559E+03    | 2.122E-06 | 1.489E+01        |
| 1s 4f $^3F_4^o$         | 1s 6h $^3H_5^o$ | 9.3170E+00    | 2.422E-09 | 1.692E+04        | 9.2773E+00    | 2.373E-09 | 1.658E+04        |
| 1s 5f $^3F_4^o$         | 1s 6h $^3H_5^o$ | 2.6394E+01    | 7.696E-10 | 6.699E+02        | 2.6281E+01    | 7.530E-10 | 6.555E+02        |
| 1s 6f $^3F_4^o$         | 1s 6h $^3H_5^o$ | 9.2055E+03    | 4.621E-14 | 3.307E-07        | 9.2780E+03    | 4.284E-14 | 2.992E-07        |
| 1s 4f $^3F_3^o$         | 1s 6h $^3H_4^o$ | 9.2640E+00    | 8.889E-15 | 7.676E-02        |               |           |                  |
| 1s 4f $^3F_4^o$         | 1s 6h $^3H_4^o$ | 9.3168E+00    | 6.293E-11 | 5.373E+02        | 9.2773E+00    | 5.395E-11 | 4.606E+02        |
| 1s 4f $^1F_3^o$         | 1s 6h $^3H_4^o$ | 9.3184E+00    | 1.950E-09 | 1.664E+04        | 9.2790E+00    | 1.890E-09 | 1.613E+04        |
| 1s 5f $^3F_3^o$         | 1s 6h $^3H_4^o$ | 2.6175E+01    | 1.242E-15 | 1.343E-03        |               |           |                  |
| 1s 5f $^3F_4^o$         | 1s 6h $^3H_4^o$ | 2.6392E+01    | 2.026E-11 | 2.156E+01        | 2.6281E+01    | 1.711E-11 | 1.820E+01        |
| 1s 5f $^1F_3^o$         | 1s 6h $^3H_4^o$ | 2.6398E+01    | 6.215E-10 | 6.610E+02        | 2.6287E+01    | 5.992E-10 | 6.372E+02        |
| 1s 6f $^3F_3^o$         | 1s 6h $^3H_4^o$ | 3.4128E+03    | 1.701E-18 | 1.082E-10        |               |           |                  |
| 1s 6f $^3F_4^o$         | 1s 6h $^3H_4^o$ | 8.9725E+03    | 8.514E-16 | 7.838E-09        | 9.2780E+03    | 9.738E-16 | 8.313E-09        |
| 1s 6f $^1F_3^o$         | 1s 6h $^3H_4^o$ | 9.4584E+03    | 3.479E-14 | 2.882E-07        | 9.2889E+03    | 3.404E-14 | 2.899E-07        |
| 1s 6h $^3H_5^o$         | 1s 6h $^3H_4^o$ | 3.5443E+05    | 5.462E-08 | 3.222E-04        |               |           |                  |
| 1s 3d $^3D_3$           | 1s 6g $^1G_4$   | 3.8727E+00    | 9.494E-14 | 4.692E+00        |               |           |                  |
| 1s 4d $^3D_3$           | 1s 6g $^1G_4$   | 9.2623E+00    | 1.894E-17 | 1.636E-04        |               |           |                  |
| 1s 5d $^3D_3$           | 1s 6g $^1G_4$   | 2.6167E+01    | 4.856E-15 | 5.256E-03        |               |           |                  |
| 1s 5g $^3G_4$           | 1s 6g $^1G_4$   | 2.6392E+01    | 7.790E-11 | 8.290E+01        | 2.6281E+01    | 7.613E-11 | 8.100E+01        |
| 1s 5g $^3G_3$           | 1s 6g $^1G_4$   | 2.6397E+01    | 2.401E-09 | 2.553E+03        | 2.6286E+01    | 2.423E-09 | 2.577E+03        |
| 1s 5g $^3G_5$           | 1s 6g $^1G_4$   | 2.6522E+01    | 1.155E-09 | 1.217E+03        | 2.6411E+01    | 1.079E-09 | 1.079E+03        |
| 1s 5g $^1G_4$           | 1s 6g $^1G_4$   | 2.6527E+01    | 4.522E-08 | 4.763E+04        | 2.6415E+01    | 4.506E-08 | 4.745E+04        |
| 1s 6d $^3D_3$           | 1s 6g $^1G_4$   | 3.3331E+03    | 4.467E-15 | 2.980E-07        |               |           |                  |
| 1s 6g $^3G_4$           | 1s 6g $^1G_4$   | 8.9597E+03    | 4.990E-08 | 4.607E-01        | 9.2558E+03    | 4.823E-08 | 4.137E-01        |
| 1s 6g $^3G_3$           | 1s 6g $^1G_4$   | 9.3244E+03    | 1.689E-06 | 1.440E+01        | 9.2557E+03    | 1.688E-06 | 1.448E+01        |
| 1s 6g $^3G_5$           | 1s 6g $^1G_4$   | 2.8974E+05    | 4.257E-08 | 3.758E-04        |               |           |                  |
| 1s 6h $^3H_5^o$         | 1s 6h $^3H_6^o$ | 1.3919E+04    | 1.709E-06 | 4.525E+00        | 1.3932E+04    | 1.704E-06 | 4.466E+00        |
| 1s 4f $^3F_4^o$         | 1s 6h $^1H_5^o$ | 9.3106E+00    | 2.276E-14 | 1.592E-01        |               |           |                  |
| 1s 5f $^3F_4^o$         | 1s 6h $^1H_5^o$ | 2.6342E+01    | 3.217E-15 | 2.811E-03        |               |           |                  |
| 1s 6f $^3F_4^o$         | 1s 6h $^1H_5^o$ | 5.4702E+03    | 1.230E-18 | 2.493E-11        |               |           |                  |
| 1s 6h $^3H_5^o$         | 1s 6h $^1H_5^o$ | 1.3481E+04    | 2.713E-08 | 9.052E-02        | 1.3932E+04    | 2.621E-08 | 8.121E-02        |
| 1s 6h $^3H_4^o$         | 1s 6h $^1H_5^o$ | 1.4014E+04    | 1.418E-06 | 4.378E+00        | 1.3932E+04    | 1.415E-06 | 4.385E+00        |
| 1s 6h $^3H_6^o$         | 1s 6h $^1H_5^o$ | 4.2819E+05    | 3.644E-08 | 1.205E-04        |               |           |                  |
| 1s <sup>2</sup> $^1S_0$ | 1s 7s $^3S_1$   | 3.1410E-01    | 6.926E-07 | 1.561E+10        | 3.1278E-01    | 6.900E-07 | 1.554E+10        |
| 1s 2s $^3S_1$           | 1s 7s $^3S_1$   | 1.3268E+00    | 5.679E-08 | 7.173E+07        | 1.3212E+00    | 5.741E-08 | 7.251E+07        |
| 1s 2s $^1S_0$           | 1s 7s $^3S_1$   | 1.3390E+00    | 3.028E-08 | 3.755E+07        | 1.3335E+00    | 2.894E-08 | 3.588E+07        |
| 1s 3s $^3S_1$           | 1s 7s $^3S_1$   | 3.3983E+00    | 1.255E-08 | 2.417E+06        | 3.3842E+00    | 1.249E-08 | 2.405E+06        |
| 1s 3s $^1S_0$           | 1s 7s $^3S_1$   | 3.4193E+00    | 6.643E-09 | 1.263E+06        | 3.4054E+00    | 6.283E-09 | 1.194E+06        |
| 1s 3d $^3D_2$           | 1s 7s $^3S_1$   | 3.5389E+00    | 1.439E-13 | 2.554E+01        |               |           |                  |
| 1s 3d $^3D_1$           | 1s 7s $^3S_1$   | 3.5404E+00    | 4.644E-12 | 8.237E+02        |               |           |                  |
| 1s 3d $^1D_2$           | 1s 7s $^3S_1$   | 3.5774E+00    | 7.601E-13 | 1.321E+02        |               |           |                  |
| 1s 4s $^3S_1$           | 1s 7s $^3S_1$   | 7.3787E+00    | 4.062E-09 | 1.659E+05        | 7.3486E+00    | 4.055E-09 | 1.655E+05        |
| 1s 4s $^1S_0$           | 1s 7s $^3S_1$   | 7.4188E+00    | 2.370E-09 | 9.573E+04        | 7.3889E+00    | 2.038E-09 | 8.229E+04        |
| 1s 4d $^3D_2$           | 1s 7s $^3S_1$   | 7.6552E+00    | 5.626E-13 | 2.135E+01        | 7.6242E+00    | 2.363E-12 | 8.964E+01        |
| 1s 4d $^3D_1$           | 1s 7s $^3S_1$   | 7.6581E+00    | 6.580E-12 | 2.495E+02        |               |           |                  |
| 1s 4d $^1D_2$           | 1s 7s $^3S_1$   | 7.7314E+00    | 9.050E-13 | 3.366E+01        |               |           |                  |
| 1s 5s $^3S_1$           | 1s 7s $^3S_1$   | 1.5931E+01    | 1.585E-09 | 1.389E+04        | 1.5867E+01    | 1.594E-09 | 1.396E+04        |
| 1s 5s $^1S_0$           | 1s 7s $^3S_1$   | 1.6025E+01    | 1.087E-09 | 9.413E+03        | 1.5961E+01    | 8.018E-10 | 6.938E+03        |
| 1s 5d $^3D_2$           | 1s 7s $^3S_1$   | 1.6590E+01    | 5.370E-13 | 4.338E+00        | 1.6526E+01    | 2.554E-12 | 2.062E+01        |
| 1s 5d $^3D_1$           | 1s 7s $^3S_1$   | 1.6597E+01    | 8.216E-12 | 6.632E+01        | 1.6532E+01    | 6.071E-13 | 4.897E+00        |
| 1s 5d $^1D_2$           | 1s 7s $^3S_1$   | 1.6773E+01    | 1.120E-12 | 8.850E+00        |               |           |                  |
| 1s 6s $^3S_1$           | 1s 7s $^3S_1$   | 4.2495E+01    | 6.431E-10 | 7.918E+02        | 4.2299E+01    | 6.487E-10 | 7.993E+02        |
| 1s 6s $^1S_0$           | 1s 7s $^3S_1$   | 4.2877E+01    | 5.937E-10 | 7.180E+02        | 4.2623E+01    | 3.267E-10 | 3.965E+02        |
| 1s 6d $^3D_2$           | 1s 7s $^3S_1$   | 4.5259E+01    | 1.365E-13 | 1.482E-01        | 4.5119E+01    | 2.252E-12 | 2.439E+00        |
| 1s 6d $^3D_1$           | 1s 7s $^3S_1$   | 4.5288E+01    | 1.227E-11 | 1.330E+01        | 4.5112E+01    | 4.512E-13 | 4.887E-01        |
| 1s 6d $^1D_2$           | 1s 7s $^3S_1$   | 4.6054E+01    | 1.888E-12 | 1.980E+00        |               |           |                  |
| 1s 2p $^3P_0^o$         | 1s 7p $^3P_0^o$ | 1.3376E+00    | 1.508E-08 | 1.873E+07        | 1.3321E+00    | 1.333E-08 | 1.656E+07        |
| 1s 2p $^3P_1^o$         | 1s 7p $^3P_1^o$ | 1.3385E+00    | 4.191E-09 | 5.202E+06        | 1.3329E+00    | 8.068E-09 | 1.001E+07        |
| 1s 2p $^3P_2^o$         | 1s 7p $^3P_2^o$ | 1.3961E+00    | 2.546E-07 | 2.904E+08        | 1.3903E+00    | 2.530E-07 | 2.886E+08        |
| 1s 2p $^1P_1^o$         | 1s 7p $^3P_1^o$ | 1.4017E+00    | 5.769E-08 | 6.529E+07        | 1.3959E+00    | 5.678E-08 | 6.424E+07        |
| 1s 3p $^3P_0^o$         | 1s 7p $^3P_0^o$ | 3.4164E+00    | 5.090E-09 | 9.696E+05        | 3.4024E+00    | 3.619E-09 | 6.892E+05        |
| 1s 3p $^3P_1^o$         | 1s 7p $^3P_1^o$ | 3.4179E+00    | 9.304E-10 | 1.771E+05        | 3.4038E+00    | 2.752E-09 | 5.236E+05        |
| 1s 3p $^3P_2^o$         | 1s 7p $^3P_2^o$ | 3.5289E+00    | 1.888E-07 | 3.370E+07        | 3.5142E+00    | 1.914E-07 | 3.417E+07        |
| 1s 3p $^1P_1^o$         | 1s 7p $^3P_1^o$ | 3.5388E+00    | 4.200E-08 | 7.456E+06        | 3.5243E+00    | 4.122E-08 | 7.316E+06        |
| 1s 4p $^3P_0^o$         | 1s 7p $^3P_0^o$ | 7.4094E+00    | 2.361E-09 | 9.563E+04        | 7.3785E+00    | 1.251E-09 | 5.067E+04        |
| 1s 4p $^3P_1^o$         | 1s 7p $^3P_1^o$ | 7.4122E+00    | 1.525E-10 | 6.170E+03        | 7.3811E+00    | 1.273E-09 | 5.152E+04        |
| 1s 4p $^3P_2^o$         | 1s 7p $^3P_2^o$ | 7.6311E+00    | 1.667E-07 | 6.363E+06        | 7.5991E+00    | 1.690E-07 | 6.451E+06        |
| 1s 4p $^1P_1^o$         | 1s 7p $^3P_0^o$ | 7.6504E+00    | 3.684E-08 | 1.400E+06        | 7.6186E+00    | 3.546E-08 | 1.347E+06        |
| 1s 4f $^3F_2^o$         | 1s 7p $^3P_1^o$ | 7.7232E+00    | 3.851E-14 | 1.436E+00        |               |           |                  |
| 1s 5p $^3P_0^o$         | 1s 7p $^3P_0^o$ | 1.5987E+01    | 1.514E-09 | 1.317E+04        | 1.5920E+01    | 4.931E-10 | 4.289E+03        |
| 1s 5p $^3P_1^o$         | 1s 7p $^3P_1^o$ | 1.5993E+01    | 6.465E-13 | 5.620E+00        | 1.5926E+01    | 7.581E-10 | 6.589E+03        |

(continued on next page)

Table 5 (continued)

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |           |                  |
|-----------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                 |                 | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 5p $^3P_2^0$ | 1s 7p $^3P_1^0$ | 1.6515E+01    | 1.788E-07 | 1.458E+06        | 1.6446E+01    | 1.815E-07 | 1.480E+06        |
| 1s 5p $^1P_1^0$ | 1s 7p $^3P_1^0$ | 1.6561E+01    | 3.921E-08 | 3.179E+05        | 1.6492E+01    | 3.741E-08 | 3.033E+05        |
| 1s 5f $^3F_2^0$ | 1s 7p $^3P_1^0$ | 1.6736E+01    | 7.663E-14 | 6.083E-01        |               |           |                  |
| 1s 6p $^3P_2^0$ | 1s 7p $^3P_0^0$ | 4.2622E+01    | 1.096E-09 | 1.342E+03        | 4.2444E+01    | 2.699E-10 | 3.304E+02        |
| 1s 6p $^3P_0^0$ | 1s 7p $^3P_1^0$ | 4.2648E+01    | 5.644E-11 | 6.899E+01        | 4.2376E+01    | 6.084E-10 | 7.470E+02        |
| 1s 6p $^3P_1^0$ | 1s 7p $^3P_0^0$ | 4.4826E+01    | 2.721E-07 | 3.011E+05        | 4.4636E+01    | 2.777E-07 | 3.073E+05        |
| 1s 6p $^1P_1^0$ | 1s 7p $^3P_1^0$ | 4.5021E+01    | 5.950E-08 | 6.527E+04        | 4.4809E+01    | 5.628E-08 | 6.180E+04        |
| 1s 6f $^3F_2^0$ | 1s 7p $^3P_0^0$ | 4.5775E+01    | 1.568E-13 | 1.663E-01        |               |           |                  |
| 1s 2s $^3S_1$   | 1s 7s $^1S_0$   | 1.3266E+00    | 2.842E-08 | 1.077E+08        | 1.3210E+00    | 2.870E-08 | 1.087E+08        |
| 1s 3s $^3S_1$   | 1s 7s $^1S_0$   | 3.3968E+00    | 5.855E-09 | 3.385E+06        | 3.3830E+00    | 6.245E-09 | 3.609E+06        |
| 1s 3d $^3D_1$   | 1s 7s $^1S_0$   | 3.5388E+00    | 6.161E-13 | 3.281E+02        |               |           |                  |
| 1s 4s $^3S_1$   | 1s 7s $^1S_0$   | 7.3716E+00    | 1.719E-09 | 2.110E+05        | 7.3425E+00    | 2.026E-09 | 2.485E+05        |
| 1s 4d $^3D_1$   | 1s 7s $^1S_0$   | 7.6504E+00    | 8.796E-13 | 1.002E+02        | 7.6206E+00    | 8.205E-13 | 9.344E+01        |
| 1s 5s $^3S_1$   | 1s 7s $^1S_0$   | 1.5898E+01    | 5.646E-10 | 1.490E+04        | 1.5839E+01    | 7.961E-10 | 2.098E+04        |
| 1s 5d $^3D_1$   | 1s 7s $^1S_0$   | 1.6561E+01    | 9.135E-13 | 2.222E+01        | 1.6502E+01    | 9.451E-13 | 2.295E+01        |
| 1s 6s $^3S_1$   | 1s 7s $^1S_0$   | 4.2259E+01    | 1.431E-10 | 5.345E+02        | 4.2100E+01    | 3.228E-10 | 1.204E+03        |
| 1s 6d $^3D_1$   | 1s 7s $^1S_0$   | 4.5020E+01    | 8.016E-13 | 2.638E+00        | 4.4886E+01    | 9.411E-13 | 3.089E+00        |
| 1s 7s $^3S_1$   | 1s 7s $^1S_0$   | 7.6139E+03    | 4.456E-09 | 5.128E-01        | 8.9405E+03    | 3.689E-09 | 3.052E-01        |
| 1s 2p $^3P_2^0$ | 1s 7p $^3P_0^0$ | 1.3376E+00    | 5.365E-09 | 2.000E+07        | 1.3321E+00    | 4.432E-09 | 1.652E+07        |
| 1s 2p $^1P_1^0$ | 1s 7p $^3P_0^0$ | 1.4016E+00    | 1.035E-07 | 3.514E+08        | 1.3959E+00    | 1.057E-07 | 3.589E+08        |
| 1s 3p $^3P_2^0$ | 1s 7p $^3P_3^0$ | 3.4163E+00    | 1.518E-09 | 8.674E+05        | 3.4026E+00    | 9.937E-10 | 5.676E+05        |
| 1s 3p $^1P_1^0$ | 1s 7p $^3P_0^0$ | 3.5387E+00    | 7.620E-08 | 4.059E+07        | 3.5246E+00    | 7.860E-08 | 4.184E+07        |
| 1s 4p $^3P_2^0$ | 1s 7p $^3P_0^0$ | 7.4089E+00    | 4.150E-10 | 5.042E+04        | 7.3797E+00    | 2.397E-10 | 2.912E+04        |
| 1s 4p $^1P_1^0$ | 1s 7p $^3P_0^0$ | 7.6499E+00    | 6.694E-08 | 7.630E+06        | 7.6199E+00    | 6.869E-08 | 7.824E+06        |
| 1s 5p $^3P_2^0$ | 1s 7p $^3P_0^0$ | 1.5984E+01    | 8.383E-11 | 2.189E+03        | 1.5926E+01    | 3.891E-11 | 1.014E+03        |
| 1s 5p $^1P_1^0$ | 1s 7p $^3P_0^0$ | 1.6558E+01    | 7.163E-08 | 1.743E+06        | 1.6498E+01    | 7.327E-08 | 1.780E+06        |
| 1s 6p $^3P_2^0$ | 1s 7p $^3P_0^0$ | 4.2605E+01    | 7.779E-12 | 2.859E+01        | 4.2486E+01    | 2.961E-11 | 1.085E+02        |
| 1s 6p $^1P_1^0$ | 1s 7p $^3P_0^0$ | 4.5003E+01    | 1.090E-07 | 3.590E+05        | 4.4856E+01    | 1.112E-07 | 3.657E+05        |
| 1s 7p $^3P_2^0$ | 1s 7p $^3P_0^0$ | 1.1050E+05    | 4.339E-08 | 2.370E-02        |               |           |                  |
| 1s 2p $^3P_1^0$ | 1s 7p $^3P_2^0$ | 1.3363E+00    | 1.183E-07 | 8.840E+07        | 1.3308E+00    | 1.215E-07 | 9.078E+07        |
| 1s 2p $^3P_2^0$ | 1s 7p $^3P_2^0$ | 1.3947E+00    | 1.912E-07 | 1.311E+08        | 1.3889E+00    | 1.835E-07 | 1.258E+08        |
| 1s 2p $^1P_1^0$ | 1s 7p $^3P_0^0$ | 1.4002E+00    | 1.400E-08 | 9.523E+06        | 1.3944E+00    | 1.676E-08 | 1.140E+07        |
| 1s 3p $^3P_1^0$ | 1s 7p $^3P_2^0$ | 3.4080E+00    | 1.229E-07 | 1.412E+07        | 3.3940E+00    | 1.242E-07 | 1.427E+07        |
| 1s 3p $^3P_2^0$ | 1s 7p $^3P_2^0$ | 3.5199E+00    | 5.498E-08 | 5.921E+06        | 3.5053E+00    | 5.309E-08 | 5.715E+06        |
| 1s 3p $^1P_1^0$ | 1s 7p $^3P_2^0$ | 3.5298E+00    | 2.478E-09 | 2.654E+05        | 3.5153E+00    | 4.084E-09 | 4.372E+05        |
| 1s 4p $^3P_2^0$ | 1s 7p $^3P_2^0$ | 7.3699E+00    | 1.253E-07 | 3.077E+06        | 7.3391E+00    | 1.273E-07 | 3.128E+06        |
| 1s 4p $^3P_1^0$ | 1s 7p $^3P_2^0$ | 7.5892E+00    | 2.251E-08 | 5.215E+05        | 7.5574E+00    | 1.936E-08 | 4.484E+05        |
| 1s 4p $^1P_1^0$ | 1s 7p $^3P_2^0$ | 7.6083E+00    | 2.879E-10 | 6.635E+03        | 7.5766E+00    | 1.124E-09 | 2.590E+04        |
| 1s 4f $^3F_3^0$ | 1s 7p $^3P_2^0$ | 7.6787E+00    | 4.986E-18 | 1.128E-04        |               |           |                  |
| 1s 4f $^3F_2^0$ | 1s 7p $^3P_2^0$ | 7.6803E+00    | 4.502E-16 | 1.018E-02        |               |           |                  |
| 1s 4f $^1F_3^0$ | 1s 7p $^3P_2^0$ | 7.7161E+00    | 5.132E-15 | 1.150E-01        |               |           |                  |
| 1s 5p $^3P_2^0$ | 1s 7p $^3P_2^0$ | 1.5804E+01    | 1.465E-07 | 7.824E+05        | 1.5738E+01    | 1.489E-07 | 7.952E+05        |
| 1s 5p $^3P_1^0$ | 1s 7p $^3P_2^0$ | 1.6320E+01    | 1.116E-08 | 5.589E+04        | 1.6251E+01    | 8.133E-09 | 4.073E+04        |
| 1s 5p $^1P_1^0$ | 1s 7p $^3P_2^0$ | 1.6364E+01    | 2.116E-11 | 1.054E+02        | 1.6297E+01    | 2.649E-10 | 1.319E+03        |
| 1s 5f $^3F_3^0$ | 1s 7p $^3P_2^0$ | 1.6532E+01    | 1.343E-13 | 6.555E-01        |               |           |                  |
| 1s 5f $^3F_2^0$ | 1s 7p $^3P_2^0$ | 1.6535E+01    | 4.833E-14 | 2.358E-01        |               |           |                  |
| 1s 5f $^1F_3^0$ | 1s 7p $^3P_2^0$ | 1.6621E+01    | 1.386E-14 | 6.691E-02        |               |           |                  |
| 1s 6p $^3P_1^0$ | 1s 7p $^3P_2^0$ | 4.1345E+01    | 2.311E-07 | 1.803E+05        | 4.1174E+01    | 2.351E-07 | 1.834E+05        |
| 1s 6p $^3P_2^0$ | 1s 7p $^3P_2^0$ | 4.3416E+01    | 5.959E-09 | 4.217E+03        | 4.3234E+01    | 3.466E-09 | 2.452E+03        |
| 1s 6p $^1P_1^0$ | 1s 7p $^3P_2^0$ | 4.3599E+01    | 5.062E-10 | 3.553E+02        |               |           |                  |
| 1s 6f $^3F_3^0$ | 1s 7p $^3P_2^0$ | 4.4291E+01    | 5.946E-13 | 4.044E-01        |               |           |                  |
| 1s 6f $^3F_2^0$ | 1s 7p $^3P_2^0$ | 4.4306E+01    | 2.356E-13 | 1.601E-01        |               |           |                  |
| 1s 6f $^1F_3^0$ | 1s 7p $^3P_2^0$ | 4.4661E+01    | 3.239E-14 | 2.166E-02        |               |           |                  |
| 1s 7p $^3P_1^0$ | 1s 7p $^3P_2^0$ | 1.3800E+03    | 5.054E-06 | 3.541E+03        | 1.3760E+03    | 5.105E-06 | 3.566E+03        |
| 1s 2s $^3S_1$   | 1s 7d $^3D_2$   | 1.3252E+00    | 3.914E-09 | 2.974E+06        | 1.3196E+00    | 4.084E-09 | 3.102E+06        |
| 1s 3s $^3S_1$   | 1s 7d $^3D_2$   | 3.3879E+00    | 7.078E-10 | 8.227E+04        | 3.3736E+00    | 7.633E-10 | 8.872E+04        |
| 1s 3d $^3D_2$   | 1s 7d $^3D_2$   | 3.5276E+00    | 1.603E-08 | 1.718E+06        | 3.5127E+00    | 1.599E-08 | 1.714E+06        |
| 1s 3d $^3D_1$   | 1s 7d $^3D_2$   | 3.5291E+00    | 1.400E-09 | 1.499E+05        | 3.5142E+00    | 1.857E-09 | 1.989E+05        |
| 1s 3d $^3D_3$   | 1s 7d $^3D_2$   | 3.5644E+00    | 2.985E-08 | 3.134E+06        | 3.5492E+00    | 2.966E-08 | 3.115E+06        |
| 1s 3d $^1D_2$   | 1s 7d $^3D_2$   | 3.5659E+00    | 2.352E-09 | 2.468E+05        | 3.5507E+00    | 2.360E-09 | 2.476E+05        |
| 1s 4s $^3S_1$   | 1s 7d $^3D_2$   | 7.3299E+00    | 1.241E-10 | 3.081E+03        | 7.2988E+00    | 1.467E-10 | 3.644E+03        |
| 1s 4d $^3D_2$   | 1s 7d $^3D_2$   | 7.6027E+00    | 8.357E-09 | 1.929E+05        | 7.5707E+00    | 8.334E-09 | 1.923E+05        |
| 1s 4d $^3D_1$   | 1s 7d $^3D_2$   | 7.6055E+00    | 6.426E-10 | 1.482E+04        | 7.5734E+00    | 9.979E-10 | 2.301E+04        |
| 1s 4d $^3D_3$   | 1s 7d $^3D_2$   | 7.6748E+00    | 3.028E-08 | 6.858E+05        | 7.6422E+00    | 3.021E-08 | 6.842E+05        |
| 1s 4d $^1D_2$   | 1s 7d $^3D_2$   | 7.6778E+00    | 2.362E-09 | 5.346E+04        | 7.6453E+00    | 2.315E-09 | 5.239E+04        |
| 1s 5s $^3S_1$   | 1s 7d $^3D_2$   | 1.5705E+01    | 1.638E-11 | 8.860E+01        | 1.5637E+01    | 2.578E-11 | 1.395E+02        |
| 1s 5d $^3D_2$   | 1s 7d $^3D_2$   | 1.6345E+01    | 4.113E-09 | 2.054E+04        | 1.6276E+01    | 4.090E-09 | 2.042E+04        |
| 1s 5d $^3D_1$   | 1s 7d $^3D_2$   | 1.6352E+01    | 2.503E-10 | 1.249E+03        | 1.6283E+01    | 5.152E-10 | 2.570E+03        |
| 1s 5d $^3D_3$   | 1s 7d $^3D_2$   | 1.6516E+01    | 3.236E-08 | 1.583E+05        | 1.6446E+01    | 3.234E-08 | 1.582E+05        |
| 1s 5d $^1D_2$   | 1s 7d $^3D_2$   | 1.6523E+01    | 2.512E-09 | 1.227E+04        | 1.6453E+01    | 2.418E-09 | 1.181E+04        |
| 1s 5g $^3G_3$   | 1s 7d $^3D_2$   | 1.6607E+01    | 9.716E-18 | 4.700E-05        |               |           |                  |

(continued on next page)

Table 5 (continued)

| Lower   | Upper   | GRASP2K       |           |                        | FAC           |            |                        |
|---|---|---------------|-----------|------------------------|---------------|------------|------------------------|
|   |   | $\lambda$ (Å) | $gf$      | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | $gf$       | $A$ (s <sup>-1</sup> ) |
| 1s6s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.0924E+01    | 1.212E-14 | 9.653E-03              |               |            |                        |
| 1s6d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.3482E+01    | 1.940E-09 | 1.369E+03              | 4.3306E+01    | 1.938E-09  | 1.367E+03              |
| 1s6d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.3508E+01    | 5.943E-11 | 4.188E+01              | 4.3299E+01    | 2.702E-10  | 1.906E+02              |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.4184E+01    | 4.703E-08 | 3.214E+04              | 4.4000E+01    | 4.706E-08  | 3.215E+04              |
| 1s6d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.4215E+01    | 3.640E-09 | 2.484E+03              | 4.4010E+01    | 3.423E-09  | 2.338E+03              |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 4.4564E+01    | 1.069E-16 | 7.182E-05              |               |            |                        |
| 1s7s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>2</sub>              | 1.1072E+03    | 3.819E-11 | 4.155E-02              | 1.0773E+03    | 1.749E-12  | 1.994E-03              |
| 1s <sup>2</sup> <sup>1</sup> S <sub>0</sub>   | 1s7d <sup>3</sup> D <sub>1</sub>              | 3.1400E-01    | 1.149E-08 | 2.591E+08              | 3.1269E-01    | 1.185E-08  | 2.673E+08              |
| 1s2s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.3252E+00    | 1.091E-09 | 1.381E+06              | 1.3196E+00    | 8.170E-10  | 1.034E+06              |
| 1s2s <sup>1</sup> S <sub>0</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.3373E+00    | 1.626E-09 | 2.021E+06              | 1.3319E+00    | 1.633E-09  | 2.029E+06              |
| 1s3s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 3.3878E+00    | 2.425E-10 | 4.698E+04              | 3.3737E+00    | 1.564E-10  | 3.030E+04              |
| 1s3s <sup>1</sup> S <sub>0</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 3.4087E+00    | 2.964E-10 | 5.672E+04              | 3.3947E+00    | 3.091E-10  | 5.914E+04              |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 3.5275E+00    | 2.219E-09 | 3.966E+05              | 3.5127E+00    | 1.737E-09  | 3.104E+05              |
| 1s3d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 3.5290E+00    | 8.898E-09 | 1.589E+06              | 3.5142E+00    | 8.895E-09  | 1.587E+06              |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 3.5657E+00    | 1.895E-08 | 3.314E+06              | 3.5507E+00    | 1.928E-08  | 3.371E+06              |
| 1s4s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 7.3294E+00    | 6.510E-11 | 2.694E+03              | 7.2989E+00    | 3.075E-11  | 1.272E+03              |
| 1s4s <sup>1</sup> S <sub>0</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 7.3689E+00    | 5.760E-11 | 2.358E+03              | 7.3387E+00    | 6.006E-11  | 2.458E+03              |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 7.6021E+00    | 1.263E-09 | 4.859E+04              | 7.5708E+00    | 8.803E-10  | 3.385E+04              |
| 1s4d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 7.6050E+00    | 4.648E-09 | 1.787E+05              | 7.5736E+00    | 4.638E-09  | 1.782E+05              |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 7.6772E+00    | 1.930E-08 | 7.282E+05              | 7.6454E+00    | 1.958E-08  | 7.388E+05              |
| 1s5s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.5703E+01    | 2.284E-11 | 2.060E+02              | 1.5638E+01    | 1.5638E-12 | 5.049E+01              |
| 1s5s <sup>1</sup> S <sub>0</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.5794E+01    | 1.050E-11 | 9.360E+01              | 1.5729E+01    | 1.078E-11  | 9.608E+01              |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.6343E+01    | 7.197E-10 | 5.991E+03              | 1.6277E+01    | 4.166E-10  | 3.466E+03              |
| 1s5d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.6349E+01    | 2.289E-09 | 1.904E+04              | 1.6283E+01    | 2.280E-09  | 1.895E+04              |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.6521E+01    | 2.062E-08 | 1.679E+05              | 1.6453E+01    | 2.091E-08  | 1.703E+05              |
| 1s6s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 4.0910E+01    | 1.214E-11 | 1.613E+01              |               |            |                        |
| 1s6s <sup>1</sup> S <sub>0</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 4.1264E+01    | 7.813E-13 | 1.020E+00              |               |            |                        |
| 1s6d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 4.3465E+01    | 4.636E-10 | 5.456E+02              | 4.3310E+01    | 1.580E-10  | 1.857E+02              |
| 1s6d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 4.3492E+01    | 1.079E-09 | 1.268E+03              | 4.3303E+01    | 1.072E-09  | 1.260E+03              |
| 1s6d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 4.4198E+01    | 2.990E-08 | 3.404E+04              | 4.4015E+01    | 3.037E-08  | 3.456E+04              |
| 1s7s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.0966E+03    | 1.138E-10 | 2.103E-01              | 1.0799E+03    | 3.492E-13  | 6.601E-04              |
| 1s7s <sup>1</sup> S <sub>0</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.2811E+03    | 1.093E-12 | 1.480E-03              | 1.2282E+03    | 6.150E-13  | 8.988E-04              |
| 1s7d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>1</sub>              | 1.1420E+05    | 8.038E-08 | 1.370E-02              |               |            |                        |
| 1s2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.3362E+00    | 2.129E-08 | 2.651E+07              | 1.3307E+00    | 2.137E-08  | 2.661E+07              |
| 1s2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.3371E+00    | 4.382E-08 | 5.450E+07              | 1.3315E+00    | 4.537E-08  | 5.642E+07              |
| 1s2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>2</sub> <sup>o</sup> | 1.3946E+00    | 2.779E-08 | 3.177E+07              | 1.3888E+00    | 2.769E-08  | 3.166E+07              |
| 1s2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.4001E+00    | 9.952E-08 | 1.129E+08              | 1.3943E+00    | 9.895E-08  | 1.122E+08              |
| 1s3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 3.4073E+00    | 2.514E-08 | 4.814E+06              | 3.3933E+00    | 2.339E-08  | 4.479E+06              |
| 1s3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.4088E+00    | 4.744E-08 | 9.077E+06              | 3.3948E+00    | 4.799E-08  | 9.180E+06              |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>2</sub> <sup>o</sup> | 3.5191E+00    | 8.199E-09 | 1.472E+06              | 3.5046E+00    | 9.472E-09  | 1.700E+06              |
| 1s3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 3.5290E+00    | 2.701E-08 | 4.823E+06              | 3.5146E+00    | 2.829E-08  | 5.050E+06              |
| 1s4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 7.3666E+00    | 2.634E-08 | 1.079E+06              | 7.3362E+00    | 2.462E-08  | 1.008E+06              |
| 1s4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.3693E+00    | 4.921E-08 | 2.015E+06              | 7.3389E+00    | 4.990E-08  | 2.042E+06              |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>2</sub> <sup>o</sup> | 7.5857E+00    | 2.994E-09 | 1.157E+05              | 7.5543E+00    | 4.311E-09  | 1.665E+05              |
| 1s4p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 7.6047E+00    | 9.460E-09 | 3.637E+05              | 7.5735E+00    | 1.015E-08  | 3.903E+05              |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 7.6767E+00    | 6.581E-16 | 2.483E-02              |               |            |                        |
| 1s5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.5788E+01    | 3.150E-08 | 2.810E+05              | 1.5725E+01    | 2.923E-08  | 2.606E+05              |
| 1s5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.5795E+01    | 5.816E-08 | 5.183E+05              | 1.5731E+01    | 5.883E-08  | 5.241E+05              |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>2</sub> <sup>o</sup> | 1.6303E+01    | 1.149E-09 | 9.614E+03              | 1.6237E+01    | 2.508E-09  | 2.097E+04              |
| 1s5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.6348E+01    | 3.464E-09 | 2.882E+04              | 1.6282E+01    | 4.145E-09  | 3.447E+04              |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.6519E+01    | 1.011E-13 | 8.235E-01              |               |            |                        |
| 1s6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 4.1241E+01    | 5.029E-08 | 6.574E+04              | 4.1082E+01    | 4.653E-08  | 6.078E+04              |
| 1s6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.1265E+01    | 9.222E-08 | 1.204E+05              | 4.1019E+01    | 9.378E-08  | 1.228E+05              |
| 1s6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>2</sub> <sup>o</sup> | 4.3302E+01    | 5.836E-10 | 6.920E+02              | 4.3133E+01    | 1.991E-09  | 2.359E+03              |
| 1s6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 4.3483E+01    | 1.175E-09 | 1.382E+03              | 4.3294E+01    | 1.809E-09  | 2.128E+03              |
| 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 4.4186E+01    | 4.893E-13 | 5.572E-01              |               |            |                        |
| 1s7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.2731E+03    | 1.019E-06 | 1.398E+03              | 1.2808E+03    | 9.958E-07  | 1.338E+03              |
| 1s7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.2879E+03    | 1.886E-06 | 2.528E+03              | 1.2433E+03    | 1.886E-06  | 2.690E+03              |
| 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7p <sup>1</sup> P <sub>2</sub> <sup>o</sup> | 1.6436E+04    | 1.261E-07 | 1.038E+00              | 1.8507E+04    | 1.091E-07  | 7.026E-01              |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 3.5248E+00    | 8.286E-09 | 6.355E+05              | 3.5099E+00    | 8.335E-09  | 6.392E+05              |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 3.5615E+00    | 7.741E-08 | 5.816E+06              | 3.5464E+00    | 7.691E-08  | 5.777E+06              |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 3.5629E+00    | 3.385E-09 | 2.541E+05              | 3.5478E+00    | 3.805E-09  | 2.856E+05              |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 7.5894E+00    | 1.320E-08 | 2.183E+05              | 7.5575E+00    | 1.324E-08  | 2.190E+05              |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 7.6613E+00    | 4.040E-08 | 6.558E+05              | 7.6289E+00    | 4.032E-08  | 6.546E+05              |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 7.6642E+00    | 1.665E-09 | 2.702E+04              | 7.6319E+00    | 1.958E-09  | 3.177E+04              |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.6284E+01    | 1.901E-08 | 6.830E+04              | 1.6216E+01    | 1.905E-08  | 6.847E+04              |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.6453E+01    | 1.990E-08 | 7.005E+04              | 1.6384E+01    | 1.990E-08  | 7.005E+04              |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.6460E+01    | 7.283E-10 | 2.561E+03              | 1.6391E+01    | 9.397E-10  | 3.304E+03              |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.6542E+01    | 1.731E-16 | 6.029E-04              |               |            |                        |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.6544E+01    | 3.024E-18 | 1.053E-05              |               |            |                        |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7d <sup>3</sup> D <sub>3</sub>              | 1.6595E+01    | 6.733E-20 | 2.330E-07              |               |            |                        |

(continued on next page)

Table 5 (continued)

| Lower  | Upper  | GRASP2K       |           |                             | FAC           |           |                             |
|--|--|---------------|-----------|-----------------------------|---------------|-----------|-----------------------------|
|  |  | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.3051E+01    | 3.466E-08 | 1.782E+04                   | 4.2880E+01    | 3.476E-08 | 1.786E+04                   |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.3740E+01    | 9.385E-09 | 4.675E+03                   | 4.3560E+01    | 9.372E-09 | 4.666E+03                   |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.3770E+01    | 2.487E-10 | 1.237E+02                   | 4.3571E+01    | 3.789E-10 | 1.886E+02                   |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.4103E+01    | 1.879E-13 | 9.204E-02                   |               |           |                             |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.4112E+01    | 7.209E-15 | 3.530E-03                   |               |           |                             |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.4321E+01    | 6.432E-18 | 3.120E-06                   |               |           |                             |
| 1s 7d <sup>3</sup> D <sub>2</sub>              | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.3459E+03    | 2.625E-06 | 1.324E+02                   | 4.3620E+03    | 2.623E-06 | 1.302E+02                   |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.3942E+00    | 8.521E-09 | 4.177E+06                   | 1.3883E+00    | 7.247E-09 | 3.552E+06                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.5164E+00    | 3.762E-10 | 2.899E+04                   | 3.5016E+00    | 4.070E-10 | 3.136E+04                   |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 7.5729E+00    | 4.137E-10 | 6.874E+03                   | 7.5406E+00    | 4.246E-10 | 7.056E+03                   |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 7.6621E+00    | 4.484E-08 | 7.279E+05                   | 7.6295E+00    | 1.331E-08 | 2.161E+05                   |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 7.6636E+00    | 1.593E-07 | 2.584E+06                   | 7.6310E+00    | 6.677E-10 | 1.083E+04                   |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 7.6982E+00    | 7.787E-09 | 1.252E+05                   | 7.6653E+00    | 7.865E-09 | 1.264E+05                   |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 7.6993E+00    | 2.637E-10 | 4.239E+03                   | 7.6665E+00    | 3.040E-10 | 4.887E+03                   |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6245E+01    | 1.679E-10 | 6.064E+02                   | 1.6174E+01    | 1.729E-10 | 6.247E+02                   |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6455E+01    | 6.347E-08 | 2.234E+05                   | 1.6385E+01    | 1.004E-08 | 3.533E+04                   |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6459E+01    | 1.769E-07 | 6.224E+05                   | 1.6388E+01    | 5.043E-10 | 1.774E+03                   |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6540E+01    | 1.096E-08 | 3.816E+04                   | 1.6469E+01    | 1.094E-08 | 3.811E+04                   |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6543E+01    | 3.832E-10 | 1.334E+03                   | 1.6472E+01    | 4.176E-10 | 1.454E+03                   |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.2891E+01    | 4.093E-11 | 2.120E+01                   | 4.2690E+01    | 4.269E-11 | 2.213E+01                   |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.3744E+01    | 4.845E-08 | 2.412E+04                   | 4.3561E+01    | 2.889E-09 | 2.889E+03                   |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.3758E+01    | 1.217E-07 | 6.059E+04                   | 4.3560E+01    | 2.919E-10 | 1.453E+02                   |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4094E+01    | 1.673E-08 | 8.197E+03                   | 4.3907E+01    | 1.663E-08 | 8.152E+03                   |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4105E+01    | 6.132E-10 | 3.004E+02                   | 4.3907E+01    | 6.178E-10 | 3.027E+02                   |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4312E+01    | 1.635E-17 | 7.936E-06                   |               |           |                             |
| 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.5436E+03    | 2.931E-12 | 2.224E-04                   | 3.3920E+03    | 4.564E-13 | 3.748E-05                   |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3358E+00    | 7.084E-12 | 5.296E+03                   | 1.3303E+00    | 5.834E-12 | 4.360E+03                   |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3942E+00    | 4.476E-10 | 3.072E+05                   | 1.3883E+00    | 5.176E-10 | 3.552E+05                   |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3997E+00    | 4.948E-09 | 3.370E+06                   | 1.3939E+00    | 4.754E-09 | 3.236E+06                   |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.4047E+00    | 9.120E-13 | 1.050E+02                   | 3.3906E+00    | 4.222E-13 | 4.858E+01                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.5163E+00    | 4.173E-11 | 4.503E+03                   | 3.5016E+00    | 2.907E-11 | 3.136E+03                   |
| 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.5262E+00    | 2.694E-10 | 2.890E+04                   | 3.5116E+00    | 2.584E-10 | 2.771E+04                   |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.3543E+00    | 9.639E-13 | 2.378E+01                   |               |           |                             |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.5727E+00    | 3.962E-11 | 9.216E+02                   | 7.5406E+00    | 3.074E-11 | 7.151E+02                   |
| 1s 4p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.5917E+00    | 2.769E-10 | 6.409E+03                   | 7.5597E+00    | 2.729E-10 | 6.316E+03                   |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.6619E+00    | 1.605E-07 | 3.648E+06                   | 7.6295E+00    | 6.748E-10 | 1.533E+04                   |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.6634E+00    | 8.990E-08 | 2.042E+06                   | 7.6310E+00    | 9.326E-09 | 2.118E+05                   |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.6990E+00    | 5.551E-09 | 1.249E+05                   | 7.6665E+00    | 5.820E-09 | 1.309E+05                   |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.5732E+01    | 5.384E-13 | 2.902E+00                   |               |           |                             |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6243E+01    | 1.702E-11 | 8.607E+01                   | 1.6174E+01    | 1.264E-11 | 6.394E+01                   |
| 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6288E+01    | 1.139E-10 | 5.729E+02                   | 1.6219E+01    | 1.117E-10 | 5.618E+02                   |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6454E+01    | 1.805E-07 | 8.896E+05                   | 1.6385E+01    | 5.107E-10 | 2.516E+03                   |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6457E+01    | 9.042E-08 | 4.454E+05                   | 1.6388E+01    | 7.034E-09 | 3.464E+04                   |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6542E+01    | 7.829E-09 | 3.817E+04                   | 1.6472E+01    | 8.100E-09 | 3.948E+04                   |
| 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.0860E+01    | 3.480E-13 | 2.781E-01                   |               |           |                             |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.2882E+01    | 5.412E-12 | 3.926E+00                   | 4.2690E+01    | 3.049E-12 | 2.213E+00                   |
| 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3060E+01    | 2.950E-11 | 2.123E+01                   | 4.2848E+01    | 2.777E-11 | 2.001E+01                   |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3735E+01    | 1.272E-07 | 8.872E+04                   | 4.3561E+01    | 2.879E-10 | 2.007E+02                   |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3749E+01    | 6.015E-08 | 4.193E+04                   | 4.3561E+01    | 4.062E-09 | 2.831E+03                   |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4096E+01    | 1.205E-08 | 8.267E+03                   | 4.3907E+01    | 1.232E-08 | 8.457E+03                   |
| 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 9.8851E+02    | 2.009E-12 | 2.742E-03                   | 9.7899E+02    | 2.186E-15 | 3.018E-06                   |
| 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.4844E+03    | 5.719E-12 | 6.284E-04                   | 3.3927E+03    | 3.259E-14 | 3.745E-06                   |
| 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4219E+03    | 9.314E-15 | 6.355E-07                   | 4.1543E+03    | 2.391E-13 | 1.833E-05                   |
| 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 2.0860E+05    | 6.413E-08 | 1.966E-03                   |               |           |                             |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.3248E+00    | 2.700E-12 | 2.052E+03                   | 1.3192E+00    | 5.989E-13 | 4.552E+02                   |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.3851E+00    | 1.746E-12 | 2.033E+02                   |               |           |                             |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.5247E+00    | 6.496E-10 | 6.976E+04                   | 3.5098E+00    | 6.265E-10 | 6.727E+04                   |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.5261E+00    | 5.200E-09 | 5.579E+05                   | 3.5113E+00    | 5.252E-09 | 5.634E+05                   |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.5614E+00    | 4.462E-09 | 4.693E+05                   | 3.5463E+00    | 4.109E-09 | 4.321E+05                   |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 3.5628E+00    | 5.333E-08 | 5.604E+06                   | 3.5477E+00    | 5.362E-08 | 5.635E+06                   |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.3170E+00    | 1.395E-12 | 3.475E+01                   |               |           |                             |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.5888E+00    | 1.014E-09 | 2.350E+04                   | 7.5573E+00    | 9.516E-10 | 2.204E+04                   |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.5916E+00    | 8.270E-09 | 1.914E+05                   | 7.5601E+00    | 8.403E-09 | 1.944E+05                   |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.6607E+00    | 2.469E-09 | 5.613E+04                   | 7.6287E+00    | 2.210E-09 | 5.023E+04                   |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 7.6636E+00    | 2.816E-08 | 6.396E+05                   | 7.6317E+00    | 2.809E-08 | 6.380E+05                   |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.5646E+01    | 1.343E-12 | 7.317E+00                   |               |           |                             |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6281E+01    | 1.459E-09 | 7.342E+03                   | 1.6215E+01    | 1.357E-09 | 6.831E+03                   |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6288E+01    | 1.195E-08 | 6.009E+04                   | 1.6221E+01    | 1.215E-08 | 6.108E+04                   |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6451E+01    | 1.339E-09 | 6.601E+03                   | 1.6383E+01    | 1.137E-09 | 5.606E+03                   |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6458E+01    | 1.394E-08 | 6.865E+04                   | 1.6390E+01    | 1.385E-08 | 6.820E+04                   |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7d <sup>1</sup> D <sub>2</sub>              | 1.6541E+01    | 8.041E-17 | 3.921E-04                   |               |           |                             |

(continued on next page)

Table 5 (continued)

| Lower   | Upper   | GRASP2K       |           |                        | FAC           |           |                        |
|---|---|---------------|-----------|------------------------|---------------|-----------|------------------------|
|   |   | $\lambda$ (Å) | $gf$      | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | $gf$      | $A$ (s <sup>-1</sup> ) |
| 1s6s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>1</sup> D <sub>2</sub>              | 4.0526E+01    | 1.824E-12 | 1.481E+00              |               |           |                        |
| 1s6d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>1</sup> D <sub>2</sub>              | 4.3033E+01    | 2.664E-09 | 1.919E+03              | 4.2873E+01    | 2.435E-09 | 1.752E+03              |
| 1s6d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>1</sup> D <sub>2</sub>              | 4.3059E+01    | 2.187E-08 | 1.574E+04              | 4.2867E+01    | 2.224E-08 | 1.601E+04              |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>1</sup> D <sub>2</sub>              | 4.3721E+01    | 7.782E-10 | 5.431E+02              | 4.3553E+01    | 5.898E-10 | 4.112E+02              |
| 1s6d <sup>1</sup> D <sub>2</sub>              | 1s7d <sup>1</sup> D <sub>2</sub>              | 4.3751E+01    | 6.584E-09 | 4.589E+03              | 4.3564E+01    | 6.539E-09 | 4.558E+03              |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7d <sup>1</sup> D <sub>2</sub>              | 4.4092E+01    | 1.366E-13 | 9.376E-02              |               |           |                        |
| 1s7s <sup>3</sup> S <sub>1</sub>              | 1s7d <sup>1</sup> D <sub>2</sub>              | 8.7478E+02    | 2.312E-11 | 4.030E-02              |               |           |                        |
| 1s7d <sup>3</sup> D <sub>2</sub>              | 1s7d <sup>1</sup> D <sub>2</sub>              | 4.1666E+03    | 1.940E-07 | 1.491E+01              | 4.2946E+03    | 1.876E-07 | 1.345E+01              |
| 1s7d <sup>3</sup> D <sub>1</sub>              | 1s7d <sup>1</sup> D <sub>2</sub>              | 4.3244E+03    | 1.655E-06 | 1.180E+02              | 4.2545E+03    | 1.654E-06 | 1.208E+02              |
| 1s7d <sup>3</sup> D <sub>3</sub>              | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.0098E+05    | 5.515E-08 | 7.215E-03              |               |           |                        |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 7.6554E+00    | 1.719E-09 | 2.174E+04              | 7.6229E+00    | 1.729E-09 | 2.187E+04              |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 7.6914E+00    | 3.672E-08 | 4.601E+05              | 7.6587E+00    | 4.082E-08 | 5.114E+05              |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 7.6926E+00    | 2.148E-09 | 2.690E+04              | 7.6598E+00    | 1.172E-09 | 1.468E+04              |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6424E+01    | 4.060E-09 | 1.116E+04              | 1.6354E+01    | 4.039E-09 | 1.109E+04              |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6509E+01    | 2.875E-08 | 7.819E+04              | 1.6439E+01    | 3.085E-08 | 8.390E+04              |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.6512E+01    | 1.249E-09 | 3.394E+03              | 1.6441E+01    | 8.891E-10 | 2.417E+03              |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.3526E+01    | 9.513E-09 | 3.722E+03              | 4.3345E+01    | 9.476E-09 | 3.706E+03              |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.3873E+01    | 1.853E-08 | 7.134E+03              | 4.3688E+01    | 1.782E-08 | 6.863E+03              |
| 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.3884E+01    | 2.962E-10 | 1.140E+02              | 4.3689E+01    | 5.068E-10 | 1.951E+02              |
| 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.4083E+01    | 8.911E-15 | 3.399E-03              |               |           |                        |
| 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.4089E+01    | 6.179E-16 | 2.356E-04              |               |           |                        |
| 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.4228E+01    | 2.315E-17 | 8.771E-06              |               |           |                        |
| 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 8.7508E+03    | 1.774E-06 | 1.717E+01              | 8.7713E+03    | 1.769E-06 | 1.690E+01              |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 3.5600E+00    | 3.651E-09 | 2.135E+05              | 3.5449E+00    | 3.702E-09 | 2.164E+05              |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 7.6543E+00    | 2.963E-11 | 3.748E+02              | 7.6223E+00    | 2.880E-11 | 3.642E+02              |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 1.6421E+01    | 2.342E-10 | 6.438E+02              | 1.6353E+01    | 2.341E-10 | 6.434E+02              |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 1.6509E+01    | 1.147E-08 | 3.119E+04              | 1.6439E+01    | 1.146E-08 | 3.116E+04              |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 1.6511E+01    | 2.735E-10 | 7.434E+02              | 1.6441E+01    | 3.276E-10 | 8.906E+02              |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 1.6560E+01    | 3.529E-09 | 9.536E+03              | 1.6490E+01    | 3.511E-09 | 9.489E+03              |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 1.6562E+01    | 8.238E-11 | 2.226E+02              | 1.6491E+01    | 8.350E-11 | 2.256E+02              |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 4.3514E+01    | 1.318E-10 | 5.160E+01              | 4.3345E+01    | 1.315E-10 | 5.144E+01              |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 4.3873E+01    | 1.072E-08 | 4.127E+03              | 4.3688E+01    | 1.069E-08 | 4.117E+03              |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 4.3882E+01    | 2.236E-10 | 8.608E+01              | 4.3688E+01    | 3.056E-10 | 1.176E+02              |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 4.4082E+01    | 7.394E-09 | 2.820E+03              | 4.3896E+01    | 7.356E-09 | 2.805E+03              |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 4.4089E+01    | 1.748E-10 | 6.664E+01              | 4.3896E+01    | 1.672E-10 | 6.377E+01              |
| 1s7d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>4</sub>              | 8.4183E+03    | 1.604E-13 | 1.677E-06              | 8.7854E+03    | 1.162E-13 | 1.106E-06              |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 3.5233E+00    | 2.179E-13 | 1.673E+01              |               |           |                        |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 3.5600E+00    | 1.630E-10 | 1.225E+04              | 3.5449E+00    | 1.371E-10 | 1.030E+04              |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 3.5614E+00    | 2.777E-09 | 2.086E+05              | 3.5464E+00    | 2.747E-09 | 2.064E+05              |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 7.5824E+00    | 3.207E-16 | 5.316E-03              |               |           |                        |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 7.6541E+00    | 9.324E-13 | 1.517E+01              | 7.6223E+00    | 1.066E-12 | 1.734E+01              |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 7.6571E+00    | 2.102E-11 | 3.417E+02              | 7.6253E+00    | 2.121E-11 | 3.447E+02              |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6252E+01    | 1.814E-14 | 6.543E-02              |               |           |                        |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6420E+01    | 9.558E-12 | 3.378E+01              | 1.6353E+01    | 8.684E-12 | 3.068E+01              |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6428E+01    | 1.752E-10 | 6.185E+02              | 1.6361E+01    | 1.734E-10 | 6.122E+02              |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6509E+01    | 3.892E-10 | 1.361E+03              | 1.6439E+01    | 3.312E-10 | 1.158E+03              |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6511E+01    | 8.849E-09 | 3.093E+04              | 1.6441E+01    | 8.844E-09 | 3.091E+04              |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6561E+01    | 2.778E-09 | 9.652E+03              | 1.6491E+01    | 2.789E-09 | 9.690E+03              |
| 1s6d <sup>3</sup> D <sub>2</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.2827E+01    | 1.476E-14 | 7.669E-03              |               |           |                        |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.3508E+01    | 5.636E-12 | 2.837E+00              | 4.3345E+01    | 4.871E-12 | 2.449E+00              |
| 1s6d <sup>1</sup> D <sub>2</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.3538E+01    | 9.946E-11 | 5.000E+01              | 4.3356E+01    | 9.747E-11 | 4.899E+01              |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.3868E+01    | 4.042E-10 | 2.002E+02              | 4.3688E+01    | 3.055E-10 | 1.512E+02              |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.3876E+01    | 8.273E-09 | 4.095E+03              | 4.3688E+01    | 8.251E-09 | 4.084E+03              |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.4084E+01    | 5.822E-09 | 2.855E+03              | 4.3896E+01    | 5.851E-09 | 2.869E+03              |
| 1s7d <sup>3</sup> D <sub>2</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 2.8438E+03    | 4.640E-15 | 5.467E-07              | 2.9148E+03    | 3.797E-17 | 4.222E-09              |
| 1s7d <sup>3</sup> D <sub>3</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 8.2277E+03    | 3.480E-15 | 4.899E-08              | 8.7854E+03    | 4.304E-15 | 5.269E-08              |
| 1s7d <sup>1</sup> D <sub>2</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 8.9575E+03    | 6.963E-14 | 8.269E-07              | 9.0724E+03    | 8.336E-14 | 9.568E-07              |
| 1s7g <sup>3</sup> G <sub>4</sub>              | 1s7g <sup>3</sup> G <sub>3</sub>              | 3.6344E+05    | 4.407E-08 | 3.179E-04              |               |           |                        |
| 1s2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.3940E+00    | 4.032E-13 | 1.977E+02              | 1.3881E+00    | 2.999E-15 | 1.470E+00              |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.5149E+00    | 1.959E-14 | 1.511E+00              | 3.5002E+00    | 1.688E-16 | 1.302E-02              |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.5662E+00    | 4.169E-14 | 6.939E-01              |               |           |                        |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.6552E+00    | 8.991E-11 | 1.462E+03              | 7.6229E+00    | 7.186E-11 | 1.168E+03              |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.6567E+00    | 1.318E-09 | 2.141E+04              | 7.6244E+00    | 1.283E-09 | 2.086E+04              |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.6912E+00    | 2.427E-09 | 3.910E+04              | 7.6586E+00    | 1.170E-09 | 1.884E+04              |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.6923E+00    | 3.464E-08 | 5.579E+05              | 7.6598E+00    | 3.148E-08 | 5.069E+05              |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6214E+01    | 4.380E-14 | 1.588E-01              |               |           |                        |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6423E+01    | 1.913E-10 | 6.757E+02              | 1.6354E+01    | 1.592E-10 | 5.624E+02              |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6427E+01    | 3.067E-09 | 1.083E+04              | 1.6358E+01    | 2.994E-09 | 1.057E+04              |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6508E+01    | 1.547E-09 | 5.408E+03              | 1.6439E+01    | 8.855E-10 | 3.096E+03              |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6511E+01    | 2.526E-08 | 8.829E+04              | 1.6441E+01    | 2.379E-08 | 8.315E+04              |
| 1s6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.2675E+01    | 5.245E-14 | 2.744E-02              |               |           |                        |

(continued on next page)

Table 5 (continued)

| Lower  | Upper  | GRASP2K       |           |                             | FAC           |           |                             |
|--|--|---------------|-----------|-----------------------------|---------------|-----------|-----------------------------|
|  |  | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3519E+01    | 4.115E-10 | 2.070E+02                   | 4.3345E+01    | 3.501E-10 | 1.760E+02                   |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3534E+01    | 7.076E-09 | 3.558E+03                   | 4.3345E+01    | 7.015E-09 | 3.528E+03                   |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3866E+01    | 5.137E-10 | 2.544E+02                   | 4.3688E+01    | 5.131E-10 | 2.540E+02                   |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3877E+01    | 1.345E-08 | 6.659E+03                   | 4.3688E+01    | 1.375E-08 | 6.807E+03                   |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.4082E+01    | 3.010E-15 | 1.476E-03                   |               |           |                             |
| 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.4995E+03    | 1.402E-12 | 2.139E-04                   |               |           |                             |
| 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 8.4824E+03    | 6.791E-08 | 8.993E-01                   | 8.7645E+03    | 6.556E-08 | 8.063E-01                   |
| 1s 7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 8.8420E+03    | 1.310E-06 | 1.597E+01                   | 8.7598E+03    | 1.309E-06 | 1.612E+01                   |
| 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.7665E+05    | 3.244E-08 | 4.039E-04                   |               |           |                             |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 1.6491E+01    | 7.591E-10 | 1.693E+03                   | 1.6420E+01    | 7.556E-10 | 1.685E+03                   |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 1.6542E+01    | 2.746E-08 | 6.085E+04                   | 1.6471E+01    | 2.743E-08 | 6.079E+04                   |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 1.6543E+01    | 4.584E-10 | 1.016E+03                   | 1.6473E+01    | 5.103E-10 | 1.130E+03                   |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 4.3743E+01    | 3.029E-09 | 9.600E+02                   | 4.3559E+01    | 3.023E-09 | 9.580E+02                   |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 4.3950E+01    | 2.568E-08 | 8.060E+03                   | 4.3765E+01    | 2.559E-08 | 8.033E+03                   |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 4.3957E+01    | 3.996E-10 | 1.254E+02                   | 4.3765E+01    | 4.739E-10 | 1.487E+02                   |
| 1s 7g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>3</sup> G <sub>5</sub>              | 1.4677E+04    | 1.341E-06 | 3.774E+00                   | 1.4692E+04    | 1.337E-06 | 3.726E+00                   |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 7.6874E+00    | 1.958E-09 | 2.009E+04                   | 7.6547E+00    | 1.933E-09 | 1.984E+04                   |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.6491E+01    | 2.258E-11 | 5.035E+01                   | 1.6420E+01    | 2.098E-11 | 4.678E+01                   |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.3742E+01    | 2.390E-10 | 7.574E+01                   | 4.3559E+01    | 2.347E-10 | 7.437E+01                   |
| 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.3951E+01    | 1.167E-08 | 3.663E+03                   | 4.3765E+01    | 1.215E-08 | 3.814E+03                   |
| 1s 6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.3956E+01    | 2.729E-10 | 8.564E+01                   | 4.3765E+01    | 2.250E-10 | 7.063E+01                   |
| 1s 6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.4090E+01    | 2.985E-09 | 9.311E+02                   | 4.3903E+01    | 2.974E-09 | 9.277E+02                   |
| 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 4.4094E+01    | 4.732E-11 | 1.476E+01                   | 4.3903E+01    | 4.575E-11 | 1.427E+01                   |
| 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1.4614E+04    | 3.511E-14 | 9.969E-08                   | 1.4763E+04    | 3.624E-14 | 1.000E-07                   |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 7.6513E+00    | 4.508E-15 | 5.707E-02                   |               |           |                             |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 7.6873E+00    | 5.158E-11 | 6.470E+02                   | 7.6547E+00    | 4.394E-11 | 5.511E+02                   |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 7.6884E+00    | 1.583E-09 | 1.985E+04                   | 7.6558E+00    | 1.539E-09 | 1.929E+04                   |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6405E+01    | 8.772E-18 | 2.416E-05                   |               |           |                             |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6490E+01    | 5.160E-13 | 1.406E+00                   | 1.6420E+01    | 4.768E-13 | 1.299E+00                   |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.6493E+01    | 1.767E-11 | 4.816E+01                   | 1.6423E+01    | 1.666E-11 | 4.540E+01                   |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.3394E+01    | 6.981E-16 | 2.748E-04                   |               |           |                             |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.3738E+01    | 6.216E-12 | 2.408E+00                   | 4.3559E+01    | 5.334E-12 | 2.065E+00                   |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.3749E+01    | 1.922E-10 | 7.442E+01                   | 4.3560E+01    | 1.866E-10 | 7.230E+01                   |
| 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.3947E+01    | 3.798E-10 | 1.458E+02                   | 4.3765E+01    | 2.250E-10 | 8.632E+01                   |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.3953E+01    | 1.029E-08 | 3.949E+03                   | 4.3765E+01    | 9.900E-09 | 3.798E+03                   |
| 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 4.4091E+01    | 2.459E-09 | 9.374E+02                   | 4.3903E+01    | 2.470E-09 | 9.420E+02                   |
| 1s 7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 5.4206E+03    | 1.109E-18 | 2.798E-11                   |               |           |                             |
| 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.4244E+04    | 7.671E-16 | 2.802E-09                   | 1.4763E+04    | 8.238E-16 | 2.777E-09                   |
| 1s 7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1.5017E+04    | 2.719E-14 | 8.935E-08                   | 1.4782E+04    | 2.879E-14 | 9.684E-08                   |
| 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 5.6215E+05    | 3.438E-08 | 8.064E-05                   |               |           |                             |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 3.5591E+00    | 4.551E-14 | 2.663E+00                   | 3.5441E+00    | 5.680E-19 | 3.323E-05                   |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 7.6502E+00    | 1.289E-15 | 1.633E-02                   | 7.6183E+00    | 4.456E-21 | 5.642E-08                   |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 1.6402E+01    | 6.373E-16 | 1.756E-03                   |               |           |                             |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 1.6490E+01    | 1.984E-11 | 5.409E+01                   | 1.6420E+01    | 1.967E-11 | 5.362E+01                   |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 1.6492E+01    | 5.980E-10 | 1.629E+03                   | 1.6423E+01    | 6.027E-10 | 1.642E+03                   |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 1.6541E+01    | 5.583E-10 | 1.512E+03                   | 1.6471E+01    | 5.080E-10 | 1.376E+03                   |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 1.6543E+01    | 2.237E-08 | 6.059E+04                   | 1.6473E+01    | 2.234E-08 | 6.052E+04                   |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 4.3381E+01    | 1.570E-15 | 6.182E-04                   |               |           |                             |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 4.3738E+01    | 7.608E-11 | 2.948E+01                   | 4.3559E+01    | 6.873E-11 | 2.662E+01                   |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 4.3747E+01    | 2.385E-09 | 9.236E+02                   | 4.3559E+01    | 2.405E-09 | 9.314E+02                   |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 4.3946E+01    | 5.553E-10 | 2.131E+02                   | 4.3765E+01    | 4.739E-10 | 1.818E+02                   |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 4.3953E+01    | 2.093E-08 | 8.029E+03                   | 4.3765E+01    | 2.085E-08 | 8.000E+03                   |
| 1s 7d <sup>3</sup> D <sub>3</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 5.2883E+03    | 3.941E-15 | 1.044E-07                   |               |           |                             |
| 1s 7g <sup>3</sup> G <sub>4</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 1.4223E+04    | 3.145E-08 | 1.152E-01                   | 1.4691E+04    | 3.040E-08 | 1.035E-01                   |
| 1s 7g <sup>3</sup> G <sub>3</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 1.4802E+04    | 1.065E-06 | 3.602E+00                   | 1.4691E+04    | 1.064E-06 | 3.623E+00                   |
| 1s 7g <sup>3</sup> G <sub>5</sub>              | 1s 7g <sup>1</sup> G <sub>4</sub>              | 4.5954E+05    | 2.680E-08 | 9.406E-05                   |               |           |                             |
| 1s 6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 4.3863E+01    | 8.357E-10 | 2.229E+02                   | 4.3678E+01    | 8.370E-10 | 2.232E+02                   |
| 1s 6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 4.4002E+01    | 2.409E-08 | 6.384E+03                   | 4.3816E+01    | 2.482E-08 | 6.577E+03                   |
| 1s 6h <sup>1</sup> H <sub>6</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 4.4006E+01    | 4.069E-10 | 1.078E+02                   | 4.3816E+01    | 3.223E-10 | 8.541E+01                   |
| 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 2.2090E+04    | 1.077E-06 | 1.133E+00                   | 2.2109E+04    | 1.074E-06 | 1.118E+00                   |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>3</sup> I <sub>6</sub>              | 1.6529E+01    | 9.680E-10 | 1.818E+03                   | 1.6459E+01    | 9.718E-10 | 1.825E+03                   |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>3</sup> I <sub>6</sub>              | 4.3863E+01    | 2.601E-10 | 6.937E+01                   | 4.3678E+01    | 2.590E-10 | 6.907E+01                   |
| 1s 7g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>3</sup> I <sub>6</sub>              | 2.2046E+04    | 8.252E-15 | 8.712E-09                   | 2.2108E+04    | 8.218E-15 | 8.555E-09                   |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 1.6478E+01    | 2.959E-15 | 6.609E-03                   |               |           |                             |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 1.6529E+01    | 1.752E-11 | 3.888E+01                   | 1.6459E+01    | 1.495E-11 | 3.318E+01                   |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 1.6531E+01    | 8.153E-10 | 1.809E+03                   | 1.6460E+01    | 8.077E-10 | 1.792E+03                   |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 4.3654E+01    | 1.569E-16 | 4.993E-05                   |               |           |                             |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 4.3861E+01    | 4.500E-12 | 1.418E+00                   | 4.3678E+01    | 3.985E-12 | 1.255E+00                   |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 4.3867E+01    | 2.181E-10 | 6.873E+01                   | 4.3678E+01    | 2.152E-10 | 6.782E+01                   |
| 1s 7g <sup>3</sup> G <sub>4</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 8.7156E+03    | 3.038E-20 | 2.425E-13                   |               |           |                             |
| 1s 7g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 2.1457E+04    | 1.337E-16 | 1.761E-10                   | 2.2108E+04    | 1.264E-16 | 1.555E-10                   |

(continued on next page)

Table 5 (continued)

| Lower  | Upper  | GRASP2K       |           |                        | FAC           |           |                        |
|--|--|---------------|-----------|------------------------|---------------|-----------|------------------------|
|  |  | $\lambda$ (Å) | $gf$      | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | $gf$      | $A$ (s <sup>-1</sup> ) |
| 1s 7g <sup>1</sup> G <sub>4</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 2.2508E+04    | 6.722E-15 | 8.045E-09              | 2.2108E+04    | 6.827E-15 | 8.399E-09              |
| 1s 7i <sup>3</sup> I <sub>6</sub>              | 1s 7i <sup>3</sup> I <sub>5</sub>              | 8.0263E+05    | 2.820E-08 | 2.655E-05              |               |           |                        |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 7.6846E+00    | 1.967E-14 | 2.020E-01              |               |           |                        |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.6478E+01    | 2.893E-16 | 6.462E-04              |               |           |                        |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3652E+01    | 9.188E-16 | 2.924E-04              |               |           |                        |
| 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3860E+01    | 1.459E-11 | 4.600E+00              | 4.3678E+01    | 1.287E-11 | 4.058E+00              |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3866E+01    | 6.893E-10 | 2.172E+02              | 4.3678E+01    | 6.953E-10 | 2.191E+02              |
| 1s 6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3999E+01    | 5.006E-10 | 1.568E+02              | 4.3816E+01    | 3.223E-10 | 1.009E+02              |
| 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.4004E+01    | 2.163E-08 | 6.773E+03              | 4.3816E+01    | 2.095E-08 | 6.561E+03              |
| 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 8.6829E+03    | 2.049E-19 | 1.648E-12              |               |           |                        |
| 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.1394E+04    | 1.710E-08 | 2.266E-02              | 2.2109E+04    | 1.653E-08 | 2.033E-02              |
| 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.2240E+04    | 8.940E-07 | 1.096E+00              | 2.2109E+04    | 8.927E-07 | 1.098E+00              |
| 1s 7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 6.7907E+05    | 2.293E-08 | 3.015E-05              |               |           |                        |
| 1s 7i <sup>3</sup> I <sub>6</sub>              | 1s 7i <sup>3</sup> I <sub>7</sub>              | 3.1014E+04    | 8.994E-07 | 4.158E-01              | 3.1015E+04    | 8.974E-07 | 4.113E-01              |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 1.6520E+01    | 6.150E-15 | 1.156E-02              |               |           |                        |
| 1s 6g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 4.3799E+01    | 5.374E-16 | 1.437E-04              |               |           |                        |
| 1s 7g <sup>3</sup> G <sub>5</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 1.2712E+04    | 7.915E-21 | 2.513E-14              |               |           |                        |
| 1s 7i <sup>3</sup> I <sub>6</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 3.0023E+04    | 1.031E-08 | 5.869E-03              | 3.1015E+04    | 9.971E-09 | 5.273E-03              |
| 1s 7i <sup>3</sup> I <sub>5</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 3.1190E+04    | 7.687E-07 | 4.055E-01              | 3.1015E+04    | 7.678E-07 | 4.060E-01              |
| 1s 7i <sup>3</sup> I <sub>7</sub>              | 1s 7i <sup>1</sup> I <sub>6</sub>              | 9.4020E+05    | 2.004E-08 | 1.163E-05              |               |           |                        |

Table 6

Magnetic quadrupole transitions  $M2$  calculated with GRASP2K and FAC for all  $n = 1-7$  configurations. For the GRASP2K calculation, the active set is expanded to  $n = 10$  (GRASP3) and only the length form is considered. A comparison between the wavelengths, weighted oscillator strengths and transition probabilities is given.

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |           |                  |
|-----------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                 |                 | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 2s $^3S_1$   | 1s 2p $^3P_0^o$ | 1.6053E+02    | 1.033E-13 | 8.911E-03        | 1.5824E+02    | 1.235E-13 | 1.087E-02        |
| 1s 2s $^1S_0$   | 1s 2p $^3P_2^o$ | 4.0520E-01    | 3.150E-04 | 2.559E+12        | 4.0356E-01    | 3.398E-04 | 2.760E+12        |
| 1s 2s $^3S_1$   | 1s 2p $^3P_2^o$ | 2.6617E+01    | 1.588E-08 | 2.990E+04        | 2.6489E+01    | 1.614E-08 | 3.043E+04        |
| 1s 2s $^1S_0$   | 1s 2p $^3P_2^o$ | 3.2564E+01    | 5.805E-09 | 7.303E+03        | 3.2508E+01    | 5.823E-09 | 7.289E+03        |
| 1s 2s $^3S_1$   | 1s 2p $^1P_1^o$ | 2.4759E+01    | 1.985E-08 | 7.200E+04        | 2.4615E+01    | 2.008E-08 | 7.308E+04        |
| 1s 2p $^3P_1^o$ | 1s 3s $^3S_1$   | 2.2065E+00    | 1.514E-09 | 6.915E+05        | 2.1974E+00    | 2.462E-09 | 1.124E+06        |
| 1s 2p $^3P_2^o$ | 1s 3s $^3S_1$   | 2.3705E+00    | 1.311E-06 | 5.189E+08        | 2.3604E+00    | 1.277E-06 | 5.054E+08        |
| 1s 2p $^1P_1^o$ | 1s 3s $^3S_1$   | 2.3864E+00    | 1.336E-06 | 5.217E+08        | 2.3765E+00    | 1.249E-06 | 4.877E+08        |
| 1s 2s $^3S_1$   | 1s 3p $^3P_0^o$ | 2.1686E+00    | 1.372E-08 | 6.484E+06        | 2.1593E+00    | 1.146E-08 | 5.418E+06        |
| 1s 3s $^3S_1$   | 1s 3p $^3P_0^o$ | 5.8954E+02    | 1.165E-14 | 7.452E-05        | 5.8484E+02    | 1.282E-14 | 8.264E-05        |
| 1s 2p $^3P_2^o$ | 1s 3s $^1S_0$   | 2.3603E+00    | 8.223E-07 | 9.845E+08        | 2.3502E+00    | 8.627E-07 | 1.032E+09        |
| 1s 2s $^1S_0$   | 1s 3p $^3P_2^o$ | 3.4470E-01    | 8.419E-05 | 9.448E+11        | 3.4333E-01    | 9.334E-05 | 1.047E+12        |
| 1s 2s $^3S_1$   | 1s 3p $^3P_2^o$ | 2.1256E+00    | 8.321E-06 | 2.457E+09        | 2.1165E+00    | 8.544E-06 | 2.522E+09        |
| 1s 2s $^1S_0$   | 1s 3p $^3P_2^o$ | 2.1571E+00    | 5.628E-06 | 1.614E+09        | 2.1483E+00    | 5.447E-06 | 1.561E+09        |
| 1s 3s $^3S_1$   | 1s 3p $^3P_2^o$ | 9.0741E+01    | 2.451E-09 | 3.972E+02        | 9.0375E+01    | 2.466E-09 | 3.995E+02        |
| 1s 3s $^1S_0$   | 1s 3p $^3P_2^o$ | 1.0861E+02    | 9.552E-10 | 1.080E+02        | 1.0840E+02    | 9.529E-10 | 1.072E+02        |
| 1s 2p $^3P_0^o$ | 1s 3d $^3D_2$   | 2.1510E+00    | 8.811E-07 | 2.541E+08        | 2.1422E+00    | 9.246E-07 | 2.665E+08        |
| 1s 2p $^3P_1^o$ | 1s 3d $^3D_2$   | 2.1533E+00    | 5.689E-07 | 1.637E+08        | 2.1443E+00    | 5.905E-07 | 1.698E+08        |
| 1s 2p $^3P_2^o$ | 1s 3d $^3D_2$   | 2.3065E+00    | 1.618E-10 | 4.057E+04        | 2.2968E+00    | 2.186E-10 | 5.482E+04        |
| 1s 2p $^1P_1^o$ | 1s 3d $^3D_2$   | 2.3216E+00    | 2.587E-10 | 6.403E+04        |               |           |                  |
| 1s 3p $^3P_0^o$ | 1s 3d $^3D_2$   | 1.0002E+02    | 4.701E-11 | 6.269E+00        | 9.9770E+01    | 4.770E-11 | 6.338E+00        |
| 1s 3p $^3P_1^o$ | 1s 3d $^3D_2$   | 1.0130E+02    | 2.911E-11 | 3.784E+00        | 1.0100E+02    | 2.943E-11 | 3.815E+00        |
| 1s 3p $^3P_2^o$ | 1s 3d $^3D_2$   | 1.4830E+03    | 2.920E-18 | 1.771E-09        |               |           |                  |
| 1s 2p $^3P_0^o$ | 1s 3d $^3D_1$   | 2.1505E+00    | 8.705E-07 | 4.185E+08        | 2.1416E+00    | 9.091E-07 | 4.370E+08        |
| 1s 2p $^3P_2^o$ | 1s 3d $^3D_1$   | 2.3059E+00    | 6.634E-13 | 2.774E+02        |               |           |                  |
| 1s 2p $^1P_1^o$ | 1s 3d $^3D_1$   | 2.3210E+00    | 1.204E-09 | 4.968E+05        | 2.3114E+00    | 1.079E-09 | 4.453E+05        |
| 1s 3p $^3P_0^o$ | 1s 3d $^3D_1$   | 9.8828E+01    | 4.804E-11 | 1.094E+01        | 9.8590E+01    | 4.859E-11 | 1.102E+01        |
| 1s 3p $^3P_1^o$ | 1s 3d $^3D_1$   | 1.2588E+03    | 1.549E-18 | 2.174E-09        |               |           |                  |
| 1s 2s $^3S_1$   | 1s 3p $^1P_1^o$ | 2.1220E+00    | 8.175E-06 | 4.037E+09        | 2.1129E+00    | 8.576E-06 | 4.234E+09        |
| 1s 3s $^3S_1$   | 1s 3p $^1P_1^o$ | 8.4608E+01    | 3.031E-09 | 9.414E+02        | 8.4198E+01    | 3.046E-09 | 9.473E+02        |
| 1s 3d $^3D_2$   | 1s 3p $^1P_1^o$ | 8.0349E+03    | 2.086E-20 | 7.185E-13        |               |           |                  |
| 1s 3d $^3D_1$   | 1s 3p $^1P_1^o$ | 2.2947E+05    | 3.151E-24 | 1.331E-19        |               |           |                  |
| 1s 2p $^3P_1^o$ | 1s 3d $^3D_3$   | 2.1376E+00    | 1.374E-05 | 2.865E+09        | 2.1288E+00    | 1.394E-05 | 2.907E+09        |
| 1s 2p $^3P_2^o$ | 1s 3d $^3D_3$   | 2.2910E+00    | 6.490E-05 | 1.178E+10        | 2.2814E+00    | 6.717E-05 | 1.219E+10        |
| 1s 2p $^1P_1^o$ | 1s 3d $^3D_3$   | 2.3059E+00    | 1.173E-05 | 2.101E+09        | 2.2965E+00    | 1.190E-05 | 2.133E+09        |
| 1s 3p $^3P_0^o$ | 1s 3d $^3D_3$   | 7.7367E+01    | 1.611E-09 | 2.565E+02        | 7.7185E+01    | 1.597E-09 | 2.533E+02        |
| 1s 3p $^3P_1^o$ | 1s 3d $^3D_3$   | 2.7769E+02    | 1.724E-10 | 2.130E+00        | 2.7772E+02    | 1.707E-10 | 2.091E+00        |
| 1s 3p $^1P_1^o$ | 1s 3d $^3D_3$   | 3.5684E+02    | 1.466E-11 | 1.097E-01        | 3.5856E+02    | 1.436E-11 | 1.055E-01        |
| 1s 2p $^3P_0^o$ | 1s 3d $^1D_2$   | 2.1371E+00    | 5.299E-06 | 1.548E+09        | 2.1283E+00    | 5.541E-06 | 1.618E+09        |
| 1s 2p $^3P_2^o$ | 1s 3d $^1D_2$   | 2.1393E+00    | 6.338E-06 | 1.847E+09        | 2.1304E+00    | 6.476E-06 | 1.887E+09        |
| 1s 2p $^1P_1^o$ | 1s 3d $^1D_2$   | 2.2905E+00    | 1.624E-05 | 4.129E+09        | 2.2809E+00    | 1.680E-05 | 4.273E+09        |
| 1s 2p $^3P_1^o$ | 1s 3d $^1D_2$   | 2.3053E+00    | 3.662E-05 | 9.192E+09        | 2.2959E+00    | 3.746E-05 | 9.401E+09        |
| 1s 3p $^3P_0^o$ | 1s 3d $^1D_2$   | 7.6708E+01    | 6.269E-10 | 1.421E+02        | 7.6517E+01    | 6.228E-10 | 1.407E+02        |
| 1s 3p $^3P_1^o$ | 1s 3d $^1D_2$   | 7.7462E+01    | 7.386E-10 | 1.642E+02        | 7.7242E+01    | 7.336E-10 | 1.626E+02        |
| 1s 3p $^3P_2^o$ | 1s 3d $^1D_2$   | 2.6938E+02    | 4.725E-11 | 8.687E-01        | 2.6926E+02    | 4.683E-11 | 8.544E-01        |
| 1s 3p $^1P_1^o$ | 1s 3d $^1D_2$   | 3.4323E+02    | 5.187E-11 | 5.874E-01        | 3.4458E+02    | 5.080E-11 | 5.659E-01        |
| 1s 2p $^3P_1^o$ | 1s 4s $^3S_1$   | 1.6341E+00    | 6.171E-10 | 5.138E+05        | 1.6274E+00    | 9.120E-10 | 7.592E+05        |
| 1s 2p $^3P_2^o$ | 1s 4s $^3S_1$   | 1.7223E+00    | 5.190E-07 | 3.890E+08        | 1.7151E+00    | 5.041E-07 | 3.778E+08        |
| 1s 2p $^1P_1^o$ | 1s 4s $^3S_1$   | 1.7308E+00    | 5.278E-07 | 3.918E+08        | 1.7236E+00    | 4.959E-07 | 3.680E+08        |
| 1s 3p $^3P_0^o$ | 1s 4s $^3S_1$   | 6.3675E+00    | 3.701E-10 | 2.029E+04        | 6.3413E+00    | 5.844E-10 | 3.204E+04        |
| 1s 3p $^3P_2^o$ | 1s 4s $^3S_1$   | 6.7695E+00    | 3.592E-07 | 1.743E+07        | 6.7412E+00    | 3.541E-07 | 1.718E+07        |
| 1s 3p $^1P_1^o$ | 1s 4s $^3S_1$   | 6.8063E+00    | 3.654E-07 | 1.754E+07        | 6.7783E+00    | 3.479E-07 | 1.669E+07        |
| 1s 2s $^3S_1$   | 1s 4p $^3P_1^o$ | 1.6159E+00    | 5.547E-09 | 4.724E+06        | 1.6090E+00    | 5.114E-09 | 4.355E+06        |
| 1s 3s $^3S_1$   | 1s 4p $^3P_1^o$ | 6.2721E+00    | 1.725E-09 | 9.747E+04        | 6.2463E+00    | 1.366E-09 | 7.720E+04        |
| 1s 3d $^3D_2$   | 1s 4p $^3P_1^o$ | 6.7686E+00    | 4.387E-09 | 2.129E+05        | 6.7403E+00    | 4.352E-09 | 2.111E+05        |
| 1s 3d $^3D_1$   | 1s 4p $^3P_1^o$ | 6.7741E+00    | 4.345E-09 | 2.105E+05        | 6.7458E+00    | 4.267E-09 | 2.067E+05        |
| 1s 3d $^3D_3$   | 1s 4p $^3P_1^o$ | 6.9054E+00    | 7.364E-08 | 3.434E+06        | 6.8762E+00    | 7.351E-08 | 3.427E+06        |
| 1s 3d $^1D_2$   | 1s 4p $^3P_1^o$ | 6.9107E+00    | 2.786E-08 | 1.297E+06        | 6.8816E+00    | 2.620E-08 | 1.219E+06        |
| 1s 4s $^3S_1$   | 1s 4p $^3P_1^o$ | 1.4439E+03    | 2.589E-15 | 2.761E-06        | 1.4544E+03    | 2.665E-15 | 2.778E-06        |
| 1s 2p $^3P_2^o$ | 1s 4s $^1S_0$   | 1.7202E+00    | 3.276E-07 | 7.385E+08        | 1.7129E+00    | 3.373E-07 | 7.604E+08        |
| 1s 3p $^3P_2^o$ | 1s 4s $^1S_0$   | 6.7361E+00    | 2.278E-07 | 3.349E+07        | 6.7077E+00    | 2.396E-07 | 3.523E+07        |
| 1s 3d $^3D_2$   | 1s 4p $^3P_0^o$ | 6.7663E+00    | 2.811E-09 | 4.096E+05        | 6.7381E+00    | 2.782E-09 | 4.052E+05        |
| 1s 3d $^1D_2$   | 1s 4p $^3P_0^o$ | 6.9083E+00    | 3.383E-08 | 4.728E+06        | 6.8793E+00    | 3.327E-08 | 4.650E+06        |
| 1s 2s $^1S_0$   | 1s 4p $^3P_2^o$ | 3.2750E-01    | 3.417E-05 | 4.249E+11        | 3.2620E-01    | 3.824E-05 | 4.754E+11        |
| 1s 2s $^3S_1$   | 1s 4p $^3P_2^o$ | 1.6057E+00    | 3.719E-06 | 1.924E+09        | 1.5989E+00    | 3.831E-06 | 1.982E+09        |
| 1s 2s $^1S_0$   | 1s 4p $^3P_2^o$ | 1.6236E+00    | 2.491E-06 | 1.261E+09        | 1.6170E+00    | 2.469E-06 | 1.249E+09        |
| 1s 3s $^3S_1$   | 1s 4p $^3P_2^o$ | 6.1216E+00    | 1.070E-06 | 3.810E+07        | 6.0965E+00    | 1.086E-06 | 3.865E+07        |
| 1s 3s $^1S_0$   | 1s 4p $^3P_2^o$ | 6.1903E+00    | 7.330E-07 | 2.552E+07        | 6.1656E+00    | 6.999E-07 | 2.435E+07        |
| 1s 3d $^3D_2$   | 1s 4p $^3P_2^o$ | 6.5936E+00    | 2.191E-13 | 6.724E+00        |               |           |                  |

(continued on next page)



Table 6 (continued)

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |            |                  |
|-----------------|-----------------|---------------|-----------|------------------|---------------|------------|------------------|
|                 |                 | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$       | $A$ ( $s^{-1}$ ) |
| 1s 3d $^3D_1$   | 1s 4p $^3P_2^0$ | 6.5989E+00    | 1.089E-12 | 3.337E+01        |               |            |                  |
| 1s 3d $^3D_3$   | 1s 4p $^3P_2^0$ | 6.7234E+00    | 2.581E-07 | 7.616E+06        | 6.6951E+00    | 2.493E-07  | 7.359E+06        |
| 1s 3d $^1D_2$   | 1s 4p $^3P_2^0$ | 6.7284E+00    | 6.488E-08 | 1.912E+06        | 6.7001E+00    | 6.220E-08  | 1.832E+06        |
| 1s 4s $^3S_1$   | 1s 4p $^3P_2^0$ | 2.1675E+02    | 6.059E-10 | 1.720E+01        | 2.1631E+02    | 6.045E-10  | 1.709E+01        |
| 1s 4s $^1S_0$   | 1s 4p $^3P_2^0$ | 2.5764E+02    | 2.410E-10 | 4.843E+00        | 2.5767E+02    | 2.384E-10  | 4.750E+00        |
| 1s 2p $^3P_1^0$ | 1s 4d $^3D_2$   | 1.6212E+00    | 2.912E-07 | 1.478E+08        | 1.6144E+00    | 3.095E-07  | 1.571E+08        |
| 1s 2p $^3P_0^0$ | 1s 4d $^3D_2$   | 1.6224E+00    | 1.846E-07 | 9.355E+07        | 1.6156E+00    | 1.932E-07  | 9.790E+07        |
| 1s 2p $^3P_2^0$ | 1s 4d $^3D_2$   | 1.7079E+00    | 1.219E-10 | 5.573E+04        | 1.7007E+00    | 1.718E-10  | 7.857E+04        |
| 1s 2p $^1P_1^0$ | 1s 4d $^3D_2$   | 1.7162E+00    | 7.192E-12 | 3.257E+03        |               |            |                  |
| 1s 3p $^3P_1^0$ | 1s 4d $^3D_2$   | 6.1751E+00    | 9.219E-08 | 3.225E+06        | 6.1494E+00    | 9.398E-08  | 3.287E+06        |
| 1s 3p $^3P_0^0$ | 1s 4d $^3D_2$   | 6.1799E+00    | 5.803E-08 | 2.027E+06        | 6.1541E+00    | 5.875E-08  | 2.051E+06        |
| 1s 3p $^3P_2^0$ | 1s 4d $^3D_2$   | 6.5523E+00    | 4.903E-11 | 1.524E+03        | 6.5248E+00    | 5.664E-11  | 1.760E+03        |
| 1s 3p $^1P_1^0$ | 1s 4d $^3D_2$   | 6.5868E+00    | 6.167E-13 | 1.896E+01        |               |            |                  |
| 1s 4p $^3P_1^0$ | 1s 4d $^3D_2$   | 2.3795E+02    | 1.520E-11 | 3.582E-01        | 2.3625E+02    | 1.552E-11  | 3.679E-01        |
| 1s 4p $^3P_0^0$ | 1s 4d $^3D_2$   | 2.4086E+02    | 9.221E-12 | 2.120E-01        | 2.3903E+02    | 9.376E-12  | 2.170E-01        |
| 1s 4p $^3P_2^0$ | 1s 4d $^3D_2$   | 3.5515E+03    | 2.231E-18 | 2.359E-10        |               |            |                  |
| 1s 2p $^3P_1^0$ | 1s 4d $^3D_1$   | 1.6210E+00    | 2.862E-07 | 2.422E+08        | 1.6143E+00    | 3.012E-07  | 2.548E+08        |
| 1s 2p $^3P_2^0$ | 1s 4d $^3D_1$   | 1.7078E+00    | 3.653E-13 | 2.785E+02        |               |            |                  |
| 1s 2p $^1P_1^0$ | 1s 4d $^3D_1$   | 1.7161E+00    | 3.609E-10 | 2.724E+05        | 1.7090E+00    | 3.716E-10  | 2.805E+05        |
| 1s 3p $^3P_1^0$ | 1s 4d $^3D_1$   | 6.1732E+00    | 8.985E-08 | 5.242E+06        | 6.1476E+00    | 9.158E-08  | 5.342E+06        |
| 1s 3p $^3P_2^0$ | 1s 4d $^3D_1$   | 6.5502E+00    | 5.443E-13 | 2.821E+01        |               |            |                  |
| 1s 3p $^1P_1^0$ | 1s 4d $^3D_1$   | 6.5847E+00    | 1.129E-10 | 5.788E+03        | 6.5574E+00    | 8.882E-11  | 4.553E+03        |
| 1s 4p $^3P_1^0$ | 1s 4d $^3D_1$   | 2.3523E+02    | 1.537E-11 | 6.175E-01        | 2.3358E+02    | 1.564E-11  | 6.320E-01        |
| 1s 4p $^3P_2^0$ | 1s 4d $^3D_1$   | 3.0279E+03    | 4.275E-19 | 1.037E-10        |               |            |                  |
| 1s 2s $^3S_1$   | 1s 4p $^1P_1^0$ | 1.6048E+00    | 3.673E-06 | 3.171E+09        | 1.5980E+00    | 3.832E-06  | 3.308E+09        |
| 1s 3s $^3S_1$   | 1s 4p $^1P_1^0$ | 6.1092E+00    | 1.049E-06 | 6.249E+07        | 6.0840E+00    | 1.091E-06  | 6.499E+07        |
| 1s 3d $^3D_2$   | 1s 4p $^1P_1^0$ | 6.5793E+00    | 6.881E-13 | 3.535E+01        |               |            |                  |
| 1s 3d $^3D_1$   | 1s 4p $^1P_1^0$ | 6.5845E+00    | 2.464E-13 | 1.264E+01        |               |            |                  |
| 1s 3d $^3D_3$   | 1s 4p $^1P_1^0$ | 6.7085E+00    | 4.497E-08 | 2.222E+06        | 6.6801E+00    | 4.629E-08  | 2.286E+06        |
| 1s 3d $^1D_2$   | 1s 4p $^1P_1^0$ | 6.7135E+00    | 1.426E-07 | 7.036E+06        | 6.6851E+00    | 1.415E-07  | 6.984E+06        |
| 1s 4s $^3S_1$   | 1s 4p $^1P_1^0$ | 2.0225E+02    | 7.466E-10 | 4.058E+01        | 2.0166E+02    | 7.451E-10  | 4.039E+01        |
| 1s 4d $^3D_2$   | 1s 4p $^1P_1^0$ | 2.0339E+04    | 7.155E-23 | 3.846E-16        |               |            |                  |
| 1s 4d $^3D_1$   | 1s 4p $^1P_1^0$ | 2.1218E+06    | 1.608E-26 | 7.940E-24        |               |            |                  |
| 1s 2p $^3P_1^0$ | 1s 4d $^3D_3$   | 1.6179E+00    | 4.628E-06 | 1.685E+09        | 1.6112E+00    | 4.723E-06  | 1.719E+09        |
| 1s 2p $^3P_2^0$ | 1s 4d $^3D_3$   | 1.7043E+00    | 2.069E-05 | 6.788E+09        | 1.6972E+00    | 2.154E-05  | 7.068E+09        |
| 1s 2p $^1P_1^0$ | 1s 4d $^3D_3$   | 1.7126E+00    | 3.719E-06 | 1.208E+09        | 1.7055E+00    | 3.855E-06  | 1.252E+09        |
| 1s 3p $^3P_1^0$ | 1s 4d $^3D_3$   | 6.1283E+00    | 1.363E-06 | 3.459E+07        | 6.1030E+00    | 1.371E-06  | 3.478E+07        |
| 1s 3p $^3P_2^0$ | 1s 4d $^3D_3$   | 6.4997E+00    | 7.099E-06 | 1.601E+08        | 6.4725E+00    | 7.232E-06  | 1.631E+08        |
| 1s 3p $^1P_1^0$ | 1s 4d $^3D_3$   | 6.5336E+00    | 1.286E-06 | 2.871E+07        | 6.5067E+00    | 1.277E-06  | 2.850E+07        |
| 1s 4p $^3P_1^0$ | 1s 4d $^3D_3$   | 1.8386E+02    | 5.115E-10 | 1.442E+01        | 1.8281E+02    | 5.134E-10  | 1.451E+01        |
| 1s 4p $^3P_2^0$ | 1s 4d $^3D_3$   | 6.5884E+02    | 5.524E-11 | 1.213E-01        | 6.5162E+02    | 5.648E-11  | 1.256E-01        |
| 1s 4p $^1P_1^0$ | 1s 4d $^3D_3$   | 8.4240E+02    | 4.763E-12 | 6.396E-03        | 8.3413E+02    | 4.865E-12  | 6.606E-03        |
| 1s 2s $^3S_1$   | 1s 4f $^3F_3^0$ | 1.6017E+00    | 1.411E-10 | 5.242E+04        |               |            |                  |
| 1s 3s $^3S_1$   | 1s 4f $^3F_3^0$ | 6.0645E+00    | 6.814E-12 | 1.765E+02        |               |            |                  |
| 1s 3d $^3D_2$   | 1s 4f $^3F_3^0$ | 6.5275E+00    | 2.415E-06 | 5.402E+07        | 6.5002E+00    | 2.450E-06  | 5.479E+07        |
| 1s 3d $^3D_1$   | 1s 4f $^3F_3^0$ | 6.5326E+00    | 4.080E-07 | 9.111E+06        | 6.5052E+00    | 4.131E-07  | 9.224E+06        |
| 1s 3d $^3D_3$   | 1s 4f $^3F_3^0$ | 6.6546E+00    | 1.660E-11 | 3.572E+02        |               |            |                  |
| 1s 3d $^1D_2$   | 1s 4f $^3F_3^0$ | 6.6595E+00    | 2.267E-10 | 4.871E+03        |               |            |                  |
| 1s 4s $^3S_1$   | 1s 4f $^3F_3^0$ | 1.6258E+02    | 2.126E-19 | 7.665E-09        | 1.6211E+02    | 1.540E-16  | 5.538E-06        |
| 1s 4d $^3D_2$   | 1s 4f $^3F_3^0$ | 7.9649E+02    | 3.345E-12 | 5.024E-03        | 8.0096E+02    | 3.264E-12  | 4.808E-03        |
| 1s 4d $^3D_1$   | 1s 4f $^3F_3^0$ | 8.2863E+02    | 5.020E-13 | 6.967E-04        | 8.3335E+02    | 4.900E-13  | 6.666E-04        |
| 1s 4d $^3D_3$   | 1s 4f $^3F_3^0$ | 5.1914E+04    | 8.399E-23 | 2.970E-17        |               |            |                  |
| 1s $^2S_1$      | 1s 4f $^3F_2^0$ | 3.2740E-01    | 1.149E-10 | 1.430E+06        | 3.2603E-01    | 4.930E-12  | 6.135E+04        |
| 1s 2s $^3S_1$   | 1s 4f $^3F_2^0$ | 1.6017E+00    | 4.643E-11 | 2.414E+04        | 1.5949E+00    | 4.969E-13  | 2.583E+02        |
| 1s 2s $^1S_0$   | 1s 4f $^3F_2^0$ | 1.6195E+00    | 4.740E-11 | 2.411E+04        | 1.6129E+00    | 3.203E-13  | 1.628E+02        |
| 1s 3s $^3S_1$   | 1s 4f $^3F_2^0$ | 6.0636E+00    | 9.483E-12 | 3.441E+02        |               |            |                  |
| 1s 3s $^1S_0$   | 1s 4f $^3F_2^0$ | 6.1310E+00    | 6.089E-12 | 2.161E+02        |               |            |                  |
| 1s 3d $^3D_2$   | 1s 4f $^3F_2^0$ | 6.5264E+00    | 6.054E-07 | 1.896E+07        | 6.4991E+00    | 6.141E-07  | 1.923E+07        |
| 1s 3d $^3D_1$   | 1s 4f $^3F_2^0$ | 6.5315E+00    | 1.411E-06 | 4.412E+07        | 6.5041E+00    | 1.429E-06  | 4.469E+07        |
| 1s 3d $^3D_3$   | 1s 4f $^3F_2^0$ | 6.6535E+00    | 1.331E-14 | 4.010E-01        |               |            |                  |
| 1s 3d $^1D_2$   | 1s 4f $^3F_2^0$ | 6.6584E+00    | 6.185E-12 | 1.861E+02        |               |            |                  |
| 1s 4s $^3S_1$   | 1s 4f $^3F_2^0$ | 1.6191E+02    | 2.730E-16 | 1.389E-05        | 1.6143E+02    | 9.377E-17  | 4.760E-06        |
| 1s 4s $^1S_0$   | 1s 4f $^3F_2^0$ | 1.8368E+02    | 2.477E-16 | 9.794E-06        | 1.8340E+02    | 8.510E-17  | 3.346E-06        |
| 1s 4d $^3D_2$   | 1s 4f $^3F_2^0$ | 7.8052E+02    | 8.910E-13 | 1.951E-03        | 7.8473E+02    | 8.697E-13  | 1.868E-03        |
| 1s 4d $^3D_1$   | 1s 4f $^3F_2^0$ | 8.1135E+02    | 1.850E-12 | 3.749E-03        | 8.1580E+02    | 1.806E-12  | 3.590E-03        |
| 1s 4d $^3D_3$   | 1s 4f $^3F_2^0$ | 2.2242E+04    | 1.812E-22 | 4.886E-16        |               |            |                  |
| 1s 2p $^3P_1^0$ | 1s 4d $^1D_2$   | 1.6178E+00    | 1.786E-06 | 9.103E+08        | 1.6111E+00    | 1.843E-06  | 9.395E+08        |
| 1s 2p $^3P_0^0$ | 1s 4d $^1D_2$   | 1.6191E+00    | 2.139E-06 | 1.089E+09        | 1.6123E+00    | 2.188E-06  | 1.113E+09        |
| 1s 2p $^3P_2^0$ | 1s 4d $^1D_2$   | 1.7042E+00    | 5.187E-06 | 2.383E+09        | 1.6970E+00    | 5.388E-06  | 2.474E+09        |
| 1s 2p $^1P_1^0$ | 1s 4d $^1D_2$   | 1.7124E+00    | 1.163E-05 | 5.291E+09        | 1.7053E+00    | 1.7053E-05 | 5.484E+09        |
| 1s 3p $^3P_1^0$ | 1s 4d $^1D_2$   | 6.1264E+00    | 5.148E-07 | 1.830E+07        | 6.1011E+00    | 5.378E-07  | 1.911E+07        |

(continued on next page)

Table 6 (continued)

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |           |                  |
|-----------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                 |                 | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 3p $^3P_0^o$ | 1s 4d $^1D_2$   | 6.1312E+00    | 6.270E-07 | 2.225E+07        | 6.1056E+00    | 6.363E-07 | 2.257E+07        |
| 1s 3p $^3P_1^o$ | 1s 4d $^1D_2$   | 6.4976E+00    | 1.773E-06 | 5.603E+07        | 6.4704E+00    | 1.809E-06 | 5.717E+07        |
| 1s 3p $^1P_1^o$ | 1s 4d $^1D_2$   | 6.5315E+00    | 4.042E-06 | 1.264E+08        | 6.5045E+00    | 4.060E-06 | 1.269E+08        |
| 1s 4p $^3P_0^o$ | 1s 4d $^1D_2$   | 1.8218E+02    | 1.978E-10 | 7.953E+00        | 1.8111E+02    | 1.990E-10 | 8.026E+00        |
| 1s 4p $^3P_1^o$ | 1s 4d $^1D_2$   | 1.8388E+02    | 2.351E-10 | 9.278E+00        | 1.8274E+02    | 2.365E-10 | 9.368E+00        |
| 1s 4p $^3P_2^o$ | 1s 4d $^1D_2$   | 6.3767E+02    | 1.524E-11 | 5.000E-02        | 6.3050E+02    | 1.558E-11 | 5.186E-02        |
| 1s 4p $^1P_1^o$ | 1s 4d $^1D_2$   | 8.0810E+02    | 1.703E-11 | 3.478E-02        | 7.9983E+02    | 1.737E-11 | 3.591E-02        |
| 1s 4f $^3F_3^o$ | 1s 4d $^1D_2$   | 3.2125E+04    | 6.900E-21 | 8.919E-15        |               |           |                  |
| 1s 4f $^3F_2^o$ | 1s 4d $^1D_2$   | 1.8409E+05    | 1.136E-24 | 4.473E-20        |               |           |                  |
| 1s 3d $^3D_2$   | 1s 4f $^3F_4^o$ | 6.5015E+00    | 4.667E-06 | 8.182E+07        | 6.4744E+00    | 4.702E-06 | 8.243E+07        |
| 1s 3d $^3D_3$   | 1s 4f $^3F_4^o$ | 6.6276E+00    | 2.919E-05 | 4.925E+08        | 6.5997E+00    | 2.959E-05 | 4.992E+08        |
| 1s 3d $^1D_2$   | 1s 4f $^3F_4^o$ | 6.6325E+00    | 2.355E-06 | 3.967E+07        | 6.6046E+00    | 2.385E-06 | 4.019E+07        |
| 1s 4d $^3D_2$   | 1s 4f $^3F_4^o$ | 5.3564E+02    | 2.134E-11 | 5.513E-02        | 5.3733E+02    | 2.081E-11 | 5.297E-02        |
| 1s 4d $^3D_3$   | 1s 4f $^3F_4^o$ | 1.5856E+03    | 5.232E-12 | 1.542E-03        | 1.6034E+03    | 5.007E-12 | 1.431E-03        |
| 1s 4d $^1D_2$   | 1s 4f $^3F_4^o$ | 1.7232E+03    | 3.306E-13 | 8.252E-05        | 1.7474E+03    | 3.143E-13 | 7.566E-05        |
| 1s 2s $^3S_1$   | 1s 4f $^1F_3^o$ | 1.6001E+00    | 2.058E-13 | 7.659E+01        |               |           |                  |
| 1s 3s $^3S_1$   | 1s 4f $^1F_3^o$ | 6.0414E+00    | 5.284E-12 | 1.380E+02        |               |           |                  |
| 1s 3d $^3D_2$   | 1s 4f $^1F_3^o$ | 6.5007E+00    | 5.480E-07 | 1.236E+07        | 6.4736E+00    | 5.559E-07 | 1.253E+07        |
| 1s 3d $^3D_1$   | 1s 4f $^1F_3^o$ | 6.5058E+00    | 3.118E-06 | 7.020E+07        | 6.4786E+00    | 3.140E-06 | 7.069E+07        |
| 1s 3d $^3D_3$   | 1s 4f $^1F_3^o$ | 6.6268E+00    | 3.503E-06 | 7.602E+07        | 6.5989E+00    | 3.552E-06 | 7.708E+07        |
| 1s 3d $^1D_2$   | 1s 4f $^1F_3^o$ | 6.6317E+00    | 2.098E-05 | 4.545E+08        | 6.6038E+00    | 2.124E-05 | 4.602E+08        |
| 1s 4s $^3S_1$   | 1s 4f $^1F_3^o$ | 1.4747E+02    | 1.639E-15 | 7.182E-05        | 1.4705E+02    | 1.598E-15 | 6.984E-05        |
| 1s 4d $^3D_2$   | 1s 4f $^1F_3^o$ | 5.3023E+02    | 2.655E-12 | 8.999E-03        | 5.3185E+02    | 2.605E-12 | 8.701E-03        |
| 1s 4d $^3D_1$   | 1s 4f $^1F_3^o$ | 5.4428E+02    | 1.364E-11 | 4.388E-02        | 5.4594E+02    | 1.331E-11 | 4.220E-02        |
| 1s 4d $^3D_3$   | 1s 4f $^1F_3^o$ | 1.5391E+03    | 6.867E-13 | 2.763E-04        | 1.5556E+03    | 6.579E-13 | 2.568E-04        |
| 1s 4d $^1D_2$   | 1s 4f $^1F_3^o$ | 1.6685E+03    | 3.227E-12 | 1.105E-03        | 1.6908E+03    | 3.068E-12 | 1.014E-03        |
| 1s 2p $^3P_0^o$ | 1s 5s $^3S_1$   | 1.4605E+00    | 3.050E-10 | 3.179E+05        | 1.4544E+00    | 4.408E-10 | 4.594E+05        |
| 1s 2p $^3P_1^o$ | 1s 5s $^3S_1$   | 1.5306E+00    | 2.559E-07 | 2.429E+08        | 1.5241E+00    | 2.484E-07 | 2.357E+08        |
| 1s 2p $^1P_1^o$ | 1s 5s $^3S_1$   | 1.5372E+00    | 2.603E-07 | 2.449E+08        | 1.5308E+00    | 2.448E-07 | 2.302E+08        |
| 1s 3p $^3P_0^o$ | 1s 5s $^3S_1$   | 4.3516E+00    | 1.805E-10 | 2.119E+04        | 4.3336E+00    | 2.612E-10 | 3.066E+04        |
| 1s 3p $^3P_1^o$ | 1s 5s $^3S_1$   | 4.5356E+00    | 1.712E-07 | 1.851E+07        | 4.5167E+00    | 1.689E-07 | 1.825E+07        |
| 1s 3p $^1P_1^o$ | 1s 5s $^3S_1$   | 4.5521E+00    | 1.739E-07 | 1.866E+07        | 4.5333E+00    | 1.668E-07 | 1.790E+07        |
| 1s 4p $^3P_0^o$ | 1s 5s $^3S_1$   | 1.3877E+01    | 1.225E-10 | 1.414E+03        | 1.3818E+01    | 1.886E-10 | 2.178E+03        |
| 1s 4p $^3P_1^o$ | 1s 5s $^3S_1$   | 1.4675E+01    | 1.220E-07 | 1.260E+06        | 1.4612E+01    | 1.208E-07 | 1.247E+06        |
| 1s 4p $^1P_1^o$ | 1s 5s $^3S_1$   | 1.4747E+01    | 1.241E-07 | 1.268E+06        | 1.4684E+01    | 1.189E-07 | 1.215E+06        |
| 1s 4f $^3F_3^o$ | 1s 5s $^3S_1$   | 1.5014E+01    | 7.117E-15 | 7.019E-02        |               |           |                  |
| 1s 4f $^3F_2^o$ | 1s 5s $^3S_1$   | 1.5020E+01    | 3.744E-18 | 3.690E-05        |               |           |                  |
| 1s 4f $^1F_3^o$ | 1s 5s $^3S_1$   | 1.5158E+01    | 4.158E-14 | 4.024E-01        |               |           |                  |
| 1s 2s $^3S_1$   | 1s 5p $^3P_0^o$ | 1.4466E+00    | 2.751E-09 | 2.923E+06        | 1.4405E+00    | 2.623E-09 | 2.787E+06        |
| 1s 3s $^3S_1$   | 1s 5p $^3P_0^o$ | 4.3132E+00    | 9.001E-10 | 1.076E+05        | 4.2953E+00    | 7.868E-10 | 9.401E+04        |
| 1s 3d $^3D_2$   | 1s 5p $^3P_0^o$ | 4.5423E+00    | 1.872E-09 | 2.018E+05        | 4.5233E+00    | 1.852E-09 | 1.996E+05        |
| 1s 3d $^3D_1$   | 1s 5p $^3P_0^o$ | 4.5448E+00    | 1.860E-09 | 2.002E+05        | 4.5258E+00    | 1.819E-09 | 1.957E+05        |
| 1s 3d $^3D_3$   | 1s 5p $^3P_0^o$ | 4.6035E+00    | 3.130E-08 | 3.284E+06        | 4.5841E+00    | 3.112E-08 | 3.264E+06        |
| 1s 3d $^1D_2$   | 1s 5p $^3P_0^o$ | 4.6059E+00    | 1.184E-08 | 1.241E+06        | 4.5865E+00    | 1.116E-08 | 1.169E+06        |
| 1s 4s $^3S_1$   | 1s 5p $^3P_0^o$ | 1.3679E+01    | 3.955E-10 | 4.699E+03        | 1.3623E+01    | 3.048E-10 | 3.621E+03        |
| 1s 4d $^3D_2$   | 1s 5p $^3P_0^o$ | 1.4661E+01    | 2.272E-09 | 2.350E+04        | 1.4602E+01    | 2.264E-09 | 2.341E+04        |
| 1s 4d $^3D_1$   | 1s 5p $^3P_0^o$ | 1.4671E+01    | 2.229E-09 | 2.302E+04        | 1.4612E+01    | 2.198E-09 | 2.269E+04        |
| 1s 4d $^3D_3$   | 1s 5p $^3P_0^o$ | 1.4932E+01    | 3.752E-08 | 3.742E+05        | 1.4871E+01    | 3.761E-08 | 3.749E+05        |
| 1s 4d $^1D_2$   | 1s 5p $^3P_0^o$ | 1.4943E+01    | 1.413E-08 | 1.408E+05        | 1.4882E+01    | 1.340E-08 | 1.334E+05        |
| 1s 5s $^3S_1$   | 1s 5p $^3P_0^o$ | 2.8648E+03    | 8.236E-16 | 2.231E-07        | 2.9004E+03    | 8.265E-16 | 2.165E-07        |
| 1s 2p $^3P_2^o$ | 1s 5s $^1S_0$   | 1.5297E+00    | 1.624E-07 | 4.628E+08        | 1.5233E+00    | 1.659E-07 | 4.728E+08        |
| 1s 3p $^3P_0^o$ | 1s 5s $^1S_0$   | 4.5281E+00    | 1.095E-07 | 3.561E+07        | 4.5091E+00    | 1.132E-07 | 3.682E+07        |
| 1s 4p $^3P_0^o$ | 1s 5s $^1S_0$   | 1.4597E+01    | 7.783E-08 | 2.437E+06        | 1.4533E+01    | 8.188E-08 | 2.563E+06        |
| 1s 4f $^3F_2^o$ | 1s 5s $^1S_0$   | 1.4938E+01    | 9.202E-15 | 2.751E-01        |               |           |                  |
| 1s 3d $^3D_2$   | 1s 5p $^3P_0^o$ | 4.5418E+00    | 1.202E-09 | 3.888E+05        | 4.5228E+00    | 1.184E-09 | 3.828E+05        |
| 1s 3d $^1D_2$   | 1s 5p $^3P_0^o$ | 4.6053E+00    | 1.441E-08 | 4.531E+06        | 4.5860E+00    | 1.410E-08 | 4.436E+06        |
| 1s 4d $^3D_2$   | 1s 5p $^3P_0^o$ | 1.4656E+01    | 1.425E-09 | 4.426E+04        | 1.4597E+01    | 1.412E-09 | 4.385E+04        |
| 1s 4d $^1D_2$   | 1s 5p $^3P_0^o$ | 1.4937E+01    | 1.725E-08 | 5.156E+05        | 1.4877E+01    | 1.705E-08 | 5.096E+05        |
| 1s $^2^1S_0$    | 1s 5p $^3P_0^o$ | 3.2010E-01    | 1.717E-05 | 2.234E+11        | 3.1883E-01    | 1.929E-05 | 2.510E+11        |
| 1s 2s $^3S_1$   | 1s 5p $^3P_0^o$ | 1.4424E+00    | 1.922E-06 | 1.232E+09        | 1.4363E+00    | 1.984E-06 | 1.272E+09        |
| 1s 2s $^1S_0$   | 1s 5p $^3P_0^o$ | 1.4568E+00    | 1.283E-06 | 8.066E+08        | 1.4509E+00    | 1.283E-06 | 8.066E+08        |
| 1s 3s $^3S_1$   | 1s 5p $^3P_0^o$ | 4.2763E+00    | 5.990E-07 | 4.370E+07        | 4.2586E+00    | 6.082E-07 | 4.435E+07        |
| 1s 3s $^1S_0$   | 1s 5p $^3P_0^o$ | 4.3097E+00    | 4.071E-07 | 2.924E+07        | 4.2923E+00    | 3.960E-07 | 2.843E+07        |
| 1s 3d $^3D_2$   | 1s 5p $^3P_0^o$ | 4.5014E+00    | 6.201E-14 | 4.082E+00        |               |           |                  |
| 1s 3d $^3D_1$   | 1s 5p $^3P_0^o$ | 4.5039E+00    | 5.894E-13 | 3.876E+01        |               |           |                  |
| 1s 3d $^3D_3$   | 1s 5p $^3P_0^o$ | 4.5615E+00    | 1.111E-07 | 7.123E+06        | 4.5423E+00    | 1.073E-07 | 6.882E+06        |
| 1s 3d $^1D_2$   | 1s 5p $^3P_0^o$ | 4.5638E+00    | 2.802E-08 | 1.794E+06        | 4.5447E+00    | 2.679E-08 | 1.716E+06        |
| 1s 4s $^3S_1$   | 1s 5p $^3P_0^o$ | 1.3315E+01    | 2.473E-07 | 1.861E+06        | 1.3261E+01    | 2.502E-07 | 1.882E+06        |
| 1s 4s $^1S_0$   | 1s 5p $^3P_0^o$ | 1.3446E+01    | 1.705E-07 | 1.258E+06        | 1.3392E+01    | 1.619E-07 | 1.194E+06        |
| 1s 4d $^3D_2$   | 1s 5p $^3P_0^o$ | 1.4243E+01    | 5.361E-13 | 3.525E+00        |               |           |                  |
| 1s 4d $^3D_1$   | 1s 5p $^3P_0^o$ | 1.4253E+01    | 3.646E-13 | 2.394E+00        |               |           |                  |

(continued on next page)

Table 6 (continued)

| Lower  | Upper  | GRASP2K       |           |                             | FAC           |           |                             |
|--|--|---------------|-----------|-----------------------------|---------------|-----------|-----------------------------|
|  |  | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.4499E+01    | 1.363E-07 | 8.649E+05                   | 1.4440E+01    | 1.327E-07 | 8.420E+05                   |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.4509E+01    | 3.425E-08 | 2.170E+05                   | 1.4450E+01    | 3.310E-08 | 2.097E+05                   |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.2565E+02    | 2.014E-10 | 1.483E+00                   | 4.2515E+02    | 2.001E-10 | 1.464E+00                   |
| 1s 5s <sup>1</sup> S <sub>0</sub>              | 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 5.0438E+02    | 8.081E-11 | 4.238E-01                   | 5.0484E+02    | 7.970E-11 | 4.136E-01                   |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4552E+00    | 1.344E-07 | 8.464E+07                   | 1.4491E+00    | 1.437E-07 | 9.054E+07                   |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4562E+00    | 8.458E-08 | 5.321E+07                   | 1.4501E+00    | 8.881E-08 | 5.586E+07                   |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.5247E+00    | 7.189E-11 | 4.125E+04                   | 1.5183E+00    | 1.049E-10 | 6.019E+04                   |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.5313E+00    | 7.295E-15 | 4.150E+00                   |               |           |                             |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.3049E+00    | 4.655E-08 | 3.351E+06                   | 4.2870E+00    | 4.769E-08 | 3.433E+06                   |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.3072E+00    | 2.903E-08 | 2.087E+06                   | 4.2892E+00    | 2.951E-08 | 2.121E+06                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.4849E+00    | 3.092E-11 | 2.051E+03                   | 4.4661E+00    | 3.730E-11 | 2.473E+03                   |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.5010E+00    | 3.286E-13 | 2.164E+01                   |               |           |                             |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.3413E+01    | 1.867E-08 | 1.385E+05                   | 1.3354E+01    | 1.890E-08 | 1.401E+05                   |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.3422E+01    | 1.165E-08 | 8.628E+04                   | 1.3363E+01    | 1.171E-08 | 8.675E+04                   |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4158E+01    | 1.382E-11 | 9.197E+01                   | 1.4095E+01    | 1.553E-11 | 1.034E+02                   |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4224E+01    | 2.600E-13 | 1.714E+00                   |               |           |                             |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4473E+01    | 7.457E-09 | 4.750E+04                   | 1.4409E+01    | 7.405E-09 | 4.718E+04                   |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4478E+01    | 1.873E-09 | 1.192E+04                   | 1.4414E+01    | 1.853E-09 | 1.179E+04                   |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4602E+01    | 1.516E-08 | 9.483E+04                   | 1.4537E+01    | 1.503E-08 | 9.412E+04                   |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 1.4606E+01    | 1.852E-09 | 1.158E+04                   | 1.4541E+01    | 1.832E-09 | 1.146E+04                   |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.6651E+02    | 5.572E-12 | 3.415E-02                   | 4.6168E+02    | 5.725E-12 | 3.553E-02                   |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 4.7209E+02    | 3.350E-12 | 2.005E-02                   | 4.6698E+02    | 3.426E-12 | 2.078E-02                   |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>2</sub>              | 6.9791E+03    | 1.076E-18 | 2.947E-11                   |               |           |                             |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.4421E+00    | 1.903E-06 | 2.034E+09                   | 1.4360E+00    | 1.983E-06 | 2.120E+09                   |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.2732E+00    | 5.899E-07 | 7.183E+07                   | 4.2555E+00    | 6.087E-07 | 7.410E+07                   |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.4980E+00    | 3.519E-13 | 3.867E+01                   |               |           |                             |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.5005E+00    | 4.503E-14 | 4.944E+00                   |               |           |                             |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.5580E+00    | 1.937E-08 | 2.073E+06                   | 4.5388E+00    | 1.975E-08 | 2.113E+06                   |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.5603E+00    | 6.171E-08 | 6.598E+06                   | 4.5411E+00    | 6.080E-08 | 6.500E+06                   |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.3285E+01    | 2.421E-07 | 3.050E+06                   | 1.3231E+01    | 2.516E-07 | 3.168E+06                   |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.4209E+01    | 7.511E-15 | 8.271E-02                   |               |           |                             |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.4219E+01    | 3.306E-10 | 3.636E+00                   |               |           |                             |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.4463E+01    | 2.382E-08 | 2.532E+05                   | 1.4404E+01    | 2.459E-08 | 2.612E+05                   |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.4474E+01    | 7.561E-08 | 8.025E+05                   | 1.4415E+01    | 7.547E-08 | 8.007E+05                   |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.9729E+02    | 2.478E-10 | 3.491E+00                   | 3.9647E+02    | 2.465E-10 | 3.457E+00                   |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.1006E+04    | 1.343E-22 | 1.776E-16                   |               |           |                             |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4551E+00    | 1.319E-07 | 1.385E+08                   | 1.4491E+00    | 1.392E-07 | 1.461E+08                   |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.5247E+00    | 2.190E-13 | 2.095E+02                   |               |           |                             |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.5313E+00    | 1.600E-10 | 1.517E+05                   | 1.5249E+00    | 1.733E-10 | 1.643E+05                   |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.3044E+00    | 4.527E-08 | 5.432E+06                   | 4.2865E+00    | 4.624E-08 | 5.548E+06                   |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.4844E+00    | 3.083E-13 | 3.408E+01                   |               |           |                             |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.5005E+00    | 5.280E-11 | 5.796E+03                   | 4.4818E+00    | 4.790E-11 | 5.257E+03                   |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.3409E+01    | 1.812E-08 | 2.241E+05                   | 1.3350E+01    | 1.835E-08 | 2.270E+05                   |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4153E+01    | 2.043E-13 | 2.268E+00                   |               |           |                             |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4219E+01    | 2.169E-11 | 2.385E+02                   | 1.4157E+01    | 1.589E-11 | 1.748E+02                   |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4467E+01    | 1.254E-09 | 1.332E+04                   | 1.4404E+01    | 1.253E-09 | 1.332E+04                   |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4473E+01    | 4.348E-09 | 4.616E+04                   | 1.4409E+01    | 4.329E-09 | 4.596E+04                   |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4601E+01    | 1.014E-08 | 1.058E+05                   | 1.4536E+01    | 1.009E-08 | 1.053E+05                   |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 4.6125E+02    | 5.605E-12 | 5.858E-02                   | 4.5655E+02    | 5.740E-12 | 6.071E-02                   |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 5.9615E+03    | 1.448E-19 | 9.058E-12                   |               |           |                             |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>1</sub>              | 1.4006E+07    | 1.496E-28 | 1.698E-27                   |               |           |                             |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4539E+00    | 2.153E-06 | 9.704E+08                   | 1.4478E+00    | 2.200E-06 | 9.919E+08                   |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.5233E+00    | 9.425E-06 | 3.871E+09                   | 1.5168E+00    | 9.852E-06 | 4.045E+09                   |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.5298E+00    | 1.691E-06 | 6.884E+08                   | 1.5235E+00    | 1.767E-06 | 7.196E+08                   |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 4.2932E+00    | 7.013E-07 | 3.626E+07                   | 4.2754E+00    | 7.111E-07 | 3.676E+07                   |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 4.4722E+00    | 3.457E-06 | 1.647E+08                   | 4.4535E+00    | 3.522E-06 | 1.678E+08                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 4.4883E+00    | 6.233E-07 | 2.948E+07                   | 4.4696E+00    | 6.279E-07 | 2.969E+07                   |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.3300E+01    | 2.701E-07 | 1.455E+06                   | 1.3242E+01    | 2.699E-07 | 1.454E+06                   |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4032E+01    | 1.483E-06 | 7.178E+06                   | 1.3970E+01    | 1.506E-06 | 7.291E+06                   |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4097E+01    | 2.694E-07 | 1.292E+06                   | 1.4036E+01    | 2.656E-07 | 1.274E+06                   |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4341E+01    | 5.108E-14 | 2.367E-01                   |               |           |                             |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4347E+01    | 1.695E-13 | 7.849E-01                   |               |           |                             |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4468E+01    | 8.474E-08 | 3.857E+05                   | 1.4405E+01    | 8.385E-08 | 3.818E+05                   |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.4472E+01    | 1.019E-08 | 4.636E+04                   | 1.4409E+01    | 1.005E-08 | 4.575E+04                   |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 3.6020E+02    | 1.859E-10 | 1.366E+00                   | 3.5728E+02    | 1.880E-10 | 1.392E+00                   |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.2888E+03    | 2.022E-11 | 1.160E-02                   | 1.2633E+03    | 2.122E-11 | 1.256E-02                   |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>3</sup> D <sub>3</sub>              | 1.6441E+03    | 1.755E-12 | 6.188E-04                   | 1.6091E+03    | 1.854E-12 | 6.766E-04                   |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4408E+00    | 9.780E-11 | 4.489E+04                   |               |           |                             |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.2620E+00    | 6.114E-13 | 3.207E+01                   |               |           |                             |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4855E+00    | 7.993E-07 | 3.786E+07                   | 4.4667E+00    | 8.162E-07 | 3.865E+07                   |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4880E+00    | 1.349E-07 | 6.380E+06                   | 4.4691E+00    | 1.376E-07 | 6.509E+06                   |

(continued on next page)

Table 6 (continued)

| Lower  | Upper  | GRASP2K       |           |                  | FAC           |           |                  |
|--|--|---------------|-----------|------------------|---------------|-----------|------------------|
|  |  | $\lambda$ (Å) | <i>gf</i> | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | <i>gf</i> | $A$ ( $s^{-1}$ ) |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.5452E+00    | 4.800E−12 | 2.214E+02        |               |           |                  |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.5475E+00    | 6.705E−11 | 3.089E+03        |               |           |                  |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.3177E+01    | 2.554E−13 | 1.402E+00        |               |           |                  |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4085E+01    | 4.505E−07 | 2.164E+06        | 1.4028E+01    | 4.534E−07 | 2.177E+06        |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4095E+01    | 7.610E−08 | 3.650E+05        | 1.4038E+01    | 7.640E−08 | 3.663E+05        |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4335E+01    | 2.763E−12 | 1.281E+01        |               |           |                  |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4345E+01    | 5.743E−11 | 2.659E+02        | 1.4286E+01    | 5.957E−11 | 2.757E+02        |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.1888E+02    | 1.023E−17 | 9.585E−08        | 3.1776E+02    | 8.216E−17 | 7.688E−07        |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.5543E+03    | 1.612E−12 | 6.359E−04        | 1.5716E+03    | 1.545E−12 | 5.911E−04        |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.6158E+03    | 2.424E−13 | 8.846E−05        | 1.6341E+03    | 2.321E−13 | 8.213E−05        |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 9.3195E+04    | 4.604E−23 | 5.051E−18        |               |           |                  |
| 1s <sup>2</sup> <sup>1</sup> S <sub>0</sub>    | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.2000E−01    | 9.916E−11 | 1.291E+06        | 3.1875E−01    | 4.044E−12 | 5.265E+04        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4408E+00    | 3.316E−11 | 2.131E+04        | 1.4347E+00    | 4.172E−13 | 2.681E+02        |
| 1s 2s <sup>1</sup> S <sub>0</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4551E+00    | 3.223E−11 | 2.030E+04        | 1.4492E+00    | 2.698E−13 | 1.699E+02        |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.2617E+00    | 1.699E−12 | 1.248E+02        |               |           |                  |
| 1s 3s <sup>1</sup> S <sub>0</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.2949E+00    | 1.182E−12 | 8.548E+01        |               |           |                  |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4853E+00    | 2.005E−07 | 1.330E+07        | 4.4664E+00    | 2.044E−07 | 1.355E+07        |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4877E+00    | 4.668E−07 | 3.092E+07        | 4.4688E+00    | 4.763E−07 | 3.155E+07        |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.5449E+00    | 4.501E−15 | 2.907E−01        |               |           |                  |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.5472E+00    | 1.914E−12 | 1.235E+02        |               |           |                  |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.3175E+01    | 1.082E−12 | 8.314E+00        |               |           |                  |
| 1s 4s <sup>1</sup> S <sub>0</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.3303E+01    | 5.809E−13 | 4.379E+00        |               |           |                  |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4083E+01    | 1.128E−07 | 7.589E+05        | 1.4025E+01    | 1.136E−07 | 7.641E+05        |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4092E+01    | 2.633E−07 | 1.768E+06        | 1.4035E+01    | 2.646E−07 | 1.776E+06        |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4332E+01    | 2.202E−14 | 1.430E−01        |               |           |                  |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.4343E+01    | 2.824E−12 | 1.832E+01        |               |           |                  |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.1755E+02    | 1.065E−16 | 1.409E−06        | 3.1643E+02    | 4.872E−17 | 6.436E−07        |
| 1s 5s <sup>1</sup> S <sub>0</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 3.5940E+02    | 1.023E−16 | 1.057E−06        | 3.5855E+02    | 4.660E−17 | 4.795E−07        |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.5232E+03    | 4.293E−13 | 2.469E−04        | 1.5396E+03    | 4.117E−13 | 2.297E−04        |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1.5821E+03    | 8.937E−13 | 4.763E−04        | 1.5996E+03    | 8.566E−13 | 4.428E−04        |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.1865E+04    | 1.183E−22 | 9.007E−17        |               |           |                  |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4538E+00    | 8.312E−07 | 5.247E+08        | 1.4478E+00    | 8.539E−07 | 5.388E+08        |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4548E+00    | 9.966E−07 | 6.282E+08        | 1.4487E+00    | 1.018E−06 | 6.420E+08        |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.5232E+00    | 2.366E−06 | 1.360E+09        | 1.5168E+00    | 2.463E−06 | 1.416E+09        |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.5298E+00    | 5.292E−06 | 3.017E+09        | 1.5234E+00    | 5.518E−06 | 3.145E+09        |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 4.2927E+00    | 2.650E−07 | 1.918E+07        | 4.2749E+00    | 2.739E−07 | 1.982E+07        |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 4.2951E+00    | 3.229E−07 | 2.335E+07        | 4.2771E+00    | 3.287E−07 | 2.377E+07        |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 4.4717E+00    | 8.646E−07 | 5.768E+07        | 4.4529E+00    | 8.809E−07 | 5.876E+07        |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 4.4877E+00    | 1.961E−06 | 1.299E+08        | 4.4691E+00    | 1.983E−06 | 1.313E+08        |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.3295E+01    | 1.013E−07 | 7.645E+05        | 1.3238E+01    | 1.057E−07 | 7.981E+05        |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.3304E+01    | 1.241E−07 | 9.356E+05        | 1.3246E+01    | 1.253E−07 | 9.450E+05        |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4027E+01    | 3.703E−07 | 2.511E+06        | 1.3965E+01    | 3.769E−07 | 2.556E+06        |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4092E+01    | 8.483E−07 | 5.699E+06        | 1.4031E+01    | 8.480E−07 | 5.698E+06        |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4336E+01    | 1.005E−12 | 6.522E+00        |               |           |                  |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4341E+01    | 4.083E−16 | 2.648E−03        |               |           |                  |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4463E+01    | 6.852E−09 | 4.371E+04        | 1.4399E+01    | 6.850E−09 | 4.370E+04        |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.4467E+01    | 6.065E−08 | 3.866E+05        | 1.4403E+01    | 6.025E−08 | 3.842E+05        |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 3.5679E+02    | 7.174E−11 | 7.518E−01        | 3.5385E+02    | 7.273E−11 | 7.683E−01        |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 3.6004E+02    | 8.559E−11 | 8.808E−01        | 3.5695E+02    | 8.675E−11 | 9.006E−01        |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.2461E+03    | 5.596E−12 | 4.807E−03        | 1.2214E+03    | 5.871E−12 | 5.205E−03        |
| 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 1.5753E+03    | 6.301E−12 | 3.387E−03        | 1.5418E+03    | 6.642E−12 | 3.695E−03        |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 6.3169E+04    | 3.487E−21 | 1.166E−15        |               |           |                  |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5d <sup>1</sup> D <sub>2</sub>              | 3.7392E+05    | 6.620E−25 | 6.316E−21        |               |           |                  |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.4792E+00    | 1.568E−06 | 5.791E+07        | 4.4604E+00    | 1.578E−06 | 5.829E+07        |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.5387E+00    | 9.572E−06 | 3.444E+08        | 4.5196E+00    | 9.774E−06 | 3.516E+08        |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 4.5410E+00    | 7.718E−07 | 2.774E+07        | 4.5219E+00    | 7.887E−07 | 2.834E+07        |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.4024E+01    | 8.559E−07 | 3.226E+06        | 1.3967E+01    | 8.610E−07 | 3.243E+06        |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.4271E+01    | 5.505E−06 | 2.003E+07        | 1.4212E+01    | 5.539E−06 | 2.015E+07        |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.4281E+01    | 4.469E−07 | 1.624E+06        | 1.4223E+01    | 4.490E−07 | 1.631E+06        |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1.0450E+03    | 1.024E−11 | 6.949E−03        | 1.0522E+03    | 9.888E−12 | 6.563E−03        |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 3.0834E+03    | 2.544E−12 | 1.984E−04        | 3.1501E+03    | 2.359E−12 | 1.747E−04        |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 3.3584E+03    | 1.601E−13 | 1.052E−05        | 3.4443E+03    | 1.470E−13 | 9.108E−06        |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 1.5225E+00    | 2.015E−11 | 6.442E+03        |               |           |                  |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 4.4657E+00    | 2.464E−11 | 9.157E+02        |               |           |                  |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 1.3968E+01    | 1.156E−12 | 4.392E+00        |               |           |                  |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 1.4275E+01    | 2.706E−06 | 9.841E+06        | 1.4214E+01    | 2.727E−06 | 9.920E+06        |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 1.4280E+01    | 2.186E−07 | 7.945E+05        | 1.4219E+01    | 2.202E−07 | 8.004E+05        |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 1.4400E+01    | 4.154E−12 | 1.485E+01        |               |           |                  |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 1.4404E+01    | 1.035E−11 | 3.695E+01        |               |           |                  |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 9.0842E+02    | 6.390E−20 | 5.739E−11        |               |           |                  |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 5g <sup>3</sup> G <sub>4</sub>              | 3.1830E+03    | 4.013E−13 | 2.936E−05        | 3.1753E+03    | 4.002E−13 | 2.917E−05        |

(continued on next page)

Table 6 (continued)

| Lower   | Upper   | GRASP2K       |           |                             | FAC           |           |                             |
|---|---|---------------|-----------|-----------------------------|---------------|-----------|-----------------------------|
|   |   | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>4</sub>              | 3.3221E+03    | 2.853E-14 | 1.916E-06                   | 3.3144E+03    | 2.845E-14 | 1.903E-06                   |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>4</sub>              | 1.7265E+06    | 3.911E-27 | 9.725E-25                   |               |           |                             |
| 1s2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.4532E+00    | 1.974E-14 | 8.909E+00                   | 1.4471E+00    | 1.086E-15 | 4.903E-01                   |
| 1s2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.5225E+00    | 2.038E-12 | 8.377E+02                   | 1.5161E+00    | 4.521E-15 | 1.858E+00                   |
| 1s2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.5291E+00    | 1.334E-11 | 5.435E+03                   |               |           |                             |
| 1s3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 4.2871E+00    | 4.526E-14 | 2.347E+00                   | 4.2694E+00    | 3.515E-16 | 1.822E-02                   |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 4.4656E+00    | 2.799E-12 | 1.337E+02                   | 4.4470E+00    | 1.621E-15 | 7.745E-02                   |
| 1s3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 4.4816E+00    | 1.566E-11 | 7.431E+02                   |               |           |                             |
| 1s4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.3242E+01    | 1.450E-15 | 8.79E-03                    |               |           |                             |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.3967E+01    | 7.954E-13 | 3.886E+00                   |               |           |                             |
| 1s4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.4032E+01    | 1.012E-12 | 4.900E+00                   |               |           |                             |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.4273E+01    | 3.250E-07 | 1.520E+06                   | 1.4213E+01    | 3.276E-07 | 1.532E+06                   |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.4278E+01    | 1.949E-06 | 9.109E+06                   | 1.4218E+01    | 1.963E-06 | 9.178E+06                   |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.4399E+01    | 1.054E-18 | 4.843E-06                   |               |           |                             |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.4403E+01    | 1.506E-12 | 6.918E+00                   |               |           |                             |
| 1s5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 3.2168E+02    | 4.463E-20 | 4.110E-10                   |               |           |                             |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 9.0225E+02    | 3.077E-18 | 3.602E-09                   |               |           |                             |
| 1s5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.0631E+03    | 3.176E-19 | 2.678E-10                   |               |           |                             |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 3.1085E+03    | 5.176E-14 | 5.104E-06                   | 3.1008E+03    | 5.161E-14 | 5.071E-06                   |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 3.2410E+03    | 2.739E-13 | 2.485E-05                   | 3.2333E+03    | 2.731E-13 | 2.468E-05                   |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>3</sub>              | 1.2333E+05    | 1.693E-26 | 1.061E-21                   |               |           |                             |
| 1s2s <sup>3</sup> S <sub>1</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4401E+00    | 1.285E-13 | 5.904E+01                   |               |           |                             |
| 1s3s <sup>3</sup> S <sub>1</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.2561E+00    | 2.007E-12 | 1.056E+02                   |               |           |                             |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.4790E+00    | 1.841E-07 | 8.745E+06                   | 4.4602E+00    | 1.862E-07 | 8.846E+06                   |
| 1s3d <sup>3</sup> D <sub>1</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.4815E+00    | 1.047E-06 | 4.968E+07                   | 4.4626E+00    | 1.054E-06 | 5.003E+07                   |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.5385E+00    | 1.150E-06 | 5.319E+07                   | 4.5194E+00    | 1.173E-06 | 5.426E+07                   |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.5408E+00    | 6.878E-06 | 3.179E+08                   | 4.5217E+00    | 7.019E-06 | 3.243E+08                   |
| 1s4s <sup>3</sup> S <sub>1</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.3121E+01    | 1.246E-12 | 6.899E+00                   |               |           |                             |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4022E+01    | 1.031E-07 | 4.999E+05                   | 1.3965E+01    | 1.047E-07 | 5.074E+05                   |
| 1s4d <sup>3</sup> D <sub>1</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4031E+01    | 5.739E-07 | 2.778E+06                   | 1.3974E+01    | 5.770E-07 | 2.791E+06                   |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4269E+01    | 6.604E-07 | 3.091E+06                   | 1.4210E+01    | 6.650E-07 | 3.111E+06                   |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.4279E+01    | 3.956E-06 | 1.849E+07                   | 1.4221E+01    | 3.974E-06 | 1.856E+07                   |
| 1s5s <sup>3</sup> S <sub>1</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.8907E+02    | 8.703E-16 | 9.925E-06                   | 2.8810E+02    | 8.531E-16 | 9.711E-06                   |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.0343E+03    | 1.288E-12 | 1.147E-03                   | 1.0413E+03    | 1.252E-12 | 1.091E-03                   |
| 1s5d <sup>3</sup> D <sub>1</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.0612E+03    | 6.565E-12 | 5.555E-03                   | 1.0684E+03    | 6.346E-12 | 5.252E-03                   |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.9925E+03    | 3.341E-13 | 3.555E-05                   | 3.0547E+03    | 3.104E-13 | 3.143E-05                   |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.2509E+03    | 1.560E-12 | 1.406E-04                   | 3.3306E+03    | 1.434E-12 | 1.221E-04                   |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.0795E+05    | 4.552E-23 | 3.723E-18                   |               |           |                             |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 5.7657E+05    | 3.514E-26 | 1.007E-22                   |               |           |                             |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>5</sub>              | 1.4237E+01    | 1.884E-06 | 5.637E+06                   | 1.4177E+01    | 1.892E-06 | 5.660E+06                   |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>5</sub>              | 1.4362E+01    | 1.643E-05 | 4.829E+07                   | 1.4301E+01    | 1.656E-05 | 4.868E+07                   |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>5</sub>              | 1.4366E+01    | 7.767E-07 | 2.282E+06                   | 1.4305E+01    | 7.827E-07 | 2.300E+06                   |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>5</sub>              | 1.9964E+03    | 1.136E-12 | 1.728E-04                   | 1.9918E+03    | 1.127E-12 | 1.708E-04                   |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>5</sub>              | 5.3388E+03    | 5.211E-13 | 1.109E-05                   | 5.3203E+03    | 5.207E-13 | 1.106E-05                   |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s5g <sup>3</sup> G <sub>5</sub>              | 5.6350E+03    | 2.097E-14 | 4.004E-07                   | 5.6164E+03    | 2.094E-14 | 3.992E-07                   |
| 1s2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5g <sup>1</sup> G <sub>4</sub>              | 1.5221E+00    | 4.230E-15 | 1.353E+00                   |               |           |                             |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5g <sup>1</sup> G <sub>4</sub>              | 4.4619E+00    | 5.547E-15 | 2.065E-01                   |               |           |                             |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5g <sup>1</sup> G <sub>4</sub>              | 1.3931E+01    | 1.748E-13 | 6.674E-01                   |               |           |                             |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s5g <sup>1</sup> G <sub>4</sub>              | 1.4236E+01    | 1.107E-07 | 4.048E+05                   | 1.4175E+01    | 1.111E-07 | 4.065E+05                   |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s5g <sup>1</sup> G <sub>4</sub>              | 1.4241E+01    | 1.421E-06 | 5.192E+06                   | 1.4181E+01    | 1.426E-06 | 5.211E+06                   |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s5g <sup>1</sup> G <sub>4</sub>              | 1.4361E+01    | 1.174E-06 | 4.218E+06                   | 1.4299E+01    | 1.183E-06 | 4.252E+06                   |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s5g <sup>1</sup> G <sub>4</sub>              | 1.4364E+01    | 1.291E-05 | 4.637E+07                   | 1.4303E+01    | 1.301E-05 | 4.673E+07                   |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s5g <sup>1</sup> G <sub>4</sub>              | 7.7310E+02    | 3.149E-18 | 3.904E-09                   |               |           |                             |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s5g <sup>1</sup> G <sub>4</sub>              | 1.9730E+03    | 6.937E-14 | 1.321E-05                   | 1.9684E+03    | 6.886E-14 | 1.306E-05                   |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s5g <sup>1</sup> G <sub>4</sub>              | 2.0256E+03    | 8.205E-13 | 1.482E-04                   | 2.0210E+03    | 8.142E-13 | 1.464E-04                   |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s5g <sup>1</sup> G <sub>4</sub>              | 5.1744E+03    | 4.089E-14 | 1.132E-06                   | 5.1563E+03    | 4.086E-14 | 1.129E-06                   |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s5g <sup>1</sup> G <sub>4</sub>              | 5.4521E+03    | 3.846E-13 | 9.589E-06                   | 5.4339E+03    | 3.841E-13 | 9.561E-06                   |
| 1s2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 1.3813E+00    | 1.649E-10 | 1.922E+05                   | 1.3756E+00    | 2.617E-10 | 3.049E+05                   |
| 1s2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 1.4438E+00    | 1.444E-07 | 1.540E+08                   | 1.4378E+00    | 1.405E-07 | 1.498E+08                   |
| 1s2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 1.4497E+00    | 1.473E-07 | 1.558E+08                   | 1.4438E+00    | 1.385E-07 | 1.465E+08                   |
| 1s3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 3.7169E+00    | 1.013E-10 | 1.630E+04                   | 3.7018E+00    | 1.480E-10 | 2.381E+04                   |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 3.8504E+00    | 9.482E-08 | 1.422E+07                   | 3.8346E+00    | 9.350E-08 | 1.401E+07                   |
| 1s3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 3.8623E+00    | 9.621E-08 | 1.434E+07                   | 3.8466E+00    | 9.250E-08 | 1.378E+07                   |
| 1s4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 8.9847E+00    | 6.745E-11 | 1.858E+03                   | 8.9484E+00    | 9.833E-11 | 2.707E+03                   |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 9.3128E+00    | 6.550E-08 | 1.679E+06                   | 9.2750E+00    | 6.491E-08 | 1.663E+06                   |
| 1s4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 9.3416E+00    | 6.643E-08 | 1.693E+06                   | 9.3040E+00    | 6.422E-08 | 1.635E+06                   |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 9.4480E+00    | 3.729E-15 | 9.287E-02                   |               |           |                             |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 9.4503E+00    | 1.759E-16 | 4.380E-03                   |               |           |                             |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 9.5047E+00    | 1.805E-14 | 4.441E-01                   |               |           |                             |
| 1s5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 2.5714E+01    | 4.946E-11 | 1.663E+02                   | 2.5617E+01    | 7.675E-11 | 2.578E+02                   |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6s <sup>3</sup> S <sub>1</sub>              | 2.7109E+01    | 4.962E-08 | 1.501E+05                   | 2.7006E+01    | 4.914E-08 | 1.485E+05                   |

(continued on next page)

Table 6 (continued)

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |           |                  |
|-----------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                 |                 | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 5p $^1P_1^o$ | 1s 6s $^3S_1$   | 2.7232E+01    | 5.040E-08 | 1.511E+05        | 2.7131E+01    | 4.840E-08 | 1.449E+05        |
| 1s 5f $^3F_3^o$ | 1s 6s $^3S_1$   | 2.7699E+01    | 4.652E-15 | 1.348E-02        |               |           |                  |
| 1s 5f $^3F_2^o$ | 1s 6s $^3S_1$   | 2.7709E+01    | 7.330E-17 | 2.123E-04        |               |           |                  |
| 1s 5f $^1F_3^o$ | 1s 6s $^3S_1$   | 2.7950E+01    | 3.169E-14 | 9.021E-02        |               |           |                  |
| 1s 2s $^3S_1$   | 1s 6p $^3P_1^o$ | 1.3692E+00    | 1.564E-09 | 1.855E+06        | 1.3634E+00    | 2.513E-09 | 2.980E+06        |
| 1s 3s $^3S_1$   | 1s 6p $^3P_0^o$ | 3.6909E+00    | 5.170E-10 | 8.438E+04        | 3.6756E+00    | 7.777E-10 | 1.269E+05        |
| 1s 3d $^3D_2$   | 1s 6p $^3P_1^o$ | 3.8574E+00    | 9.776E-10 | 1.461E+05        | 3.8413E+00    | 9.678E-10 | 1.445E+05        |
| 1s 3d $^3D_1$   | 1s 6p $^3P_0^o$ | 3.8592E+00    | 9.778E-10 | 1.460E+05        | 3.8431E+00    | 9.506E-10 | 1.419E+05        |
| 1s 3d $^3D_3$   | 1s 6p $^3P_0^o$ | 3.9015E+00    | 1.634E-08 | 2.387E+06        | 3.8850E+00    | 1.597E-08 | 2.333E+06        |
| 1s 3d $^1D_2$   | 1s 6p $^3P_1^o$ | 3.9032E+00    | 6.202E-09 | 9.052E+05        | 3.8868E+00    | 6.120E-09 | 8.930E+05        |
| 1s 4s $^3S_1$   | 1s 6p $^3P_0^o$ | 8.9132E+00    | 2.368E-10 | 6.628E+03        | 8.8765E+00    | 3.358E-10 | 9.397E+03        |
| 1s 4d $^3D_2$   | 1s 6p $^3P_0^o$ | 9.3198E+00    | 1.118E-09 | 2.863E+04        | 9.2819E+00    | 1.114E-09 | 2.851E+04        |
| 1s 4d $^3D_1$   | 1s 6p $^3P_1^o$ | 9.3241E+00    | 1.101E-09 | 2.815E+04        | 9.2861E+00    | 1.082E-09 | 2.767E+04        |
| 1s 4d $^3D_3$   | 1s 6p $^3P_0^o$ | 9.4285E+00    | 1.839E-08 | 4.600E+05        | 9.3898E+00    | 1.808E-08 | 4.521E+05        |
| 1s 4d $^1D_2$   | 1s 6p $^3P_0^o$ | 9.4329E+00    | 6.934E-09 | 1.733E+05        | 9.3943E+00    | 6.934E-09 | 1.732E+05        |
| 1s 5s $^3S_1$   | 1s 6p $^3P_0^o$ | 2.5356E+01    | 1.264E-10 | 4.372E+02        | 2.5254E+01    | 1.596E-10 | 5.519E+02        |
| 1s 5d $^3D_2$   | 1s 6p $^3P_0^o$ | 2.7067E+01    | 1.122E-09 | 3.406E+03        | 2.6964E+01    | 1.119E-09 | 3.395E+03        |
| 1s 5d $^3D_1$   | 1s 6p $^3P_0^o$ | 2.7084E+01    | 1.096E-09 | 3.323E+03        | 2.6981E+01    | 1.082E-09 | 3.276E+03        |
| 1s 5d $^3D_3$   | 1s 6p $^3P_0^o$ | 2.7538E+01    | 1.837E-08 | 5.387E+04        | 2.7432E+01    | 1.814E-08 | 5.314E+04        |
| 1s 5d $^1D_2$   | 1s 6p $^3P_1^o$ | 2.7558E+01    | 6.906E-09 | 2.022E+04        | 2.7452E+01    | 6.892E-09 | 2.016E+04        |
| 1s 5g $^3G_3$   | 1s 6p $^3P_0^o$ | 2.7793E+01    | 9.899E-18 | 2.850E-05        |               |           |                  |
| 1s 6s $^3S_1$   | 1s 6p $^3P_0^o$ | 4.9854E+03    | 3.274E-16 | 2.929E-08        | 4.6146E+03    | 7.235E-16 | 7.490E-08        |
| 1s 2p $^3P_2^o$ | 1s 6s $^1S_0$   | 1.4434E+00    | 9.229E-08 | 2.955E+08        | 1.4374E+00    | 9.373E-08 | 3.000E+08        |
| 1s 3p $^3P_2^o$ | 1s 6s $^1S_0$   | 3.8473E+00    | 6.108E-08 | 2.753E+07        | 3.8320E+00    | 6.246E-08 | 2.813E+07        |
| 1s 4p $^3P_2^o$ | 1s 6s $^1S_0$   | 9.2946E+00    | 4.218E-08 | 3.257E+06        | 9.2596E+00    | 4.349E-08 | 3.354E+06        |
| 1s 4f $^3F_2^o$ | 1s 6s $^1S_0$   | 9.4316E+00    | 4.585E-15 | 3.438E-01        |               |           |                  |
| 1s 5p $^3P_2^o$ | 1s 6s $^1S_0$   | 2.6955E+01    | 3.177E-08 | 2.917E+05        | 2.6876E+01    | 3.323E-08 | 3.043E+05        |
| 1s 5f $^3F_2^o$ | 1s 6s $^1S_0$   | 2.7549E+01    | 6.717E-15 | 5.903E-02        |               |           |                  |
| 1s 3d $^3D_2$   | 1s 6p $^3P_0^o$ | 3.8572E+00    | 6.303E-10 | 2.826E+05        | 3.8418E+00    | 6.184E-10 | 2.771E+05        |
| 1s 3d $^1D_2$   | 1s 6p $^3P_0^o$ | 3.9029E+00    | 7.563E-09 | 3.312E+06        | 3.8873E+00    | 7.362E-09 | 3.222E+06        |
| 1s 4d $^3D_2$   | 1s 6p $^3P_0^o$ | 9.3186E+00    | 7.033E-10 | 5.403E+04        | 9.2852E+00    | 6.944E-10 | 5.327E+04        |
| 1s 4d $^1D_2$   | 1s 6p $^3P_0^o$ | 9.4317E+00    | 8.476E-09 | 6.355E+05        | 9.3976E+00    | 8.342E-09 | 6.247E+05        |
| 1s 5d $^3D_2$   | 1s 6p $^3P_0^o$ | 2.7056E+01    | 6.977E-10 | 6.357E+03        | 2.6991E+01    | 6.888E-10 | 6.253E+03        |
| 1s 5d $^1D_2$   | 1s 6p $^3P_0^o$ | 2.7547E+01    | 8.449E-09 | 7.426E+04        | 2.7481E+01    | 8.332E-09 | 7.297E+04        |
| 1s $^2^1S_0$    | 1s 6p $^3P_2^o$ | 3.1630E-01    | 9.827E-06 | 1.310E+11        | 3.1498E-01    | 1.106E-05 | 1.475E+11        |
| 1s 2s $^3S_1$   | 1s 6p $^3P_2^o$ | 1.3670E+00    | 1.115E-06 | 7.956E+08        | 1.3612E+00    | 1.152E-06 | 8.224E+08        |
| 1s 2s $^1S_0$   | 1s 6p $^3P_2^o$ | 1.3800E+00    | 7.427E-07 | 5.203E+08        | 1.3743E+00    | 7.463E-07 | 5.226E+08        |
| 1s 3s $^3S_1$   | 1s 6p $^3P_2^o$ | 3.6753E+00    | 3.545E-07 | 3.501E+07        | 3.6601E+00    | 3.604E-07 | 3.559E+07        |
| 1s 3s $^1S_0$   | 1s 6p $^3P_2^o$ | 3.6999E+00    | 2.408E-07 | 2.347E+07        | 3.6849E+00    | 2.354E-07 | 2.293E+07        |
| 1s 3d $^3D_2$   | 1s 6p $^3P_2^o$ | 3.8403E+00    | 1.356E-14 | 1.227E+00        |               |           |                  |
| 1s 3d $^3D_1$   | 1s 6p $^3P_2^o$ | 3.8421E+00    | 3.557E-13 | 3.214E+01        |               |           |                  |
| 1s 3d $^3D_3$   | 1s 6p $^3P_2^o$ | 3.8840E+00    | 5.812E-08 | 5.139E+06        | 3.8677E+00    | 5.623E-08 | 4.972E+06        |
| 1s 3d $^1D_2$   | 1s 6p $^3P_2^o$ | 3.8856E+00    | 1.476E-08 | 1.304E+06        | 3.8694E+00    | 1.403E-08 | 1.240E+06        |
| 1s 4s $^3S_1$   | 1s 6p $^3P_2^o$ | 8.8224E+00    | 1.571E-07 | 2.692E+06        | 8.7863E+00    | 1.589E-07 | 2.723E+06        |
| 1s 4s $^1S_0$   | 1s 6p $^3P_2^o$ | 8.8798E+00    | 1.078E-07 | 1.824E+06        | 8.8440E+00    | 1.038E-07 | 1.756E+06        |
| 1s 4d $^3D_2$   | 1s 6p $^3P_2^o$ | 9.2206E+00    | 2.240E-13 | 3.514E+00        |               |           |                  |
| 1s 4d $^3D_1$   | 1s 6p $^3P_2^o$ | 9.2248E+00    | 2.274E-13 | 3.564E+00        |               |           |                  |
| 1s 4d $^3D_3$   | 1s 6p $^3P_2^o$ | 9.3270E+00    | 6.780E-08 | 1.040E+06        | 9.2888E+00    | 6.619E-08 | 1.014E+06        |
| 1s 4d $^1D_2$   | 1s 6p $^3P_2^o$ | 9.3314E+00    | 1.709E-08 | 2.619E+05        | 9.2933E+00    | 1.652E-08 | 2.530E+05        |
| 1s 5s $^3S_1$   | 1s 6p $^3P_2^o$ | 2.4635E+01    | 7.930E-08 | 1.743E+05        | 2.4537E+01    | 8.016E-08 | 1.761E+05        |
| 1s 5s $^1S_0$   | 1s 6p $^3P_2^o$ | 2.4860E+01    | 5.498E-08 | 1.187E+05        | 2.4762E+01    | 5.199E-08 | 1.121E+05        |
| 1s 5d $^3D_2$   | 1s 6p $^3P_2^o$ | 2.6247E+01    | 4.110E-13 | 7.959E-01        |               |           |                  |
| 1s 5d $^3D_1$   | 1s 6p $^3P_2^o$ | 2.6264E+01    | 1.397E-13 | 2.703E-01        |               |           |                  |
| 1s 5d $^3D_3$   | 1s 6p $^3P_2^o$ | 2.6690E+01    | 6.829E-08 | 1.279E+05        | 2.6588E+01    | 6.672E-08 | 1.248E+05        |
| 1s 5d $^1D_2$   | 1s 6p $^3P_2^o$ | 2.6709E+01    | 1.716E-08 | 3.210E+04        | 2.6607E+01    | 1.664E-08 | 3.110E+04        |
| 1s 5g $^3G_4$   | 1s 6p $^3P_2^o$ | 2.6923E+01    | 3.604E-16 | 6.634E-04        |               |           |                  |
| 1s 5g $^3G_3$   | 1s 6p $^3P_2^o$ | 2.6929E+01    | 8.766E-16 | 1.613E-03        |               |           |                  |
| 1s 5g $^1G_4$   | 1s 6p $^3P_2^o$ | 2.7064E+01    | 1.057E-15 | 1.924E-03        |               |           |                  |
| 1s 6s $^3S_1$   | 1s 6p $^3P_2^o$ | 7.3822E+02    | 8.147E-11 | 1.994E-01        | 7.2782E+02    | 8.413E-11 | 2.100E-01        |
| 1s 6s $^1S_0$   | 1s 6p $^3P_2^o$ | 8.7342E+02    | 3.282E-11 | 5.739E-02        | 8.3711E+02    | 3.686E-11 | 6.958E-02        |
| 1s 2p $^3P_0^o$ | 1s 6d $^3D_2$   | 1.3786E+00    | 7.357E-08 | 5.164E+07        | 1.3729E+00    | 8.090E-08 | 5.677E+07        |
| 1s 2p $^3P_1^o$ | 1s 6d $^3D_2$   | 1.3795E+00    | 4.617E-08 | 3.237E+07        | 1.3737E+00    | 4.698E-08 | 3.293E+07        |
| 1s 2p $^3P_2^o$ | 1s 6d $^3D_2$   | 1.4409E+00    | 4.355E-11 | 2.798E+04        | 1.4348E+00    | 1.874E-10 | 1.204E+05        |
| 1s 2p $^1P_1^o$ | 1s 6d $^3D_2$   | 1.4467E+00    | 3.892E-13 | 2.481E+02        | 1.4407E+00    | 1.020E-10 | 6.504E+04        |
| 1s 3p $^3P_0^o$ | 1s 6d $^3D_2$   | 3.6972E+00    | 2.620E-08 | 2.557E+06        | 3.6817E+00    | 2.754E-08 | 2.688E+06        |
| 1s 3p $^3P_1^o$ | 1s 6d $^3D_2$   | 3.6989E+00    | 1.627E-08 | 1.586E+06        | 3.6834E+00    | 1.603E-08 | 1.563E+06        |
| 1s 3p $^3P_2^o$ | 1s 6d $^3D_2$   | 3.8292E+00    | 1.916E-11 | 1.744E+03        | 3.8130E+00    | 6.803E-11 | 6.189E+03        |
| 1s 3p $^1P_1^o$ | 1s 6d $^3D_2$   | 3.8409E+00    | 6.830E-13 | 6.176E+01        | 3.8249E+00    | 4.396E-11 | 3.974E+03        |
| 1s 4p $^3P_0^o$ | 1s 6d $^3D_2$   | 8.8702E+00    | 1.140E-08 | 1.933E+05        | 8.8316E+00    | 1.183E-08 | 2.006E+05        |
| 1s 4p $^3P_1^o$ | 1s 6d $^3D_2$   | 8.8742E+00    | 7.076E-09 | 1.199E+05        | 8.8354E+00    | 6.901E-09 | 1.169E+05        |
| 1s 4p $^3P_2^o$ | 1s 6d $^3D_2$   | 9.1898E+00    | 9.056E-12 | 1.431E+02        | 9.1496E+00    | 3.048E-11 | 4.816E+02        |

(continued on next page)

Table 6 (continued)

| Lower  | Upper  | GRASP2K       |           |                             | FAC           |           |                             |
|--|--|---------------|-----------|-----------------------------|---------------|-----------|-----------------------------|
|  |  | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 9.2178E+00    | 4.459E-13 | 7.001E+00                   | 9.1778E+00    | 2.140E-11 | 3.361E+02                   |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 9.3215E+00    | 3.189E-09 | 4.896E+04                   | 9.2809E+00    | 3.158E-09 | 4.849E+04                   |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 9.3237E+00    | 8.011E-10 | 1.229E+04                   | 9.2831E+00    | 7.907E-10 | 1.213E+04                   |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 9.3749E+00    | 6.477E-09 | 9.832E+04                   | 9.3339E+00    | 6.370E-09 | 9.671E+04                   |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 9.3766E+00    | 7.961E-10 | 1.208E+04                   | 9.3356E+00    | 8.302E-10 | 1.260E+04                   |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 2.4798E+01    | 5.473E-09 | 1.187E+04                   | 2.4683E+01    | 5.652E-09 | 1.227E+04                   |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 2.4813E+01    | 3.400E-09 | 7.368E+03                   | 2.4698E+01    | 3.305E-09 | 7.167E+03                   |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 2.6092E+01    | 4.739E-12 | 9.286E+00                   | 2.5970E+01    | 1.516E-11 | 2.974E+01                   |
| 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 2.6207E+01    | 2.750E-13 | 5.341E-01                   | 2.6085E+01    | 1.163E-11 | 2.262E+01                   |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 2.6639E+01    | 5.658E-09 | 1.064E+04                   | 2.6517E+01    | 5.635E-09 | 1.060E+04                   |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 2.6648E+01    | 1.421E-09 | 2.669E+03                   | 2.6526E+01    | 1.410E-09 | 2.651E+03                   |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 2.6863E+01    | 1.142E-08 | 2.112E+04                   | 2.6740E+01    | 1.129E-08 | 2.089E+04                   |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 2.6870E+01    | 1.403E-09 | 2.593E+03                   | 2.6747E+01    | 1.470E-09 | 2.718E+03                   |
| 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 8.0869E+02    | 2.361E-12 | 4.815E-03                   | 7.9302E+02    | 2.548E-12 | 5.360E-03                   |
| 1s 6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 8.1823E+02    | 1.413E-12 | 2.816E-03                   | 7.6994E+02    | 1.621E-12 | 3.618E-03                   |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>2</sub>              | 1.2115E+04    | 5.193E-19 | 4.720E-12                   |               |           |                             |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.3668E+00    | 1.105E-06 | 1.315E+09                   | 1.3611E+00    | 1.149E-06 | 1.368E+09                   |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.6740E+00    | 3.498E-07 | 5.762E+07                   | 3.6589E+00    | 3.600E-07 | 5.928E+07                   |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.8389E+00    | 2.598E-13 | 3.919E+01                   |               |           |                             |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.8407E+00    | 1.055E-14 | 1.590E+00                   |               |           |                             |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.8825E+00    | 1.013E-08 | 1.494E+06                   | 3.8664E+00    | 1.059E-08 | 1.562E+06                   |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.8842E+00    | 3.253E-08 | 4.794E+06                   | 3.8681E+00    | 3.153E-08 | 4.646E+06                   |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 8.8149E+00    | 1.545E-07 | 4.420E+06                   | 8.7796E+00    | 1.589E-07 | 4.545E+06                   |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 9.2125E+00    | 1.128E-14 | 2.955E-01                   |               |           |                             |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 9.2166E+00    | 1.136E-13 | 2.974E+00                   |               |           |                             |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 9.3186E+00    | 1.187E-08 | 3.038E+05                   | 9.2814E+00    | 1.247E-08 | 3.192E+05                   |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 9.3230E+00    | 3.780E-08 | 9.670E+05                   | 9.2858E+00    | 3.718E-08 | 9.507E+05                   |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.4577E+01    | 7.756E-08 | 2.855E+05                   | 2.4485E+01    | 8.050E-08 | 2.960E+05                   |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.6180E+01    | 9.174E-15 | 2.976E-02                   |               |           |                             |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.6197E+01    | 2.364E-13 | 7.658E-01                   |               |           |                             |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.6621E+01    | 1.196E-08 | 3.753E+04                   | 2.6527E+01    | 1.267E-08 | 3.970E+04                   |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.6640E+01    | 3.799E-08 | 1.190E+05                   | 2.6546E+01    | 3.758E-08 | 1.175E+05                   |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 2.6859E+01    | 8.269E-18 | 2.548E-05                   |               |           |                             |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 6.8918E+02    | 1.001E-10 | 4.688E-01                   | 6.8482E+02    | 1.007E-10 | 4.737E-01                   |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.2196E+04    | 1.674E-22 | 7.143E-17                   |               |           |                             |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 1.3786E+00    | 7.220E-08 | 8.447E+07                   | 1.3729E+00    | 7.636E-08 | 8.932E+07                   |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 1.4408E+00    | 1.425E-13 | 1.527E+02                   |               |           |                             |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 1.4467E+00    | 8.401E-11 | 8.924E+04                   | 1.4407E+00    | 1.079E-10 | 1.146E+05                   |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 3.6970E+00    | 2.546E-08 | 4.142E+06                   | 3.6817E+00    | 2.602E-08 | 4.232E+06                   |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 3.8290E+00    | 1.910E-13 | 2.896E+01                   |               |           |                             |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 3.8407E+00    | 2.859E-11 | 4.309E+03                   | 3.8249E+00    | 3.310E-11 | 4.989E+03                   |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 8.8691E+00    | 1.105E-08 | 3.125E+05                   | 8.8318E+00    | 1.118E-08 | 3.161E+05                   |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 9.1886E+00    | 1.273E-13 | 3.352E+00                   |               |           |                             |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 9.2166E+00    | 1.238E-11 | 3.240E+02                   | 9.1781E+00    | 1.357E-11 | 3.553E+02                   |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 9.3202E+00    | 5.366E-10 | 1.374E+04                   | 9.2811E+00    | 5.341E-10 | 1.367E+04                   |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 9.3225E+00    | 1.860E-09 | 4.759E+04                   | 9.2834E+00    | 1.845E-09 | 4.719E+04                   |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 9.3753E+00    | 4.340E-09 | 1.098E+05                   | 9.3359E+00    | 4.305E-09 | 1.088E+05                   |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.4789E+01    | 5.299E-09 | 1.917E+04                   | 2.4685E+01    | 5.349E-09 | 1.935E+04                   |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6083E+01    | 8.543E-14 | 2.792E-01                   |               |           |                             |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6197E+01    | 6.135E-12 | 1.988E+01                   | 2.6087E+01    | 6.049E-12 | 1.959E+01                   |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6629E+01    | 9.512E-10 | 2.983E+03                   | 2.6519E+01    | 9.521E-10 | 2.984E+03                   |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6638E+01    | 3.300E-09 | 1.034E+04                   | 2.6529E+01    | 3.290E-09 | 1.030E+04                   |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 2.6860E+01    | 7.654E-09 | 2.359E+04                   | 2.6749E+01    | 7.630E-09 | 2.351E+04                   |
| 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 7.9964E+02    | 2.369E-12 | 8.238E-03                   | 7.9517E+02    | 2.385E-12 | 8.315E-03                   |
| 1s 6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 1.0358E+04    | 5.839E-20 | 1.210E-12                   |               |           |                             |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>1</sub>              | 6.7159E+06    | 2.936E-27 | 1.447E-25                   |               |           |                             |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 1.3779E+00    | 1.185E-06 | 5.945E+08                   | 1.3722E+00    | 1.211E-06 | 6.080E+08                   |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 1.4401E+00    | 5.129E-06 | 2.357E+09                   | 1.4340E+00    | 5.376E-06 | 2.470E+09                   |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 1.4460E+00    | 9.200E-07 | 4.193E+08                   | 1.4400E+00    | 9.661E-07 | 4.402E+08                   |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 3.6922E+00    | 3.978E-07 | 2.780E+07                   | 3.6768E+00    | 4.047E-07 | 2.829E+07                   |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 3.8238E+00    | 1.918E-06 | 1.250E+08                   | 3.8077E+00    | 1.956E-06 | 1.275E+08                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 3.8355E+00    | 3.451E-07 | 2.236E+07                   | 3.8195E+00    | 3.499E-07 | 2.266E+07                   |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 8.8415E+00    | 1.680E-07 | 2.047E+06                   | 8.8033E+00    | 1.690E-07 | 2.060E+06                   |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.1590E+00    | 8.734E-07 | 9.922E+06                   | 9.1192E+00    | 8.851E-07 | 1.005E+07                   |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.1868E+00    | 1.579E-07 | 1.783E+06                   | 9.1472E+00    | 1.575E-07 | 1.778E+06                   |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.2898E+00    | 2.242E-14 | 2.476E-01                   |               |           |                             |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.2920E+00    | 9.727E-14 | 1.074E+00                   |               |           |                             |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.3429E+00    | 3.624E-08 | 3.957E+05                   | 9.3023E+00    | 3.574E-08 | 3.903E+05                   |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 9.3445E+00    | 4.358E-09 | 4.756E+04                   | 9.3039E+00    | 4.287E-09 | 4.679E+04                   |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.4575E+01    | 7.820E-08 | 1.234E+05                   | 2.4463E+01    | 7.792E-08 | 1.230E+05                   |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 6d <sup>3</sup> D <sub>3</sub>              | 2.5845E+01    | 4.441E-07 | 6.335E+05                   | 2.5726E+01    | 4.508E-07 | 6.436E+05                   |

(continued on next page)

Table 6 (continued)

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |           |                  |
|-----------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                 |                 | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 5p $^1P_1^o$ | 1s 6d $^3D_3$   | 2.5958E+01    | 8.083E-08 | 1.143E+05        | 2.5839E+01    | 7.947E-08 | 1.124E+05        |
| 1s 5f $^3F_2^o$ | 1s 6d $^3D_3$   | 2.6382E+01    | 3.376E-14 | 4.622E-02        |               |           |                  |
| 1s 5f $^3F_0^o$ | 1s 6d $^3D_3$   | 2.6391E+01    | 8.504E-14 | 1.163E-01        |               |           |                  |
| 1s 5f $^3F_4^o$ | 1s 6d $^3D_3$   | 2.6602E+01    | 6.478E-08 | 8.723E+04        | 2.6482E+01    | 6.437E-08 | 8.672E+04        |
| 1s 5f $^1F_3^o$ | 1s 6d $^3D_3$   | 2.6609E+01    | 7.788E-09 | 1.048E+04        | 2.6489E+01    | 7.718E-09 | 1.039E+04        |
| 1s 6p $^3P_0^o$ | 1s 6d $^3D_3$   | 6.2409E+02    | 7.844E-11 | 1.919E-01        | 6.1530E+02    | 7.917E-11 | 1.975E-01        |
| 1s 6p $^3P_2^o$ | 1s 6d $^3D_3$   | 2.2306E+03    | 8.574E-12 | 1.642E-03        | 2.1370E+03    | 9.635E-12 | 1.993E-03        |
| 1s 6p $^1P_1^o$ | 1s 6d $^3D_3$   | 2.8416E+03    | 7.471E-13 | 8.817E-05        | 2.6199E+03    | 9.643E-13 | 1.327E-04        |
| 1s 2s $^3S_1$   | 1s 6f $^3F_3^o$ | 1.3662E+00    | 6.354E-11 | 3.244E+04        |               |           |                  |
| 1s 3s $^3S_1$   | 1s 6f $^3F_3^o$ | 3.6691E+00    | 3.991E-14 | 2.825E+00        |               |           |                  |
| 1s 3d $^3D_2$   | 1s 6f $^3F_3^o$ | 3.8336E+00    | 3.774E-07 | 2.447E+07        | 3.8174E+00    | 3.877E-07 | 2.513E+07        |
| 1s 3d $^3D_1$   | 1s 6f $^3F_3^o$ | 3.8354E+00    | 6.366E-08 | 4.124E+06        | 3.8192E+00    | 6.429E-08 | 4.164E+06        |
| 1s 3d $^3D_3$   | 1s 6f $^3F_3^o$ | 3.8771E+00    | 2.152E-12 | 1.364E+02        |               |           |                  |
| 1s 3d $^1D_2$   | 1s 6f $^3F_3^o$ | 3.8788E+00    | 2.980E-11 | 1.887E+03        |               |           |                  |
| 1s 4s $^3S_1$   | 1s 6f $^3F_3^o$ | 8.7872E+00    | 1.208E-13 | 1.491E+00        |               |           |                  |
| 1s 4d $^3D_2$   | 1s 6f $^3F_3^o$ | 9.1821E+00    | 2.268E-07 | 2.563E+06        | 9.1440E+00    | 2.296E-07 | 2.595E+06        |
| 1s 4d $^3D_1$   | 1s 6f $^3F_3^o$ | 9.1863E+00    | 3.827E-08 | 4.321E+05        | 9.1480E+00    | 3.808E-08 | 4.299E+05        |
| 1s 4d $^3D_3$   | 1s 6f $^3F_3^o$ | 9.2876E+00    | 1.258E-12 | 1.390E+01        |               |           |                  |
| 1s 4d $^1D_2$   | 1s 6f $^3F_3^o$ | 9.2919E+00    | 2.710E-11 | 2.991E+02        |               |           |                  |
| 1s 5s $^3S_1$   | 1s 6f $^3F_3^o$ | 2.4362E+01    | 5.695E-15 | 9.143E-03        |               |           |                  |
| 1s 5d $^3D_2$   | 1s 6f $^3F_3^o$ | 2.5937E+01    | 1.250E-07 | 1.770E+05        | 2.5831E+01    | 1.257E-07 | 1.780E+05        |
| 1s 5d $^3D_1$   | 1s 6f $^3F_3^o$ | 2.5954E+01    | 2.111E-08 | 2.987E+04        | 2.5848E+01    | 2.083E-08 | 2.946E+04        |
| 1s 5d $^3D_3$   | 1s 6f $^3F_3^o$ | 2.6370E+01    | 7.159E-13 | 9.810E-01        |               |           |                  |
| 1s 5d $^1D_2$   | 1s 6f $^3F_3^o$ | 2.6388E+01    | 1.786E-11 | 2.444E+01        |               |           |                  |
| 1s 5g $^3G_4$   | 1s 6f $^3F_3^o$ | 2.6598E+01    | 6.169E-09 | 8.309E+03        | 2.6482E+01    | 6.138E-09 | 8.270E+03        |
| 1s 5g $^3G_3$   | 1s 6f $^3F_3^o$ | 2.6603E+01    | 7.426E-10 | 9.999E+02        | 2.6487E+01    | 7.367E-10 | 9.922E+02        |
| 1s 5g $^3G_5$   | 1s 6f $^3F_3^o$ | 2.6730E+01    | 4.453E-09 | 5.938E+03        | 2.6614E+01    | 4.418E-09 | 5.893E+03        |
| 1s 5g $^1G_4$   | 1s 6f $^3F_3^o$ | 2.6735E+01    | 2.634E-10 | 3.512E+02        | 2.6618E+01    | 2.759E-10 | 3.679E+02        |
| 1s 6s $^3S_1$   | 1s 6f $^3F_3^o$ | 5.5267E+02    | 1.173E-17 | 3.658E-08        |               |           |                  |
| 1s 6d $^3D_2$   | 1s 6f $^3F_3^o$ | 2.6863E+03    | 7.605E-13 | 1.004E-04        | 2.7429E+03    | 7.086E-13 | 8.898E-05        |
| 1s 6d $^3D_1$   | 1s 6f $^3F_3^o$ | 2.7912E+03    | 1.144E-13 | 1.399E-05        | 2.7175E+03    | 1.210E-13 | 1.548E-05        |
| 1s 6d $^3D_3$   | 1s 6f $^3F_3^o$ | 1.5394E+05    | 2.306E-23 | 9.272E-19        |               |           |                  |
| 1s $^2S_0$      | 1s 6f $^3F_2^o$ | 3.1620E-01    | 6.848E-11 | 9.134E+05        |               |           |                  |
| 1s 2s $^3S_1$   | 1s 6f $^3F_2^o$ | 1.3662E+00    | 2.222E-11 | 1.588E+04        |               |           |                  |
| 1s 2s $^1S_0$   | 1s 6f $^3F_2^o$ | 1.3791E+00    | 2.075E-11 | 1.456E+04        |               |           |                  |
| 1s 3s $^3S_1$   | 1s 6f $^3F_2^o$ | 3.6690E+00    | 4.287E-13 | 4.249E+01        |               |           |                  |
| 1s 3s $^1S_0$   | 1s 6f $^3F_2^o$ | 3.6936E+00    | 3.226E-13 | 3.155E+01        |               |           |                  |
| 1s 3d $^3D_2$   | 1s 6f $^3F_2^o$ | 3.8335E+00    | 9.471E-08 | 8.598E+06        | 3.8174E+00    | 9.688E-08 | 8.794E+06        |
| 1s 3d $^3D_1$   | 1s 6f $^3F_2^o$ | 3.8353E+00    | 2.205E-07 | 2.000E+07        | 3.8192E+00    | 2.257E-07 | 2.047E+07        |
| 1s 3d $^3D_3$   | 1s 6f $^3F_2^o$ | 3.8770E+00    | 1.142E-18 | 1.013E-04        |               |           |                  |
| 1s 3d $^1D_2$   | 1s 6f $^3F_2^o$ | 3.8787E+00    | 8.803E-13 | 7.806E+01        |               |           |                  |
| 1s 4s $^3S_1$   | 1s 6f $^3F_2^o$ | 8.7866E+00    | 5.076E-13 | 8.772E+00        |               |           |                  |
| 1s 4s $^1S_0$   | 1s 6f $^3F_2^o$ | 8.8435E+00    | 3.256E-13 | 5.554E+00        |               |           |                  |
| 1s 4d $^3D_2$   | 1s 6f $^3F_2^o$ | 9.1815E+00    | 5.683E-08 | 8.994E+05        | 9.1440E+00    | 5.738E-08 | 9.077E+05        |
| 1s 4d $^3D_1$   | 1s 6f $^3F_2^o$ | 9.1856E+00    | 1.325E-07 | 2.095E+06        | 9.1480E+00    | 1.337E-07 | 2.113E+06        |
| 1s 4d $^3D_3$   | 1s 6f $^3F_2^o$ | 9.2869E+00    | 1.242E-14 | 1.921E-01        |               |           |                  |
| 1s 4d $^1D_2$   | 1s 6f $^3F_2^o$ | 9.2913E+00    | 1.382E-12 | 2.135E+01        |               |           |                  |
| 1s 5s $^3S_1$   | 1s 6f $^3F_2^o$ | 2.4358E+01    | 1.928E-13 | 4.335E-01        |               |           |                  |
| 1s 5s $^1S_0$   | 1s 6f $^3F_2^o$ | 2.4577E+01    | 9.292E-14 | 2.052E-01        |               |           |                  |
| 1s 5d $^3D_2$   | 1s 6f $^3F_2^o$ | 2.5932E+01    | 3.129E-08 | 6.207E+04        | 2.5831E+01    | 3.141E-08 | 6.227E+04        |
| 1s 5d $^3D_1$   | 1s 6f $^3F_2^o$ | 2.5948E+01    | 7.306E-08 | 1.447E+05        | 2.5848E+01    | 7.316E-08 | 1.448E+05        |
| 1s 5d $^3D_3$   | 1s 6f $^3F_2^o$ | 2.6365E+01    | 1.482E-14 | 2.845E-02        |               |           |                  |
| 1s 5d $^1D_2$   | 1s 6f $^3F_2^o$ | 2.6383E+01    | 1.033E-12 | 1.979E+00        |               |           |                  |
| 1s 5g $^3G_4$   | 1s 6f $^3F_2^o$ | 2.6592E+01    | 4.970E-10 | 9.377E+02        | 2.6482E+01    | 4.963E-10 | 9.362E+02        |
| 1s 5g $^3G_3$   | 1s 6f $^3F_2^o$ | 2.6598E+01    | 4.442E-09 | 8.376E+03        | 2.6488E+01    | 4.420E-09 | 8.334E+03        |
| 1s 5g $^1G_4$   | 1s 6f $^3F_2^o$ | 2.6729E+01    | 3.356E-09 | 6.266E+03        | 2.6618E+01    | 3.343E-09 | 6.241E+03        |
| 1s 6s $^3S_1$   | 1s 6f $^3F_2^o$ | 5.5035E+02    | 4.304E-17 | 1.896E-07        |               |           |                  |
| 1s 6s $^1S_0$   | 1s 6f $^3F_2^o$ | 6.2215E+02    | 4.276E-17 | 1.474E-07        |               |           |                  |
| 1s 6d $^3D_2$   | 1s 6f $^3F_2^o$ | 2.6325E+03    | 2.025E-13 | 3.898E-05        | 2.7436E+03    | 1.769E-13 | 3.109E-05        |
| 1s 6d $^3D_1$   | 1s 6f $^3F_2^o$ | 2.7332E+03    | 4.220E-13 | 7.536E-05        | 2.7182E+03    | 4.245E-13 | 7.601E-05        |
| 1s 6d $^3D_3$   | 1s 6f $^3F_2^o$ | 7.0900E+04    | 6.510E-23 | 1.728E-17        |               |           |                  |
| 1s 2p $^3P_0^o$ | 1s 6d $^1D_2$   | 1.3779E+00    | 4.573E-07 | 3.213E+08        | 1.3722E+00    | 4.669E-07 | 3.280E+08        |
| 1s 2p $^3P_1^o$ | 1s 6d $^1D_2$   | 1.3788E+00    | 5.490E-07 | 3.852E+08        | 1.3730E+00    | 5.623E-07 | 3.945E+08        |
| 1s 2p $^3P_2^o$ | 1s 6d $^1D_2$   | 1.4401E+00    | 1.289E-06 | 8.293E+08        | 1.4340E+00    | 1.343E-06 | 8.644E+08        |
| 1s 2p $^1P_1^o$ | 1s 6d $^1D_2$   | 1.4459E+00    | 2.881E-06 | 1.839E+09        | 1.4399E+00    | 3.012E-06 | 1.921E+09        |
| 1s 3p $^3P_0^o$ | 1s 6d $^1D_2$   | 3.6920E+00    | 1.505E-07 | 1.472E+07        | 3.6767E+00    | 1.542E-07 | 1.509E+07        |
| 1s 3p $^3P_1^o$ | 1s 6d $^1D_2$   | 3.6937E+00    | 1.833E-07 | 1.793E+07        | 3.6783E+00    | 1.874E-07 | 1.832E+07        |
| 1s 3p $^3P_2^o$ | 1s 6d $^1D_2$   | 3.8236E+00    | 4.803E-07 | 4.383E+07        | 3.8077E+00    | 4.891E-07 | 4.462E+07        |
| 1s 3p $^1P_1^o$ | 1s 6d $^1D_2$   | 3.8353E+00    | 1.087E-06 | 9.861E+07        | 3.8195E+00    | 1.102E-06 | 9.999E+07        |
| 1s 4p $^3P_0^o$ | 1s 6d $^1D_2$   | 8.8403E+00    | 6.306E-08 | 1.076E+06        | 8.8028E+00    | 6.473E-08 | 1.104E+06        |
| 1s 4p $^3P_1^o$ | 1s 6d $^1D_2$   | 8.8442E+00    | 7.726E-08 | 1.318E+06        | 8.8066E+00    | 7.837E-08 | 1.336E+06        |

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Table 6 (continued)

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |           |                  |
|-----------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                 |                 | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 4p $^3P_2^0$ | 1s 6d $^1D_2$   | 9.1577E+00    | 2.183E-07 | 3.473E+06        | 9.1187E+00    | 2.212E-07 | 3.520E+06        |
| 1s 4p $^1P_1^0$ | 1s 6d $^3D_2$   | 9.1855E+00    | 4.979E-07 | 7.872E+06        | 9.1467E+00    | 4.996E-07 | 7.900E+06        |
| 1s 4f $^3F_3^0$ | 1s 6d $^1D_2$   | 9.2884E+00    | 4.634E-13 | 7.165E+00        |               |           |                  |
| 1s 4f $^3F_2^0$ | 1s 6d $^1D_2$   | 9.2907E+00    | 4.578E-18 | 7.075E-05        |               |           |                  |
| 1s 4f $^3F_4^0$ | 1s 6d $^1D_2$   | 9.3415E+00    | 2.936E-09 | 4.489E+04        | 9.3018E+00    | 2.962E-09 | 4.529E+04        |
| 1s 4f $^1F_3^0$ | 1s 6d $^1D_2$   | 9.3432E+00    | 2.595E-08 | 3.966E+05        | 9.3035E+00    | 2.562E-08 | 3.915E+05        |
| 1s 5p $^3P_0^0$ | 1s 6d $^1D_2$   | 2.4566E+01    | 2.924E-08 | 6.463E+04        | 2.4460E+01    | 3.038E-08 | 6.718E+04        |
| 1s 5p $^3P_1^0$ | 1s 6d $^1D_2$   | 2.4581E+01    | 3.593E-08 | 7.934E+04        | 2.4474E+01    | 3.629E-08 | 8.014E+04        |
| 1s 5p $^3P_2^0$ | 1s 6d $^1D_2$   | 2.5835E+01    | 1.108E-07 | 2.215E+05        | 2.5723E+01    | 1.127E-07 | 2.254E+05        |
| 1s 5p $^1P_1^0$ | 1s 6d $^1D_2$   | 2.5947E+01    | 2.547E-07 | 5.046E+05        | 2.5836E+01    | 2.540E-07 | 5.034E+05        |
| 1s 5f $^3F_3^0$ | 1s 6d $^1D_2$   | 2.6371E+01    | 7.765E-13 | 1.490E+00        |               |           |                  |
| 1s 5f $^3F_2^0$ | 1s 6d $^1D_2$   | 2.6380E+01    | 5.047E-15 | 9.676E-03        |               |           |                  |
| 1s 5f $^3F_4^0$ | 1s 6d $^1D_2$   | 2.6591E+01    | 5.248E-09 | 9.902E+03        | 2.6478E+01    | 5.337E-09 | 1.006E+04        |
| 1s 5f $^1F_3^0$ | 1s 6d $^1D_2$   | 2.6598E+01    | 4.638E-08 | 8.747E+04        | 2.6485E+01    | 4.613E-08 | 8.700E+04        |
| 1s 6p $^3P_0^0$ | 1s 6d $^1D_2$   | 6.1807E+02    | 3.022E-11 | 1.055E-01        | 6.1320E+02    | 3.228E-11 | 1.135E-01        |
| 1s 6p $^3P_1^0$ | 1s 6d $^1D_2$   | 6.2363E+02    | 3.613E-11 | 1.239E-01        | 5.9930E+02    | 4.033E-11 | 1.485E-01        |
| 1s 6p $^3P_2^0$ | 1s 6d $^1D_2$   | 2.1556E+03    | 2.376E-12 | 6.821E-04        | 2.1118E+03    | 2.495E-12 | 7.402E-04        |
| 1s 6p $^1P_1^0$ | 1s 6d $^1D_2$   | 2.7210E+03    | 2.688E-12 | 4.843E-04        | 2.5822E+03    | 3.083E-12 | 6.116E-04        |
| 1s 6f $^3F_3^0$ | 1s 6d $^1D_2$   | 1.0989E+05    | 1.664E-21 | 1.838E-16        |               |           |                  |
| 1s 6f $^3F_2^0$ | 1s 6d $^1D_2$   | 6.7056E+05    | 3.229E-25 | 9.582E-22        |               |           |                  |
| 1s 6f $^3F_4^0$ | 1s 6d $^1D_2$   | 3.8310E+00    | 7.454E-07 | 3.764E+07        | 3.8148E+00    | 7.494E-07 | 3.784E+07        |
| 1s 3d $^3D_3$   | 1s 6f $^3F_4^0$ | 3.8744E+00    | 4.504E-06 | 2.224E+08        | 3.8580E+00    | 4.617E-06 | 2.279E+08        |
| 1s 3d $^1D_2$   | 1s 6f $^3F_4^0$ | 3.8761E+00    | 3.632E-07 | 1.792E+07        | 3.8597E+00    | 3.727E-07 | 1.838E+07        |
| 1s 4d $^3D_2$   | 1s 6f $^3F_4^0$ | 9.1669E+00    | 4.363E-07 | 3.848E+06        | 9.1288E+00    | 4.400E-07 | 3.879E+06        |
| 1s 4d $^3D_3$   | 1s 6f $^3F_4^0$ | 9.2719E+00    | 2.746E-06 | 2.367E+07        | 9.2331E+00    | 2.774E-06 | 2.391E+07        |
| 1s 4d $^1D_2$   | 1s 6f $^3F_4^0$ | 9.2763E+00    | 2.228E-07 | 1.919E+06        | 9.2375E+00    | 2.251E-07 | 1.938E+06        |
| 1s 5d $^3D_2$   | 1s 6f $^3F_4^0$ | 2.5816E+01    | 2.354E-07 | 2.617E+05        | 2.5711E+01    | 2.362E-07 | 2.625E+05        |
| 1s 5d $^3D_3$   | 1s 6f $^3F_4^0$ | 2.6244E+01    | 1.538E-06 | 1.656E+06        | 2.6136E+01    | 1.544E-06 | 1.661E+06        |
| 1s 5d $^1D_2$   | 1s 6f $^3F_4^0$ | 2.6262E+01    | 1.253E-07 | 1.346E+05        | 2.6155E+01    | 1.254E-07 | 1.347E+05        |
| 1s 5g $^3G_4$   | 1s 6f $^3F_4^0$ | 2.6470E+01    | 8.803E-15 | 9.312E-03        |               |           |                  |
| 1s 5g $^3G_3$   | 1s 6f $^3F_4^0$ | 2.6475E+01    | 7.111E-16 | 7.519E-04        |               |           |                  |
| 1s 5g $^3G_5$   | 1s 6f $^3F_4^0$ | 2.6601E+01    | 3.646E-08 | 3.819E+04        | 2.6486E+01    | 3.625E-08 | 3.797E+04        |
| 1s 5g $^1G_4$   | 1s 6f $^3F_4^0$ | 2.6606E+01    | 2.610E-09 | 2.732E+03        | 2.6491E+01    | 2.588E-09 | 2.710E+03        |
| 1s 6d $^3D_2$   | 1s 6f $^3F_4^0$ | 1.8056E+03    | 4.817E-12 | 1.095E-03        | 1.8327E+03    | 4.512E-12 | 9.871E-04        |
| 1s 6d $^3D_3$   | 1s 6f $^3F_4^0$ | 5.3175E+03    | 1.207E-12 | 3.163E-05        | 5.5117E+03    | 1.070E-12 | 2.590E-05        |
| 1s 6d $^1D_2$   | 1s 6f $^3F_4^0$ | 5.7984E+03    | 7.578E-14 | 1.670E-06        | 5.6864E+03    | 8.061E-14 | 1.832E-06        |
| 1s 2p $^3P_2^0$ | 1s 6g $^3G_4$   | 1.4397E+00    | 2.007E-11 | 7.176E+03        |               |           |                  |
| 1s 3p $^3P_2^0$ | 1s 6g $^3G_4$   | 3.8211E+00    | 1.773E-11 | 9.000E+02        |               |           |                  |
| 1s 4p $^3P_2^0$ | 1s 6g $^3G_4$   | 9.1432E+00    | 1.834E-14 | 1.626E-01        |               |           |                  |
| 1s 4f $^3F_3^0$ | 1s 6g $^3G_4$   | 9.2736E+00    | 8.732E-07 | 7.525E+06        | 9.2341E+00    | 8.851E-07 | 7.628E+06        |
| 1s 4f $^3F_2^0$ | 1s 6g $^3G_4$   | 9.2758E+00    | 7.052E-08 | 6.074E+05        | 9.2363E+00    | 7.076E-08 | 6.095E+05        |
| 1s 4f $^3F_4^0$ | 1s 6g $^3G_4$   | 9.3264E+00    | 1.314E-12 | 1.120E+01        |               |           |                  |
| 1s 4f $^1F_3^0$ | 1s 6g $^3G_4$   | 9.3281E+00    | 3.260E-12 | 2.776E+01        |               |           |                  |
| 1s 5p $^3P_2^0$ | 1s 6g $^3G_4$   | 2.5720E+01    | 1.495E-13 | 1.675E-01        |               |           |                  |
| 1s 5f $^3F_3^0$ | 1s 6g $^3G_4$   | 2.6251E+01    | 7.032E-07 | 7.563E+05        | 2.6139E+01    | 7.069E-07 | 7.603E+05        |
| 1s 5f $^3F_2^0$ | 1s 6g $^3G_4$   | 2.6260E+01    | 5.684E-08 | 6.109E+04        | 2.6148E+01    | 5.650E-08 | 6.072E+04        |
| 1s 5f $^3F_4^0$ | 1s 6g $^3G_4$   | 2.6469E+01    | 1.089E-12 | 1.152E+00        |               |           |                  |
| 1s 5f $^1F_3^0$ | 1s 6g $^3G_4$   | 2.6476E+01    | 3.093E-12 | 3.270E+00        |               |           |                  |
| 1s 6p $^3P_2^0$ | 1s 6g $^3G_4$   | 1.5705E+03    | 1.699E-21 | 5.106E-13        |               |           |                  |
| 1s 6f $^3F_3^0$ | 1s 6g $^3G_4$   | 5.4970E+03    | 2.497E-13 | 6.123E-06        | 5.5303E+03    | 2.427E-13 | 5.831E-06        |
| 1s 6f $^3F_2^0$ | 1s 6g $^3G_4$   | 5.7369E+03    | 1.775E-14 | 3.997E-07        | 5.5276E+03    | 1.944E-14 | 4.676E-07        |
| 1s 6f $^3F_4^0$ | 1s 6g $^3G_4$   | 2.7996E+06    | 2.940E-27 | 2.780E-25        |               |           |                  |
| 1s 2p $^3P_0^0$ | 1s 6g $^3G_3$   | 1.3775E+00    | 8.809E-15 | 4.423E+00        |               |           |                  |
| 1s 2p $^3P_1^0$ | 1s 6g $^3G_3$   | 1.4397E+00    | 2.018E-12 | 9.277E+02        |               |           |                  |
| 1s 2p $^1P_1^0$ | 1s 6g $^3G_3$   | 1.4456E+00    | 1.399E-11 | 6.382E+03        |               |           |                  |
| 1s 3p $^3P_0^0$ | 1s 6g $^3G_3$   | 3.6896E+00    | 3.546E-14 | 2.482E+00        |               |           |                  |
| 1s 3p $^3P_1^0$ | 1s 6g $^3G_3$   | 3.8210E+00    | 2.034E-12 | 1.327E+02        |               |           |                  |
| 1s 3p $^1P_1^0$ | 1s 6g $^3G_3$   | 3.8327E+00    | 1.119E-11 | 7.261E+02        |               |           |                  |
| 1s 4p $^3P_0^0$ | 1s 6g $^3G_3$   | 8.8264E+00    | 1.545E-16 | 1.889E-03        |               |           |                  |
| 1s 4p $^3P_1^0$ | 1s 6g $^3G_3$   | 9.1429E+00    | 6.432E-14 | 7.331E-01        |               |           |                  |
| 1s 4p $^1P_1^0$ | 1s 6g $^3G_3$   | 9.1706E+00    | 4.170E-16 | 4.725E-03        |               |           |                  |
| 1s 4f $^3F_3^0$ | 1s 6g $^3G_3$   | 9.2732E+00    | 1.050E-07 | 1.163E+06        | 9.2341E+00    | 1.062E-07 | 1.176E+06        |
| 1s 4f $^3F_2^0$ | 1s 6g $^3G_3$   | 9.2754E+00    | 6.289E-07 | 6.966E+06        | 9.2363E+00    | 6.368E-07 | 7.053E+06        |
| 1s 4f $^3F_4^0$ | 1s 6g $^3G_3$   | 9.3261E+00    | 1.641E-18 | 1.798E-05        |               |           |                  |
| 1s 4f $^1F_3^0$ | 1s 6g $^3G_3$   | 9.3277E+00    | 4.791E-13 | 5.247E+00        |               |           |                  |
| 1s 5p $^3P_0^0$ | 1s 6g $^3G_3$   | 2.4459E+01    | 1.101E-16 | 1.754E-04        |               |           |                  |
| 1s 5p $^3P_1^0$ | 1s 6g $^3G_3$   | 2.5717E+01    | 2.230E-13 | 3.213E-01        |               |           |                  |
| 1s 5p $^1P_1^0$ | 1s 6g $^3G_3$   | 2.5829E+01    | 1.653E-13 | 2.361E-01        |               |           |                  |
| 1s 5f $^3F_3^0$ | 1s 6g $^3G_3$   | 2.6248E+01    | 8.445E-08 | 1.168E+05        | 2.6139E+01    | 8.483E-08 | 1.173E+05        |
| 1s 5f $^3F_2^0$ | 1s 6g $^3G_3$   | 2.6257E+01    | 5.627E-07 | 7.003E+05        | 2.6148E+01    | 5.085E-07 | 7.026E+05        |
| 1s 5f $^3F_4^0$ | 1s 6g $^3G_3$   | 2.6466E+01    | 3.237E-17 | 4.403E-05        |               |           |                  |

(continued on next page)

Table 6 (continued)

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |           |                  |
|-----------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                 |                 | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 5f $^1F_3^0$ | 1s 6g $^3G_3$   | 2.6473E+01    | 3.503E-13 | 4.762E-01        |               |           |                  |
| 1s 6p $^3P_1^0$ | 1s 6g $^3G_3$   | 5.5707E+02    | 5.442E-20 | 1.671E-10        |               |           |                  |
| 1s 6p $^3P_2^0$ | 1s 6g $^3G_3$   | 1.5598E+03    | 2.160E-18 | 8.458E-10        |               |           |                  |
| 1s 6p $^1P_1^0$ | 1s 6g $^3G_3$   | 1.8359E+03    | 1.466E-19 | 4.146E-11        |               |           |                  |
| 1s 6f $^3F_3^0$ | 1s 6g $^3G_3$   | 5.3682E+03    | 3.220E-14 | 1.065E-06        | 5.5303E+03    | 2.912E-14 | 8.997E-07        |
| 1s 6f $^3F_2^0$ | 1s 6g $^3G_3$   | 5.5968E+03    | 1.704E-13 | 5.185E-06        | 5.5277E+03    | 1.750E-13 | 5.411E-06        |
| 1s 6f $^3F_4^0$ | 1s 6g $^3G_3$   | 2.1175E+05    | 1.685E-26 | 3.580E-22        |               |           |                  |
| 1s 2s $^3S_1$   | 1s 6f $^1F_3^0$ | 1.3658E+00    | 9.089E-14 | 4.643E+01        |               |           |                  |
| 1s 3s $^3S_1$   | 1s 6f $^1F_3^0$ | 3.6666E+00    | 9.718E-13 | 6.888E+01        |               |           |                  |
| 1s 3d $^3D_2$   | 1s 6f $^1F_3^0$ | 3.8309E+00    | 8.752E-08 | 5.683E+06        | 3.8148E+00    | 8.744E-08 | 5.677E+06        |
| 1s 3d $^3D_1$   | 1s 6f $^1F_3^0$ | 3.8326E+00    | 4.980E-07 | 3.230E+07        | 3.8165E+00    | 5.017E-07 | 3.254E+07        |
| 1s 3d $^3D_3$   | 1s 6f $^1F_3^0$ | 3.8743E+00    | 5.411E-07 | 3.435E+07        | 3.8580E+00    | 5.541E-07 | 3.517E+07        |
| 1s 3d $^1D_2$   | 1s 6f $^1F_3^0$ | 3.8760E+00    | 3.237E-06 | 2.053E+08        | 3.8597E+00    | 3.316E-06 | 2.103E+08        |
| 1s 4s $^3S_1$   | 1s 6f $^1F_3^0$ | 8.7727E+00    | 6.785E-13 | 8.401E+00        |               |           |                  |
| 1s 4d $^3D_2$   | 1s 6f $^1F_3^0$ | 9.1664E+00    | 5.257E-08 | 5.962E+05        | 9.1288E+00    | 5.284E-08 | 5.991E+05        |
| 1s 4d $^3D_1$   | 1s 6f $^1F_3^0$ | 9.1705E+00    | 2.925E-07 | 3.314E+06        | 9.1329E+00    | 2.954E-07 | 3.347E+06        |
| 1s 4d $^3D_3$   | 1s 6f $^1F_3^0$ | 9.2714E+00    | 3.296E-07 | 3.654E+06        | 9.2331E+00    | 3.328E-07 | 3.689E+06        |
| 1s 4d $^1D_2$   | 1s 6f $^1F_3^0$ | 9.2758E+00    | 1.973E-06 | 2.185E+07        | 9.2375E+00    | 1.990E-06 | 2.204E+07        |
| 1s 5s $^3S_1$   | 1s 6f $^1F_3^0$ | 2.4251E+01    | 3.672E-13 | 5.949E-01        |               |           |                  |
| 1s 5d $^3D_2$   | 1s 6f $^1F_3^0$ | 2.5812E+01    | 2.867E-08 | 4.101E+04        | 2.5711E+01    | 2.878E-08 | 4.113E+04        |
| 1s 5d $^3D_1$   | 1s 6f $^1F_3^0$ | 2.5828E+01    | 1.581E-07 | 2.258E+05        | 2.5727E+01    | 1.587E-07 | 2.266E+05        |
| 1s 5d $^3D_3$   | 1s 6f $^1F_3^0$ | 2.6240E+01    | 1.845E-07 | 2.554E+05        | 2.6136E+01    | 1.853E-07 | 2.562E+05        |
| 1s 5d $^1D_2$   | 1s 6f $^1F_3^0$ | 2.6259E+01    | 1.106E-06 | 1.528E+06        | 2.6155E+01    | 1.107E-06 | 1.529E+06        |
| 1s 5g $^3G_4$   | 1s 6f $^1F_3^0$ | 2.6466E+01    | 2.632E-14 | 3.580E-02        |               |           |                  |
| 1s 5g $^3G_3$   | 1s 6f $^1F_3^0$ | 2.6471E+01    | 3.695E-15 | 5.025E-03        |               |           |                  |
| 1s 5g $^3G_5$   | 1s 6f $^1F_3^0$ | 2.6597E+01    | 1.722E-09 | 2.319E+03        | 2.6486E+01    | 1.729E-09 | 2.329E+03        |
| 1s 5g $^1G_4$   | 1s 6f $^1F_3^0$ | 2.6601E+01    | 2.865E-08 | 3.857E+04        | 2.6490E+01    | 2.846E-08 | 3.832E+04        |
| 1s 6s $^3S_1$   | 1s 6f $^1F_3^0$ | 5.0083E+02    | 4.301E-16 | 1.634E-06        |               |           |                  |
| 1s 6d $^3D_2$   | 1s 6f $^1F_3^0$ | 1.7871E+03    | 6.094E-13 | 1.818E-04        | 1.8323E+03    | 5.891E-13 | 1.658E-04        |
| 1s 6d $^3D_1$   | 1s 6f $^1F_3^0$ | 1.8330E+03    | 3.093E-12 | 8.773E-04        | 1.8209E+03    | 3.120E-12 | 8.892E-04        |
| 1s 6d $^3D_3$   | 1s 6f $^1F_3^0$ | 5.1604E+03    | 1.585E-13 | 5.671E-06        | 5.5079E+03    | 1.287E-13 | 4.010E-06        |
| 1s 6d $^1D_2$   | 1s 6f $^1F_3^0$ | 5.6121E+03    | 7.375E-13 | 2.231E-05        | 5.6823E+03    | 7.009E-13 | 2.051E-05        |
| 1s 6g $^3G_4$   | 1s 6f $^1F_3^0$ | 1.8628E+05    | 3.059E-23 | 8.401E-19        |               |           |                  |
| 1s 6g $^3G_3$   | 1s 6f $^1F_3^0$ | 9.9701E+05    | 2.038E-26 | 1.953E-23        |               |           |                  |
| 1s 4f $^3F_3^0$ | 1s 6g $^3G_5$   | 9.2643E+00    | 6.142E-07 | 4.339E+06        | 9.2249E+00    | 6.158E-07 | 4.350E+06        |
| 1s 4f $^3F_2^0$ | 1s 6g $^3G_5$   | 9.3170E+00    | 5.280E-06 | 3.688E+07        | 9.2773E+00    | 5.351E-06 | 3.738E+07        |
| 1s 4f $^1F_3^0$ | 1s 6g $^3G_5$   | 9.3187E+00    | 2.496E-07 | 1.743E+06        | 9.2790E+00    | 2.529E-07 | 1.766E+06        |
| 1s 5f $^3F_3^0$ | 1s 6g $^3G_5$   | 2.6177E+01    | 4.863E-07 | 4.304E+05        | 2.6065E+01    | 4.885E-07 | 4.323E+05        |
| 1s 5f $^3F_4^0$ | 1s 6g $^3G_5$   | 2.6394E+01    | 4.285E-06 | 3.730E+06        | 2.6281E+01    | 4.304E-06 | 3.747E+06        |
| 1s 5f $^1F_3^0$ | 1s 6g $^3G_5$   | 2.6400E+01    | 2.028E-07 | 1.764E+05        | 2.6287E+01    | 2.035E-07 | 1.771E+05        |
| 1s 6f $^3F_3^0$ | 1s 6g $^3G_5$   | 3.4474E+03    | 7.054E-13 | 3.599E-05        | 3.4619E+03    | 6.849E-13 | 3.436E-05        |
| 1s 6f $^3F_2^0$ | 1s 6g $^3G_5$   | 9.2152E+03    | 3.245E-13 | 2.317E-06        | 9.2775E+03    | 3.143E-13 | 2.195E-06        |
| 1s 6f $^1F_3^0$ | 1s 6g $^3G_5$   | 9.7284E+03    | 1.305E-14 | 8.363E-08        | 9.2884E+03    | 1.494E-14 | 1.041E-07        |
| 1s 3d $^3D_3$   | 1s 6h $^3H_5^0$ | 3.8728E+00    | 5.411E-12 | 2.188E+02        |               |           |                  |
| 1s 4d $^3D_3$   | 1s 6h $^3H_5^0$ | 9.2626E+00    | 5.290E-12 | 3.739E+01        |               |           |                  |
| 1s 5d $^3D_3$   | 1s 6h $^3H_5^0$ | 2.6170E+01    | 2.629E-13 | 2.328E-01        |               |           |                  |
| 1s 5g $^3G_4$   | 1s 6h $^3H_5^0$ | 2.6394E+01    | 2.528E-06 | 2.200E+06        | 2.6281E+01    | 2.542E-06 | 2.212E+06        |
| 1s 5g $^3G_3$   | 1s 6h $^3H_5^0$ | 2.6399E+01    | 1.213E-07 | 1.055E+05        | 2.6286E+01    | 1.209E-07 | 1.052E+05        |
| 1s 5g $^3G_5$   | 1s 6h $^3H_5^0$ | 2.6525E+01    | 1.198E-12 | 1.032E+00        |               |           |                  |
| 1s 5g $^1G_4$   | 1s 6h $^3H_5^0$ | 2.6529E+01    | 2.458E-12 | 2.118E+00        |               |           |                  |
| 1s 6d $^3D_3$   | 1s 6h $^3H_5^0$ | 3.3705E+03    | 7.804E-21 | 4.165E-13        |               |           |                  |
| 1s 6g $^3G_4$   | 1s 6h $^3H_5^0$ | 9.2359E+03    | 7.177E-14 | 5.102E-07        | 9.2564E+03    | 7.054E-14 | 4.950E-07        |
| 1s 6g $^3G_3$   | 1s 6h $^3H_5^0$ | 9.6239E+03    | 3.044E-15 | 1.993E-08        | 9.2564E+03    | 3.359E-15 | 2.357E-08        |
| 1s 6g $^3G_5$   | 1s 6h $^3H_5^0$ | 8.7873E+06    | 3.968E-29 | 3.115E-28        |               |           |                  |
| 1s 3d $^3D_2$   | 1s 6h $^3H_4^0$ | 3.8293E+00    | 6.327E-16 | 3.198E-02        |               |           |                  |
| 1s 3d $^3D_3$   | 1s 6h $^3H_4^0$ | 3.8727E+00    | 3.323E-13 | 1.642E+01        |               |           |                  |
| 1s 3d $^1D_2$   | 1s 6h $^3H_4^0$ | 3.8744E+00    | 4.003E-12 | 1.976E+02        |               |           |                  |
| 1s 4d $^3D_2$   | 1s 6h $^3H_4^0$ | 9.1575E+00    | 7.295E-16 | 6.448E-03        |               |           |                  |
| 1s 4d $^3D_3$   | 1s 6h $^3H_4^0$ | 9.2624E+00    | 3.180E-13 | 2.747E+00        |               |           |                  |
| 1s 4d $^1D_2$   | 1s 6h $^3H_4^0$ | 9.2667E+00    | 3.921E-12 | 3.384E+01        |               |           |                  |
| 1s 5d $^3D_2$   | 1s 6h $^3H_4^0$ | 2.5741E+01    | 3.296E-17 | 3.686E-05        |               |           |                  |
| 1s 5d $^3D_3$   | 1s 6h $^3H_4^0$ | 2.6168E+01    | 2.500E-14 | 2.706E-02        |               |           |                  |
| 1s 5d $^1D_2$   | 1s 6h $^3H_4^0$ | 2.6186E+01    | 2.013E-13 | 2.176E-01        |               |           |                  |
| 1s 5g $^3G_4$   | 1s 6h $^3H_4^0$ | 2.6392E+01    | 1.806E-07 | 1.922E+05        | 2.6281E+01    | 1.815E-07 | 1.931E+05        |
| 1s 5g $^3G_3$   | 1s 6h $^3H_4^0$ | 2.6397E+01    | 1.986E-06 | 2.113E+06        | 2.6286E+01    | 1.996E-06 | 2.123E+06        |
| 1s 5g $^3G_5$   | 1s 6h $^3H_4^0$ | 2.6523E+01    | 4.039E-17 | 4.255E-05        |               |           |                  |
| 1s 5g $^1G_4$   | 1s 6h $^3H_4^0$ | 2.6527E+01    | 6.353E-13 | 6.691E-01        |               |           |                  |
| 1s 6d $^3D_2$   | 1s 6h $^3H_4^0$ | 1.5031E+03    | 4.993E-24 | 1.638E-15        |               |           |                  |
| 1s 6d $^3D_3$   | 1s 6h $^3H_4^0$ | 3.3388E+03    | 3.254E-21 | 2.163E-13        |               |           |                  |
| 1s 6d $^1D_2$   | 1s 6h $^3H_4^0$ | 3.5222E+03    | 6.134E-21 | 3.664E-13        |               |           |                  |
| 1s 6g $^3G_4$   | 1s 6h $^3H_4^0$ | 9.0013E+03    | 5.541E-15 | 5.068E-08        | 9.2564E+03    | 5.038E-15 | 4.321E-08        |

(continued on next page)

Table 6 (continued)

| Lower   | Upper   | GRASP2K       |           |                             | FAC           |           |                             |
|---|---|---------------|-----------|-----------------------------|---------------|-----------|-----------------------------|
|   |   | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 9.3695E+03    | 5.404E-14 | 4.562E-07                   | 9.2564E+03    | 5.542E-14 | 4.753E-07                   |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 3.4069E+05    | 1.141E-30 | 7.288E-27                   |               |           |                             |
| 1s2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 1.4395E+00    | 5.680E-15 | 2.031E+00                   |               |           |                             |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 3.8194E+00    | 3.778E-15 | 1.919E-01                   |               |           |                             |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 9.1339E+00    | 6.563E-14 | 5.830E-01                   |               |           |                             |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 9.2640E+00    | 3.610E-08 | 3.117E+05                   | 9.2249E+00    | 3.550E-08 | 3.065E+05                   |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 9.2662E+00    | 4.630E-07 | 3.997E+06                   | 9.2271E+00    | 4.648E-07 | 4.012E+06                   |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 9.3167E+00    | 3.774E-07 | 3.222E+06                   | 9.2773E+00    | 3.822E-07 | 3.263E+06                   |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 9.3184E+00    | 4.149E-06 | 3.541E+07                   | 9.2790E+00    | 4.203E-06 | 3.587E+07                   |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.5647E+01    | 7.477E-14 | 8.425E-02                   |               |           |                             |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.6175E+01    | 2.866E-08 | 3.100E+04                   | 2.6065E+01    | 2.825E-08 | 3.055E+04                   |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.6184E+01    | 3.669E-07 | 3.966E+05                   | 2.6074E+01    | 3.687E-07 | 3.985E+05                   |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.6391E+01    | 3.061E-07 | 3.257E+05                   | 2.6281E+01    | 3.074E-07 | 3.271E+05                   |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.6398E+01    | 3.368E-06 | 3.582E+06                   | 2.6287E+01    | 3.380E-06 | 3.595E+06                   |
| 1s6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 1.3363E+03    | 2.421E-18 | 1.005E-09                   |               |           |                             |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 3.4068E+03    | 4.316E-14 | 2.756E-06                   | 3.4619E+03    | 4.205E-14 | 2.578E-06                   |
| 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 3.4975E+03    | 5.097E-13 | 3.088E-05                   | 3.4608E+03    | 5.197E-13 | 3.188E-05                   |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 8.9311E+03    | 2.547E-14 | 2.366E-07                   | 9.2773E+03    | 2.245E-14 | 1.917E-07                   |
| 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 9.4124E+03    | 2.394E-13 | 2.002E-06                   | 9.2882E+03    | 2.460E-13 | 2.096E-06                   |
| 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 2.9962E+05    | 2.062E-24 | 1.703E-20                   |               |           |                             |
| 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s6g <sup>1</sup> G <sub>4</sub>              | 1.9372E+06    | 1.973E-27 | 3.896E-25                   |               |           |                             |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 2.6344E+01    | 8.894E-07 | 6.576E+05                   | 2.6232E+01    | 8.917E-07 | 6.593E+05                   |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 2.6474E+01    | 1.048E-05 | 7.674E+06                   | 2.6361E+01    | 1.054E-05 | 7.716E+06                   |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 2.6478E+01    | 3.306E-07 | 2.420E+05                   | 2.6365E+01    | 3.324E-07 | 2.432E+05                   |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 5.5520E+03    | 1.164E-13 | 1.938E-06                   | 5.5614E+03    | 1.139E-13 | 1.874E-06                   |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1.3897E+04    | 8.779E-14 | 2.332E-07                   | 1.3933E+04    | 8.611E-14 | 2.256E-07                   |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1.4598E+04    | 2.390E-15 | 5.755E-09                   | 1.3934E+04    | 2.733E-15 | 7.163E-09                   |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 3.8717E+00    | 4.245E-16 | 1.717E-02                   |               |           |                             |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 9.2562E+00    | 4.469E-16 | 3.163E-03                   |               |           |                             |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.6119E+01    | 2.181E-16 | 1.939E-04                   |               |           |                             |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.6342E+01    | 3.299E-08 | 2.883E+04                   | 2.6232E+01    | 3.216E-08 | 2.810E+04                   |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.6348E+01    | 7.157E-07 | 6.251E+05                   | 2.6237E+01    | 7.181E-07 | 6.272E+05                   |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.6473E+01    | 4.992E-07 | 4.320E+05                   | 2.6361E+01    | 5.019E-07 | 4.342E+05                   |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.6477E+01    | 8.653E-06 | 7.485E+06                   | 2.6365E+01    | 8.697E-06 | 7.523E+06                   |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.6964E+03    | 7.459E-22 | 6.221E-14                   |               |           |                             |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 5.4809E+03    | 4.490E-15 | 9.064E-08                   | 5.5614E+03    | 4.383E-15 | 8.520E-08                   |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 5.6153E+03    | 9.058E-14 | 1.742E-06                   | 5.5614E+03    | 9.204E-14 | 1.789E-06                   |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.3461E+04    | 4.602E-15 | 1.540E-08                   | 1.3933E+04    | 4.100E-15 | 1.269E-08                   |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.4116E+04    | 6.916E-14 | 2.105E-07                   | 1.3934E+04    | 7.107E-14 | 2.201E-07                   |
| 1s2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 1.3378E+00    | 7.061E-11 | 8.772E+04                   | 1.3323E+00    | 1.617E-10 | 2.008E+05                   |
| 1s2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 1.3964E+00    | 8.788E-08 | 1.002E+08                   | 1.3905E+00    | 8.717E-08 | 9.938E+07                   |
| 1s2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 1.4019E+00    | 9.183E-08 | 1.039E+08                   | 1.3961E+00    | 8.599E-08 | 9.725E+07                   |
| 1s3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 3.4180E+00    | 6.412E-11 | 1.220E+04                   | 3.4039E+00    | 8.987E-11 | 1.710E+04                   |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 3.5305E+00    | 5.822E-08 | 1.038E+07                   | 3.5159E+00    | 5.726E-08 | 1.021E+07                   |
| 1s3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 3.5405E+00    | 5.893E-08 | 1.045E+07                   | 3.5260E+00    | 5.669E-08 | 1.005E+07                   |
| 1s4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 7.4166E+00    | 4.198E-11 | 1.697E+03                   | 7.3859E+00    | 5.786E-11 | 2.338E+03                   |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 7.6388E+00    | 3.929E-08 | 1.497E+06                   | 7.6070E+00    | 3.893E-08 | 1.483E+06                   |
| 1s4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 7.6581E+00    | 3.974E-08 | 1.507E+06                   | 7.6265E+00    | 3.858E-08 | 1.462E+06                   |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 7.7295E+00    | 3.020E-15 | 1.124E-01                   |               |           |                             |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 7.7310E+00    | 4.463E-16 | 1.660E-02                   |               |           |                             |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 7.7674E+00    | 9.051E-15 | 3.336E-01                   |               |           |                             |
| 1s5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 1.6020E+01    | 2.993E-11 | 2.593E+02                   | 1.5955E+01    | 4.220E-11 | 3.655E+02                   |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 1.6551E+01    | 2.882E-08 | 2.340E+05                   | 1.6483E+01    | 2.871E-08 | 2.329E+05                   |
| 1s5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 1.6597E+01    | 2.919E-08 | 2.356E+05                   | 1.6529E+01    | 2.843E-08 | 2.294E+05                   |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 1.6769E+01    | 2.832E-15 | 2.239E-02                   |               |           |                             |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 1.6773E+01    | 2.941E-17 | 2.324E-04                   |               |           |                             |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 1.6860E+01    | 1.476E-14 | 1.154E-01                   |               |           |                             |
| 1s6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 4.2860E+01    | 2.300E-11 | 2.784E+01                   | 4.2690E+01    | 5.831E-11 | 7.054E+01                   |
| 1s6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 4.5091E+01    | 2.306E-08 | 2.522E+04                   | 4.4909E+01    | 2.285E-08 | 2.498E+04                   |
| 1s6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 4.5287E+01    | 2.341E-08 | 2.537E+04                   | 4.5084E+01    | 2.254E-08 | 2.444E+04                   |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 4.6035E+01    | 2.643E-15 | 2.773E-03                   |               |           |                             |
| 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 4.6051E+01    | 1.251E-16 | 1.312E-04                   |               |           |                             |
| 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7s <sup>3</sup> S <sub>1</sub>              | 4.6435E+01    | 1.966E-14 | 2.027E-02                   |               |           |                             |
| 1s2s <sup>3</sup> S <sub>1</sub>              | 1s7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.3266E+00    | 9.923E-10 | 1.254E+06                   | 1.3210E+00    | 1.573E-09 | 1.987E+06                   |
| 1s3s <sup>3</sup> S <sub>1</sub>              | 1s7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 3.3968E+00    | 3.292E-10 | 6.343E+04                   | 3.3827E+00    | 4.928E-10 | 9.495E+04                   |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 3.5373E+00    | 5.806E-10 | 1.032E+05                   | 3.5225E+00    | 5.732E-10 | 1.018E+05                   |
| 1s3d <sup>3</sup> D <sub>1</sub>              | 1s7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 3.5388E+00    | 5.924E-10 | 1.052E+05                   | 3.5240E+00    | 5.632E-10 | 9.998E+04                   |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 3.5743E+00    | 9.720E-09 | 1.692E+06                   | 3.5593E+00    | 9.462E-09 | 1.646E+06                   |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 3.5757E+00    | 3.723E-09 | 6.474E+05                   | 3.5607E+00    | 3.624E-09 | 6.301E+05                   |
| 1s4s <sup>3</sup> S <sub>1</sub>              | 1s7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 7.3716E+00    | 1.514E-10 | 6.195E+03                   | 7.3412E+00    | 1.484E-10 | 8.937E+03                   |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 7.6476E+00    | 6.420E-10 | 2.441E+04                   | 7.6163E+00    | 6.362E-10 | 2.418E+04                   |

(continued on next page)

Table 6 (continued)

| Lower  | Upper  | GRASP2K       |           |                  | FAC           |           |                  |
|--|--|---------------|-----------|------------------|---------------|-----------|------------------|
|  |  | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 7.6504E+00    | 6.386E−10 | 2.426E+04        | 7.6191E+00    | 6.185E−10 | 2.348E+04        |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7p <sup>3</sup> P <sub>3</sub> <sup>o</sup> | 7.7206E+00    | 1.056E−08 | 3.939E+05        | 7.6888E+00    | 1.031E−08 | 3.845E+05        |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 7.7236E+00    | 4.009E−09 | 1.494E+05        | 7.6918E+00    | 3.961E−09 | 1.476E+05        |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.5898E+01    | 8.382E−11 | 7.373E+02        | 1.5833E+01    | 1.150E−10 | 1.011E+03        |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.6554E+01    | 6.141E−10 | 4.983E+03        | 1.6489E+01    | 6.088E−10 | 4.936E+03        |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.6561E+01    | 6.033E−10 | 4.891E+03        | 1.6495E+01    | 5.889E−10 | 4.771E+03        |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7p <sup>3</sup> P <sub>3</sub> <sup>o</sup> | 1.6729E+01    | 1.001E−08 | 7.953E+04        | 1.6663E+01    | 9.785E−09 | 7.770E+04        |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.6737E+01    | 3.776E−09 | 2.997E+04        | 1.6670E+01    | 3.758E−09 | 2.981E+04        |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1.6823E+01    | 5.398E−18 | 4.241E−05        |               |           |                  |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.2260E+01    | 5.061E−11 | 6.301E+01        | 4.2057E+01    | 6.306E−11 | 7.859E+01        |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.4993E+01    | 5.884E−10 | 6.463E+02        | 4.4844E+01    | 5.978E−10 | 6.553E+02        |
| 1s 6d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.5021E+01    | 5.741E−10 | 6.298E+02        | 4.4837E+01    | 5.631E−10 | 6.175E+02        |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7p <sup>3</sup> P <sub>3</sub> <sup>o</sup> | 4.5746E+01    | 9.580E−09 | 1.018E+04        | 4.5589E+01    | 9.401E−09 | 9.972E+03        |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 4.5778E+01    | 3.602E−09 | 3.821E+03        | 4.5600E+01    | 3.564E−09 | 3.779E+03        |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.6153E+01    | 1.003E−17 | 1.047E−05        |               |           |                  |
| 1s 7s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 7.6504E+03    | 1.709E−16 | 6.493E−09        | 7.3461E+03    | 3.329E−16 | 1.360E−08        |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7s <sup>1</sup> S <sub>0</sub>              | 1.3961E+00    | 5.700E−08 | 1.951E+08        | 1.3903E+00    | 5.814E−08 | 1.989E+08        |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7s <sup>1</sup> S <sub>0</sub>              | 3.5288E+00    | 3.806E−08 | 2.038E+07        | 3.5145E+00    | 3.822E−08 | 2.046E+07        |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7s <sup>1</sup> S <sub>0</sub>              | 7.6311E+00    | 2.568E−08 | 2.941E+06        | 7.6005E+00    | 2.602E−08 | 2.979E+06        |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7s <sup>1</sup> S <sub>0</sub>              | 7.7232E+00    | 2.042E−15 | 2.284E−01        |               |           |                  |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7s <sup>1</sup> S <sub>0</sub>              | 1.6515E+01    | 1.876E−08 | 4.589E+05        | 1.6452E+01    | 1.924E−08 | 4.702E+05        |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7s <sup>1</sup> S <sub>0</sub>              | 1.6736E+01    | 3.426E−15 | 8.160E−02        |               |           |                  |
| 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7s <sup>1</sup> S <sub>0</sub>              | 4.4825E+01    | 1.486E−08 | 4.934E+04        | 4.4685E+01    | 1.546E−08 | 5.123E+04        |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7s <sup>1</sup> S <sub>0</sub>              | 4.5774E+01    | 4.081E−15 | 1.299E−02        |               |           |                  |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 3.5372E+00    | 3.772E−10 | 2.011E+05        | 3.5228E+00    | 3.663E−10 | 1.952E+05        |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 3.5756E+00    | 4.547E−09 | 2.372E+06        | 3.5610E+00    | 4.361E−09 | 2.274E+06        |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 7.6470E+00    | 4.064E−10 | 4.636E+04        | 7.6177E+00    | 3.968E−10 | 4.522E+04        |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 7.7230E+00    | 4.905E−09 | 5.486E+05        | 7.6932E+00    | 4.762E−09 | 5.322E+05        |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.6552E+01    | 3.834E−10 | 9.335E+03        | 1.6495E+01    | 3.754E−10 | 9.126E+03        |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1.6734E+01    | 4.624E−09 | 1.101E+05        | 1.6677E+01    | 4.518E−09 | 1.074E+05        |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.4975E+01    | 3.644E−10 | 1.202E+03        | 4.4891E+01    | 3.446E−10 | 1.131E+03        |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 4.5759E+01    | 4.411E−09 | 1.405E+04        | 4.5649E+01    | 4.337E−09 | 1.376E+04        |
| 1s <sup>2</sup> <sup>1</sup> S <sub>0</sub>    | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.1400E−01    | 6.200E−06 | 8.387E+10        | 3.1270E−01    | 6.930E−06 | 9.375E+10        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.3253E+00    | 7.079E−07 | 5.377E+08        | 1.3197E+00    | 7.260E−07 | 5.513E+08        |
| 1s 2s <sup>1</sup> S <sub>0</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.3374E+00    | 4.714E−07 | 3.516E+08        | 1.3320E+00    | 4.707E−07 | 3.509E+08        |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.3884E+00    | 2.267E−07 | 2.634E+07        | 3.3744E+00    | 2.291E−07 | 2.661E+07        |
| 1s 3s <sup>1</sup> S <sub>0</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.4094E+00    | 1.548E−07 | 1.776E+07        | 3.3955E+00    | 1.499E−07 | 1.720E+07        |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.5282E+00    | 1.202E−17 | 1.288E−03        |               |           |                  |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.5297E+00    | 2.420E−13 | 2.591E+01        |               |           |                  |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.5650E+00    | 3.454E−08 | 3.626E+06        | 3.5501E+00    | 3.333E−08 | 3.499E+06        |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 3.5665E+00    | 8.900E−09 | 9.335E+05        | 3.5515E+00    | 8.324E−09 | 8.730E+05        |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.3324E+00    | 1.020E−07 | 2.530E+06        | 7.3023E+00    | 1.027E−07 | 2.547E+06        |
| 1s 4s <sup>1</sup> S <sub>0</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.3720E+00    | 7.087E−08 | 1.740E+06        | 7.3421E+00    | 6.736E−08 | 1.652E+06        |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.6054E+00    | 7.859E−14 | 1.813E+00        |               |           |                  |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.6082E+00    | 1.657E−13 | 3.818E+00        |               |           |                  |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.6776E+00    | 3.901E−08 | 8.828E+05        | 7.6461E+00    | 3.790E−08 | 8.575E+05        |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 7.6806E+00    | 9.934E−09 | 2.246E+05        | 7.6491E+00    | 9.464E−09 | 2.139E+05        |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.5717E+01    | 5.498E−08 | 2.969E+05        | 1.5653E+01    | 5.521E−08 | 2.980E+05        |
| 1s 5s <sup>1</sup> S <sub>0</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.5808E+01    | 3.839E−08 | 2.049E+05        | 1.5745E+01    | 3.617E−08 | 1.930E+05        |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6358E+01    | 1.841E−13 | 9.179E−01        |               |           |                  |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6364E+01    | 1.037E−13 | 5.164E−01        |               |           |                  |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6529E+01    | 3.782E−08 | 1.847E+05        | 1.6463E+01    | 3.680E−08 | 1.796E+05        |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6536E+01    | 9.557E−09 | 4.663E+04        | 1.6471E+01    | 9.189E−09 | 4.480E+04        |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6618E+01    | 1.900E−16 | 9.176E−04        |               |           |                  |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6620E+01    | 4.014E−16 | 1.939E−03        |               |           |                  |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.6671E+01    | 5.026E−16 | 2.413E−03        |               |           |                  |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.1005E+01    | 3.153E−08 | 2.501E+04        | 4.0810E+01    | 3.175E−08 | 2.522E+04        |
| 1s 6s <sup>1</sup> S <sub>0</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.1360E+01    | 2.208E−08 | 1.722E+04        | 4.1111E+01    | 2.071E−08 | 1.620E+04        |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.3572E+01    | 2.575E−13 | 1.809E−01        |               |           |                  |
| 1s 6d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.3599E+01    | 6.437E−14 | 4.518E−02        |               |           |                  |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4278E+01    | 3.619E−08 | 2.463E+04        | 4.4127E+01    | 3.518E−08 | 2.389E+04        |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4308E+01    | 9.105E−09 | 6.187E+03        | 4.4138E+01    | 8.787E−09 | 5.966E+03        |
| 1s 6g <sup>3</sup> G <sub>4</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4650E+01    | 3.033E−16 | 2.030E−04        |               |           |                  |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4659E+01    | 1.017E−15 | 6.805E−04        |               |           |                  |
| 1s 6g <sup>1</sup> G <sub>4</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 4.4874E+01    | 1.154E−15 | 7.646E−04        |               |           |                  |
| 1s 7s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.1691E+03    | 3.824E−11 | 3.733E−02        | 1.1590E+03    | 3.901E−11 | 3.842E−02        |
| 1s 7s <sup>1</sup> S <sub>0</sub>              | 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1.3812E+03    | 1.542E−11 | 1.078E−02        | 1.3316E+03    | 1.714E−11 | 1.279E−02        |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.3362E+00    | 4.478E−08 | 3.345E+07        | 1.3307E+00    | 4.941E−08 | 3.691E+07        |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.3371E+00    | 2.808E−08 | 2.095E+07        | 1.3315E+00    | 2.860E−08 | 2.133E+07        |
| 1s 2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.3946E+00    | 2.722E−11 | 1.867E+04        | 1.3888E+00    | 1.197E−10 | 8.211E+04        |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.4001E+00    | 5.100E−13 | 3.471E+02        | 1.3943E+00    | 6.804E−11 | 4.629E+04        |

(continued on next page)

Table 6 (continued)

| Lower  | Upper  | GRASP2K       |           |                             | FAC           |           |                             |
|--|--|---------------|-----------|-----------------------------|---------------|-----------|-----------------------------|
|  |  | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 3.4075E+00    | 1.627E-08 | 1.869E+06                   | 3.3932E+00    | 1.702E-08 | 1.956E+06                   |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 3.4089E+00    | 1.009E-08 | 1.158E+06                   | 3.3946E+00    | 9.875E-09 | 1.133E+06                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 3.5193E+00    | 1.222E-11 | 1.316E+03                   | 3.5045E+00    | 4.385E-11 | 4.723E+03                   |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 3.5292E+00    | 7.061E-13 | 7.563E+01                   | 3.5145E+00    | 2.920E-11 | 3.127E+03                   |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.3673E+00    | 7.197E-09 | 1.769E+05                   | 7.3356E+00    | 7.478E-09 | 1.838E+05                   |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.3700E+00    | 4.458E-09 | 1.095E+05                   | 7.3382E+00    | 4.345E-09 | 1.067E+05                   |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.5864E+00    | 5.874E-12 | 1.361E+02                   | 7.5537E+00    | 2.000E-11 | 4.636E+02                   |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.6055E+00    | 4.053E-13 | 9.348E+00                   | 7.5729E+00    | 1.427E-11 | 3.293E+02                   |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.6759E+00    | 1.692E-09 | 3.830E+04                   | 7.6429E+00    | 1.661E-09 | 3.762E+04                   |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.6774E+00    | 4.251E-10 | 9.622E+03                   | 7.6444E+00    | 4.160E-10 | 9.418E+03                   |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.7121E+00    | 3.413E-09 | 7.654E+04                   | 7.6789E+00    | 3.354E-09 | 7.524E+04                   |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 7.7133E+00    | 4.204E-10 | 9.426E+03                   | 7.6800E+00    | 4.388E-10 | 9.841E+03                   |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.5792E+01    | 3.717E-09 | 1.988E+04                   | 1.5722E+01    | 3.848E-09 | 2.059E+04                   |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.5798E+01    | 2.303E-09 | 1.231E+04                   | 1.5728E+01    | 2.239E-09 | 1.197E+04                   |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.6307E+01    | 3.226E-12 | 1.619E+01                   | 1.6234E+01    | 1.060E-11 | 5.324E+01                   |
| 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.6352E+01    | 2.514E-13 | 1.255E+00                   | 1.6279E+01    | 7.983E-12 | 3.984E+01                   |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.6519E+01    | 2.775E-09 | 1.357E+04                   | 1.6446E+01    | 2.756E-09 | 1.347E+04                   |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.6522E+01    | 6.968E-10 | 3.405E+03                   | 1.6450E+01    | 6.900E-10 | 3.373E+03                   |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.6605E+01    | 5.591E-09 | 2.705E+04                   | 1.6532E+01    | 5.516E-09 | 2.669E+04                   |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.6607E+01    | 6.887E-10 | 3.331E+03                   | 1.6535E+01    | 7.220E-10 | 3.493E+03                   |
| 1s 6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.1263E+01    | 2.028E-09 | 1.589E+03                   | 4.1063E+01    | 2.093E-09 | 1.641E+03                   |
| 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.1288E+01    | 1.257E-09 | 9.836E+02                   | 4.1000E+01    | 1.227E-09 | 9.657E+02                   |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.3326E+01    | 1.907E-12 | 1.355E+00                   | 4.3112E+01    | 6.034E-12 | 4.294E+00                   |
| 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.3508E+01    | 1.635E-13 | 1.152E-01                   | 4.3273E+01    | 3.074E-12 | 2.171E+00                   |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.4197E+01    | 3.605E-09 | 2.462E+03                   | 4.4000E+01    | 3.604E-09 | 2.462E+03                   |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.4212E+01    | 9.051E-10 | 6.177E+02                   | 4.4000E+01    | 9.006E-10 | 6.153E+02                   |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.4555E+01    | 7.249E-09 | 4.871E+03                   | 4.4354E+01    | 7.175E-09 | 4.824E+03                   |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.4566E+01    | 8.930E-10 | 5.998E+02                   | 4.4354E+01    | 9.294E-10 | 6.249E+02                   |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 4.4777E+01    | 1.788E-21 | 1.190E-09                   |               |           |                             |
| 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.2946E+03    | 1.100E-12 | 8.757E-04                   | 1.2624E+03    | 1.212E-12 | 1.006E-03                   |
| 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 1.3100E+03    | 6.563E-13 | 5.102E-04                   | 1.2259E+03    | 7.685E-13 | 6.764E-04                   |
| 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>2</sub>              | 2.0924E+04    | 2.094E-19 | 6.381E-13                   |               |           |                             |
| 1s 2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.3362E+00    | 4.400E-08 | 5.479E+07                   | 1.3307E+00    | 4.658E-08 | 5.799E+07                   |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.3946E+00    | 9.500E-14 | 1.086E+02                   |               |           |                             |
| 1s 2p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.4001E+00    | 4.968E-11 | 5.634E+04                   | 1.3943E+00    | 6.617E-11 | 7.503E+04                   |
| 1s 3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 3.4074E+00    | 1.582E-08 | 3.030E+06                   | 3.3932E+00    | 1.606E-08 | 3.075E+06                   |
| 1s 3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 3.5192E+00    | 1.300E-13 | 2.334E+01                   |               |           |                             |
| 1s 3p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 3.5291E+00    | 1.664E-11 | 2.970E+03                   | 3.5145E+00    | 2.062E-11 | 3.680E+03                   |
| 1s 4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 7.3668E+00    | 6.984E-09 | 2.861E+05                   | 7.3357E+00    | 7.059E-09 | 2.892E+05                   |
| 1s 4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 7.5859E+00    | 8.791E-14 | 3.396E+00                   |               |           |                             |
| 1s 4p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 7.6050E+00    | 7.421E-12 | 2.853E+02                   | 7.5730E+00    | 8.740E-12 | 3.359E+02                   |
| 1s 4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 7.6754E+00    | 2.849E-10 | 1.075E+04                   | 7.6430E+00    | 2.810E-10 | 1.060E+04                   |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 7.6769E+00    | 9.882E-10 | 3.728E+04                   | 7.6445E+00    | 9.709E-10 | 3.662E+04                   |
| 1s 4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 7.7127E+00    | 2.289E-09 | 8.555E+04                   | 7.6801E+00    | 2.268E-09 | 8.477E+04                   |
| 1s 5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.5790E+01    | 3.602E-09 | 3.212E+04                   | 1.5722E+01    | 3.635E-09 | 3.241E+04                   |
| 1s 5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.6305E+01    | 5.927E-14 | 4.957E-01                   |               |           |                             |
| 1s 5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.6349E+01    | 3.876E-12 | 3.224E+01                   | 1.6280E+01    | 4.371E-12 | 3.635E+01                   |
| 1s 5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.6516E+01    | 4.669E-10 | 3.806E+03                   | 1.6447E+01    | 4.657E-10 | 3.795E+03                   |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.6520E+01    | 1.620E-09 | 1.320E+04                   | 1.6451E+01    | 1.610E-09 | 1.311E+04                   |
| 1s 5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.6605E+01    | 3.751E-09 | 3.025E+04                   | 1.6535E+01    | 3.730E-09 | 3.008E+04                   |
| 1s 6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 4.1248E+01    | 1.91E-09  | 2.563E+03                   | 4.1067E+01    | 1.974E-09 | 2.581E+03                   |
| 1s 6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 4.3310E+01    | 4.142E-14 | 4.910E-02                   |               |           |                             |
| 1s 6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 4.3491E+01    | 2.199E-12 | 2.585E+00                   | 4.3277E+01    | 3.706E-12 | 4.363E+00                   |
| 1s 6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 4.4180E+01    | 6.062E-10 | 6.905E+02                   | 4.4005E+01    | 5.983E-10 | 6.812E+02                   |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 4.4195E+01    | 2.104E-09 | 2.395E+03                   | 4.4004E+01    | 2.101E-09 | 2.392E+03                   |
| 1s 6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 4.4549E+01    | 4.862E-09 | 5.447E+03                   | 4.4358E+01    | 4.862E-09 | 5.447E+03                   |
| 1s 7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.2801E+03    | 1.102E-12 | 1.496E-03                   | 1.2659E+03    | 1.132E-12 | 1.558E-03                   |
| 1s 7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>1</sub>              | 1.7684E+04    | 2.108E-20 | 1.499E-13                   |               |           |                             |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.3252E+00    | 7.024E-07 | 8.893E+08                   | 1.3196E+00    | 7.245E-07 | 9.173E+08                   |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.3877E+00    | 2.240E-07 | 4.340E+07                   | 3.3738E+00    | 2.287E-07 | 4.430E+07                   |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.5275E+00    | 2.870E-13 | 5.129E+01                   |               |           |                             |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.5290E+00    | 3.245E-15 | 5.794E-01                   |               |           |                             |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.5643E+00    | 6.031E-09 | 1.055E+06                   | 3.5494E+00    | 6.273E-09 | 1.097E+06                   |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 3.5657E+00    | 1.963E-08 | 3.433E+06                   | 3.5508E+00    | 1.869E-08 | 3.269E+06                   |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.3292E+00    | 1.005E-07 | 4.160E+06                   | 7.2994E+00    | 1.026E-07 | 4.245E+06                   |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.6019E+00    | 3.982E-14 | 1.532E+00                   |               |           |                             |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.6047E+00    | 4.575E-14 | 1.759E+00                   |               |           |                             |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.6740E+00    | 6.836E-09 | 2.581E+05                   | 7.6429E+00    | 7.123E-09 | 2.688E+05                   |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 7.6770E+00    | 2.199E-08 | 8.294E+05                   | 7.6459E+00    | 2.128E-08 | 8.026E+05                   |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.5702E+01    | 5.403E-08 | 4.873E+05                   | 1.5640E+01    | 5.523E-08 | 4.978E+05                   |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1.6342E+01    | 9.126E-20 | 7.599E-07                   |               |           |                             |

(continued on next page)

Table 6 (continued)

| Lower  | Upper  | GRASP2K       |           |                  | FAC           |           |                  |
|--|--|---------------|-----------|------------------|---------------|-----------|------------------|
|  |  | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.6348E+01    | 1.012E-13 | 8.420E-01        |               |           |                  |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.6512E+01    | 6.645E-09 | 5.418E+04        | 1.6449E+01    | 6.925E-09 | 5.643E+04        |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.6520E+01    | 2.120E-08 | 1.727E+05        | 1.6456E+01    | 2.069E-08 | 1.684E+05        |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.6603E+01    | 6.845E-18 | 5.521E-05        |               |           |                  |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 4.0902E+01    | 3.083E-08 | 4.097E+04        | 4.0720E+01    | 3.189E-08 | 4.241E+04        |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 4.3457E+01    | 1.217E-14 | 1.433E-02        |               |           |                  |
| 1s 6d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 4.3483E+01    | 1.543E-13 | 1.814E-01        |               |           |                  |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 4.4159E+01    | 6.358E-09 | 7.250E+03        | 4.4022E+01    | 6.675E-09 | 7.593E+03        |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 4.4189E+01    | 2.019E-08 | 2.299E+04        | 4.4032E+01    | 1.986E-08 | 2.258E+04        |
| 1s 6g <sup>3</sup> G <sub>3</sub>              | 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 4.4538E+01    | 9.976E-19 | 1.118E-06        |               |           |                  |
| 1s 7s <sup>3</sup> S <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1.0915E+03    | 4.698E-11 | 8.768E-02        | 1.0907E+03    | 4.671E-11 | 8.656E-02        |
| 1s 7d <sup>3</sup> D <sub>2</sub>              | 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 7.6625E+04    | 4.221E-22 | 1.598E-16        |               |           |                  |
| 1s 7d <sup>3</sup> D <sub>1</sub>              | 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 2.3287E+05    | 1.361E-22 | 5.579E-18        |               |           |                  |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.3358E+00    | 7.245E-07 | 3.869E+08        | 1.3303E+00    | 7.408E-07 | 3.955E+08        |
| 1s 2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.3942E+00    | 3.102E-06 | 1.520E+09        | 1.3883E+00    | 3.269E-06 | 1.602E+09        |
| 1s 2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.3997E+00    | 5.609E-07 | 2.728E+08        | 1.3939E+00    | 5.880E-07 | 2.859E+08        |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 3.4048E+00    | 2.467E-07 | 2.028E+07        | 3.3906E+00    | 2.512E-07 | 2.065E+07        |
| 1s 3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 3.5164E+00    | 1.176E-06 | 9.066E+07        | 3.5016E+00    | 1.199E-06 | 9.241E+07        |
| 1s 3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 3.5263E+00    | 2.112E-07 | 1.619E+07        | 3.5116E+00    | 2.148E-07 | 1.645E+07        |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 7.3548E+00    | 1.069E-07 | 1.882E+06        | 7.3233E+00    | 1.078E-07 | 1.899E+06        |
| 1s 4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 7.5732E+00    | 5.437E-07 | 9.033E+06        | 7.5406E+00    | 5.503E-07 | 9.145E+06        |
| 1s 4p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 7.5922E+00    | 9.799E-08 | 1.620E+06        | 7.5597E+00    | 9.827E-08 | 1.624E+06        |
| 1s 4f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 7.6624E+00    | 1.187E-14 | 1.927E-01        |               |           |                  |
| 1s 4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 7.6639E+00    | 5.976E-14 | 9.696E-01        |               |           |                  |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 7.6985E+00    | 1.906E-08 | 3.064E+05        | 7.6654E+00    | 1.878E-08 | 3.020E+05        |
| 1s 4f <sup>1</sup> F <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 7.6996E+00    | 2.291E-09 | 3.683E+04        | 7.6665E+00    | 2.252E-09 | 3.621E+04        |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.5735E+01    | 5.408E-08 | 2.082E+05        | 1.5665E+01    | 5.427E-08 | 2.089E+05        |
| 1s 5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.6246E+01    | 2.913E-07 | 1.052E+06        | 1.6174E+01    | 2.949E-07 | 1.065E+06        |
| 1s 5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.6290E+01    | 5.274E-08 | 1.894E+05        | 1.6219E+01    | 5.244E-08 | 1.883E+05        |
| 1s 5f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.6456E+01    | 1.679E-14 | 5.907E-02        |               |           |                  |
| 1s 5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.6460E+01    | 5.449E-14 | 1.917E-01        |               |           |                  |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.6542E+01    | 3.177E-08 | 1.106E+05        | 1.6469E+01    | 3.151E-08 | 1.097E+05        |
| 1s 5f <sup>1</sup> F <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 1.6544E+01    | 3.820E-09 | 1.330E+04        | 1.6472E+01    | 3.779E-09 | 1.316E+04        |
| 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.0875E+01    | 2.875E-08 | 1.639E+04        | 4.0680E+01    | 2.791E-08 | 1.593E+04        |
| 1s 6p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.2898E+01    | 1.671E-07 | 8.652E+04        | 4.2690E+01    | 1.695E-07 | 8.791E+04        |
| 1s 6p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.3077E+01    | 3.045E-08 | 1.563E+04        | 4.2848E+01    | 3.049E-08 | 1.569E+04        |
| 1s 6f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.3752E+01    | 1.969E-14 | 9.804E-03        |               |           |                  |
| 1s 6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.3767E+01    | 4.018E-14 | 1.999E-02        |               |           |                  |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.4102E+01    | 4.150E-08 | 2.033E+04        | 4.3907E+01    | 4.131E-08 | 2.024E+04        |
| 1s 6f <sup>1</sup> F <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.4114E+01    | 4.989E-09 | 2.443E+03        | 4.3908E+01    | 4.957E-09 | 2.429E+03        |
| 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.4315E+01    | 9.137E-18 | 4.434E-06        |               |           |                  |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.4320E+01    | 2.233E-18 | 1.083E-06        |               |           |                  |
| 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.4461E+01    | 1.723E-18 | 8.305E-07        |               |           |                  |
| 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 9.9748E+02    | 3.656E-11 | 3.502E-02        | 9.7908E+02    | 3.761E-11 | 3.707E-02        |
| 1s 7p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 3.5985E+03    | 3.897E-12 | 2.868E-04        | 3.3938E+03    | 4.609E-12 | 3.780E-04        |
| 1s 7p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s 7d <sup>3</sup> D <sub>3</sub>              | 4.6072E+03    | 3.345E-13 | 1.502E-05        | 4.1560E+03    | 4.627E-13 | 2.531E-05        |
| 1s 2s <sup>3</sup> S <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.3248E+00    | 4.372E-11 | 2.374E+04        |               |           |                  |
| 1s 3s <sup>3</sup> S <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 3.3852E+00    | 9.240E-15 | 7.683E-01        |               |           |                  |
| 1s 3d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 3.5247E+00    | 2.120E-07 | 1.626E+07        | 3.5099E+00    | 2.183E-07 | 1.674E+07        |
| 1s 3d <sup>3</sup> D <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 3.5262E+00    | 3.577E-08 | 2.742E+06        | 3.5113E+00    | 3.619E-08 | 2.773E+06        |
| 1s 3d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 3.5615E+00    | 1.257E-12 | 9.441E+01        |               |           |                  |
| 1s 3d <sup>1</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 3.5629E+00    | 1.636E-11 | 1.228E+03        |               |           |                  |
| 1s 4s <sup>3</sup> S <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 7.3173E+00    | 6.507E-14 | 1.158E+00        |               |           |                  |
| 1s 4d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 7.5891E+00    | 1.297E-07 | 2.146E+06        | 7.5575E+00    | 1.316E-07 | 2.177E+06        |
| 1s 4d <sup>3</sup> D <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 7.5919E+00    | 2.189E-08 | 3.619E+05        | 7.5603E+00    | 2.182E-08 | 3.607E+05        |
| 1s 4d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 7.6610E+00    | 6.830E-13 | 1.109E+01        |               |           |                  |
| 1s 4d <sup>1</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 7.6640E+00    | 1.512E-11 | 2.452E+02        |               |           |                  |
| 1s 5s <sup>3</sup> S <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.5648E+01    | 8.099E-15 | 3.152E-02        |               |           |                  |
| 1s 5d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.6283E+01    | 7.588E-08 | 2.727E+05        | 1.6216E+01    | 7.648E-08 | 2.748E+05        |
| 1s 5d <sup>3</sup> D <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.6289E+01    | 1.281E-08 | 4.601E+04        | 1.6222E+01    | 1.268E-08 | 4.552E+04        |
| 1s 5d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.6452E+01    | 4.024E-13 | 1.417E+00        |               |           |                  |
| 1s 5d <sup>1</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.6459E+01    | 1.044E-11 | 3.671E+01        |               |           |                  |
| 1s 5g <sup>3</sup> G <sub>4</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.6541E+01    | 2.537E-09 | 8.837E+03        | 1.6470E+01    | 2.522E-09 | 8.786E+03        |
| 1s 5g <sup>3</sup> G <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.6543E+01    | 3.069E-10 | 1.069E+03        | 1.6472E+01    | 3.028E-10 | 1.054E+03        |
| 1s 5g <sup>3</sup> G <sub>5</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.6592E+01    | 1.834E-09 | 6.348E+03        | 1.6521E+01    | 1.818E-09 | 6.295E+03        |
| 1s 5g <sup>1</sup> G <sub>4</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 1.6593E+01    | 1.091E-10 | 3.777E+02        | 1.6522E+01    | 1.137E-10 | 3.937E+02        |
| 1s 6s <sup>3</sup> S <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 4.0535E+01    | 3.060E-16 | 1.774E-04        |               |           |                  |
| 1s 6d <sup>3</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 4.3043E+01    | 4.447E-08 | 2.287E+04        | 4.2880E+01    | 4.463E-08 | 2.293E+04        |
| 1s 6d <sup>3</sup> D <sub>1</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 4.3069E+01    | 7.515E-09 | 3.860E+03        | 4.2873E+01    | 7.412E-09 | 3.810E+03        |
| 1s 6d <sup>3</sup> D <sub>3</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 4.3731E+01    | 2.440E-13 | 1.216E-01        |               |           |                  |
| 1s 6d <sup>1</sup> D <sub>2</sub>              | 1s 7f <sup>3</sup> F <sub>0</sub> <sup>o</sup> | 4.3761E+01    | 6.745E-12 | 3.356E+00        |               |           |                  |

(continued on next page)

Table 6 (continued)

| Lower   | Upper   | GRASP2K       |           |                        | FAC           |           |                        |
|---|---|---------------|-----------|------------------------|---------------|-----------|------------------------|
|   |   | $\lambda$ (Å) | <i>gf</i> | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | $A$ (s <sup>-1</sup> ) |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4095E+01    | 5.957E-09 | 2.919E+03              | 4.3907E+01    | 5.943E-09 | 2.912E+03              |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4103E+01    | 7.176E-10 | 3.515E+02              | 4.3907E+01    | 7.132E-10 | 3.495E+02              |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4306E+01    | 4.285E-09 | 2.080E+03              | 4.4116E+01    | 4.256E-09 | 2.066E+03              |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4313E+01    | 2.540E-10 | 1.233E+02              | 4.4116E+01    | 2.616E-10 | 1.270E+02              |
| 1s7s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 8.7909E+02    | 9.255E-18 | 1.141E-08              |               |           |                        |
| 1s7d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.2661E+03    | 3.833E-13 | 2.007E-05              | 4.3591E+03    | 3.562E-13 | 1.771E-05              |
| 1s7d <sup>3</sup> D <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 4.4317E+03    | 5.768E-14 | 2.799E-06              | 4.3178E+03    | 6.085E-14 | 3.083E-06              |
| 1s7d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 2.3237E+05    | 1.291E-23 | 2.278E-19              |               |           |                        |
| 1s <sup>2</sup> <sup>1</sup> S <sub>0</sub>   | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.1390E-01    | 4.947E-11 | 6.694E+05              |               |           |                        |
| 1s2s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3248E+00    | 1.507E-11 | 1.146E+04              |               |           |                        |
| 1s2s <sup>1</sup> S <sub>0</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.3369E+00    | 1.400E-11 | 1.045E+04              |               |           |                        |
| 1s3s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.3851E+00    | 1.421E-13 | 1.654E+01              |               |           |                        |
| 1s3s <sup>1</sup> S <sub>0</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.4060E+00    | 5.718E-14 | 6.576E+00              |               |           |                        |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.5247E+00    | 5.320E-08 | 5.713E+06              | 3.5099E+00    | 5.455E-08 | 5.857E+06              |
| 1s3d <sup>3</sup> D <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.5262E+00    | 1.239E-07 | 1.330E+07              | 3.5113E+00    | 1.271E-07 | 1.363E+07              |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.5614E+00    | 1.346E-14 | 1.416E+00              |               |           |                        |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 3.5628E+00    | 5.049E-13 | 5.306E+01              |               |           |                        |
| 1s4s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.3170E+00    | 2.407E-13 | 5.998E+00              |               |           |                        |
| 1s4s <sup>1</sup> S <sub>0</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.3564E+00    | 1.604E-13 | 3.954E+00              |               |           |                        |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.5889E+00    | 3.251E-08 | 7.530E+05              | 7.5575E+00    | 3.288E-08 | 7.616E+05              |
| 1s4d <sup>3</sup> D <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.5917E+00    | 7.584E-08 | 1.755E+06              | 7.5603E+00    | 7.665E-08 | 1.773E+06              |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.6607E+00    | 6.576E-15 | 1.495E-01              |               |           |                        |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 7.6637E+00    | 7.964E-13 | 1.809E+01              |               |           |                        |
| 1s5s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.5646E+01    | 1.174E-13 | 6.400E-01              |               |           |                        |
| 1s5s <sup>1</sup> S <sub>0</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.5737E+01    | 7.104E-14 | 3.827E-01              |               |           |                        |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6281E+01    | 1.900E-08 | 9.564E+04              | 1.6216E+01    | 1.911E-08 | 9.613E+04              |
| 1s5d <sup>3</sup> D <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6288E+01    | 4.437E-08 | 2.231E+05              | 1.6222E+01    | 4.453E-08 | 2.238E+05              |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6451E+01    | 9.948E-15 | 4.904E-02              |               |           |                        |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6458E+01    | 6.222E-13 | 3.064E+00              |               |           |                        |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6539E+01    | 2.043E-10 | 9.963E+02              | 1.6470E+01    | 2.039E-10 | 9.947E+02              |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6541E+01    | 1.835E-09 | 8.949E+03              | 1.6472E+01    | 1.817E-09 | 8.858E+03              |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.6592E+01    | 1.387E-09 | 6.722E+03              | 1.6522E+01    | 1.376E-09 | 6.669E+03              |
| 1s6s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.0528E+01    | 4.682E-14 | 3.803E-02              |               |           |                        |
| 1s6s <sup>1</sup> S <sub>0</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.0875E+01    | 2.291E-14 | 1.830E-02              |               |           |                        |
| 1s6d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3034E+01    | 1.113E-08 | 8.018E+03              | 4.2880E+01    | 1.115E-08 | 8.022E+03              |
| 1s6d <sup>3</sup> D <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3060E+01    | 2.601E-08 | 1.871E+04              | 4.2874E+01    | 2.603E-08 | 1.873E+04              |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3722E+01    | 9.348E-15 | 6.523E-03              |               |           |                        |
| 1s6d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3752E+01    | 4.162E-13 | 2.900E-01              |               |           |                        |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4085E+01    | 4.800E-10 | 3.295E+02              | 4.3907E+01    | 4.754E-10 | 3.262E+02              |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4094E+01    | 4.293E-09 | 2.946E+03              | 4.3907E+01    | 4.279E-09 | 2.936E+03              |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.4303E+01    | 3.232E-09 | 2.197E+03              | 4.4116E+01    | 3.227E-09 | 2.193E+03              |
| 1s7s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 8.7540E+02    | 1.929E-17 | 3.359E-08              |               |           |                        |
| 1s7s <sup>1</sup> S <sub>0</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 9.8912E+02    | 1.980E-17 | 2.700E-08              |               |           |                        |
| 1s7d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.1806E+03    | 1.020E-13 | 7.789E-06              | 4.3602E+03    | 8.894E-14 | 6.188E-06              |
| 1s7d <sup>3</sup> D <sub>1</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 4.3395E+03    | 2.128E-13 | 1.508E-05              | 4.3189E+03    | 2.135E-13 | 1.514E-05              |
| 1s7d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1.0992E+05    | 3.776E-23 | 4.169E-18              |               |           |                        |
| 1s2p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.3358E+00    | 2.774E-07 | 2.074E+08              | 1.3303E+00    | 2.850E-07 | 2.130E+08              |
| 1s2p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.3367E+00    | 3.356E-07 | 2.506E+08              | 1.3311E+00    | 3.437E-07 | 2.566E+08              |
| 1s2p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.3942E+00    | 7.807E-07 | 5.358E+08              | 1.3883E+00    | 8.173E-07 | 5.609E+08              |
| 1s2p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.3997E+00    | 1.753E-06 | 1.194E+09              | 1.3939E+00    | 1.832E-06 | 1.247E+09              |
| 1s3p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 3.4047E+00    | 9.352E-08 | 1.076E+07              | 3.3905E+00    | 9.546E-08 | 1.098E+07              |
| 1s3p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 3.4061E+00    | 1.139E-07 | 1.310E+07              | 3.3919E+00    | 1.162E-07 | 1.336E+07              |
| 1s3p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 3.5163E+00    | 2.950E-07 | 3.183E+07              | 3.5016E+00    | 2.998E-07 | 3.234E+07              |
| 1s3p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 3.5262E+00    | 6.667E-07 | 7.153E+07              | 3.5116E+00    | 6.762E-07 | 7.254E+07              |
| 1s4p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 7.3543E+00    | 4.023E-08 | 9.922E+05              | 7.3231E+00    | 4.103E-08 | 1.012E+06              |
| 1s4p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 7.3570E+00    | 4.925E-08 | 1.214E+06              | 7.3257E+00    | 4.994E-08 | 1.230E+06              |
| 1s4p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 7.5726E+00    | 1.361E-07 | 3.167E+06              | 7.5404E+00    | 1.375E-07 | 3.200E+06              |
| 1s4p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 7.5916E+00    | 3.096E-07 | 7.166E+06              | 7.5595E+00    | 3.110E-07 | 7.199E+06              |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 7.6618E+00    | 2.579E-13 | 5.861E+00              |               |           |                        |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 7.6633E+00    | 1.012E-18 | 2.299E-05              |               |           |                        |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 7.6979E+00    | 1.547E-09 | 3.482E+04              | 7.6651E+00    | 1.558E-09 | 3.507E+04              |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 7.6990E+00    | 1.365E-08 | 3.073E+05              | 7.6663E+00    | 1.346E-08 | 3.029E+05              |
| 1s5p <sup>3</sup> P <sub>0</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.5732E+01    | 2.027E-08 | 1.093E+05              | 1.5665E+01    | 2.079E-08 | 1.121E+05              |
| 1s5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.5738E+01    | 2.489E-08 | 1.341E+05              | 1.5671E+01    | 2.518E-08 | 1.356E+05              |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.6243E+01    | 7.285E-08 | 3.683E+05              | 1.6173E+01    | 7.372E-08 | 3.728E+05              |
| 1s5p <sup>1</sup> P <sub>0</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.6288E+01    | 1.665E-07 | 8.375E+05              | 1.6218E+01    | 1.667E-07 | 8.385E+05              |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.6454E+01    | 4.024E-13 | 1.983E+00              |               |           |                        |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.6457E+01    | 1.812E-15 | 8.923E-03              |               |           |                        |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.6539E+01    | 2.579E-09 | 1.258E+04              | 1.6468E+01    | 2.613E-09 | 1.274E+04              |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 1.6542E+01    | 2.277E-08 | 1.110E+05              | 1.6471E+01    | 2.258E-08 | 1.101E+05              |
| 1s6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7d <sup>1</sup> D <sub>2</sub>              | 4.0858E+01    | 1.073E-08 | 8.576E+03              | 4.0674E+01    | 1.190E-08 | 9.521E+03              |

(continued on next page)

Table 6 (continued)

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |           |                  |
|-----------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                 |                 | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 6p $^3P_0^o$ | 1s 7d $^1D_2$   | 4.0882E+01    | 1.321E-08 | 1.055E+04        | 4.0612E+01    | 1.340E-08 | 1.074E+04        |
| 1s 6p $^3P_2^o$ | 1s 7d $^1D_2$   | 4.2880E+01    | 4.171E-08 | 3.026E+04        | 4.2684E+01    | 4.240E-08 | 3.079E+04        |
| 1s 6p $^1P_1^o$ | 1s 7d $^1D_2$   | 4.3058E+01    | 9.601E-08 | 6.908E+04        | 4.2841E+01    | 9.514E-08 | 6.856E+04        |
| 1s 6f $^3F_3^o$ | 1s 7d $^1D_2$   | 4.3733E+01    | 5.031E-13 | 3.509E-01        |               |           |                  |
| 1s 6f $^3F_2^o$ | 1s 7d $^1D_2$   | 4.3748E+01    | 6.962E-15 | 4.853E-03        |               |           |                  |
| 1s 6f $^3F_4^o$ | 1s 7d $^1D_2$   | 4.4083E+01    | 3.368E-09 | 2.312E+03        | 4.3900E+01    | 3.427E-09 | 2.352E+03        |
| 1s 6f $^1F_3^o$ | 1s 7d $^1D_2$   | 4.4094E+01    | 2.973E-08 | 2.040E+04        | 4.3901E+01    | 2.963E-08 | 2.033E+04        |
| 1s 6h $^3H_4^o$ | 1s 7d $^1D_2$   | 4.4301E+01    | 4.583E-18 | 3.115E-06        |               |           |                  |
| 1s 7p $^3P_0^o$ | 1s 7d $^1D_2$   | 9.8772E+01    | 1.410E-11 | 1.928E-02        | 9.7564E+02    | 1.532E-11 | 2.128E-02        |
| 1s 7p $^3P_1^o$ | 1s 7d $^1D_2$   | 9.9663E+02    | 1.685E-11 | 2.263E-02        | 9.5369E+02    | 1.915E-11 | 2.785E-02        |
| 1s 7p $^3P_2^o$ | 1s 7d $^1D_2$   | 3.4747E+03    | 1.082E-12 | 1.196E-04        | 3.3529E+03    | 1.194E-12 | 1.405E-04        |
| 1s 7p $^1P_1^o$ | 1s 7d $^1D_2$   | 4.4062E+03    | 1.207E-12 | 8.296E-05        | 4.0947E+03    | 1.481E-12 | 1.169E-04        |
| 1s 7f $^3F_3^o$ | 1s 7d $^1D_2$   | 1.7858E+05    | 7.949E-22 | 3.325E-17        |               |           |                  |
| 1s 7f $^3F_2^o$ | 1s 7d $^1D_2$   | 1.2412E+06    | 1.105E-25 | 9.570E-23        |               |           |                  |
| 1s 3d $^3D_2$   | 1s 7f $^3F_4^o$ | 3.5233E+00    | 4.205E-07 | 2.510E+07        | 3.5085E+00    | 4.222E-07 | 2.520E+07        |
| 1s 3d $^3D_3$   | 1s 7f $^3F_4^o$ | 3.5600E+00    | 2.526E-06 | 1.477E+08        | 3.5449E+00    | 2.596E-06 | 1.518E+08        |
| 1s 3d $^1D_2$   | 1s 7f $^3F_4^o$ | 3.5614E+00    | 2.038E-07 | 1.191E+07        | 3.5463E+00    | 2.095E-07 | 1.224E+07        |
| 1s 4d $^3D_2$   | 1s 7f $^3F_4^o$ | 7.5826E+00    | 2.510E-07 | 3.235E+06        | 7.5510E+00    | 2.533E-07 | 3.265E+06        |
| 1s 4d $^3D_3$   | 1s 7f $^3F_4^o$ | 7.6543E+00    | 1.564E-06 | 1.979E+07        | 7.6222E+00    | 1.584E-06 | 2.003E+07        |
| 1s 4d $^1D_2$   | 1s 7f $^3F_4^o$ | 7.6573E+00    | 1.270E-07 | 1.605E+06        | 7.6252E+00    | 1.286E-07 | 1.625E+06        |
| 1s 5d $^3D_2$   | 1s 7f $^3F_4^o$ | 1.6252E+01    | 1.445E-07 | 4.054E+05        | 1.6186E+01    | 1.453E-07 | 4.077E+05        |
| 1s 5d $^3D_3$   | 1s 7f $^3F_4^o$ | 1.6421E+01    | 9.255E-07 | 2.544E+06        | 1.6353E+01    | 9.309E-07 | 2.558E+06        |
| 1s 5d $^1D_2$   | 1s 7f $^3F_4^o$ | 1.6428E+01    | 7.534E-08 | 2.069E+05        | 1.6360E+01    | 7.572E-08 | 2.078E+05        |
| 1s 5g $^3G_4$   | 1s 7f $^3F_4^o$ | 1.6509E+01    | 3.180E-15 | 8.647E-03        |               |           |                  |
| 1s 5g $^3G_3$   | 1s 7f $^3F_4^o$ | 1.6511E+01    | 4.291E-16 | 1.166E-03        |               |           |                  |
| 1s 5g $^3G_5$   | 1s 7f $^3F_4^o$ | 1.6560E+01    | 1.498E-08 | 4.050E+04        | 1.6489E+01    | 1.487E-08 | 4.021E+04        |
| 1s 5g $^1G_4$   | 1s 7f $^3F_4^o$ | 1.6562E+01    | 1.077E-09 | 2.909E+03        | 1.6491E+01    | 1.062E-09 | 2.871E+03        |
| 1s 6d $^3D_2$   | 1s 7f $^3F_4^o$ | 4.2832E+01    | 8.329E-08 | 3.365E+04        | 4.2671E+01    | 8.278E-08 | 3.340E+04        |
| 1s 6d $^3D_3$   | 1s 7f $^3F_4^o$ | 4.3514E+01    | 5.502E-07 | 2.154E+05        | 4.3345E+01    | 5.513E-07 | 2.156E+05        |
| 1s 6d $^1D_2$   | 1s 7f $^3F_4^o$ | 4.3544E+01    | 4.488E-08 | 1.754E+04        | 4.3355E+01    | 4.548E-08 | 1.778E+04        |
| 1s 6g $^3G_4$   | 1s 7f $^3F_4^o$ | 4.3874E+01    | 8.351E-15 | 3.215E-03        |               |           |                  |
| 1s 6g $^3G_3$   | 1s 7f $^3F_4^o$ | 4.3882E+01    | 5.086E-16 | 1.957E-04        |               |           |                  |
| 1s 6g $^3G_5$   | 1s 7f $^3F_4^o$ | 4.4083E+01    | 3.532E-08 | 1.347E+04        | 4.3895E+01    | 3.519E-08 | 1.342E+04        |
| 1s 6g $^1G_4$   | 1s 7f $^3F_4^o$ | 4.4090E+01    | 2.529E-09 | 9.643E+02        | 4.3895E+01    | 2.514E-09 | 9.588E+02        |
| 1s 7d $^3D_2$   | 1s 7f $^3F_4^o$ | 2.8680E+03    | 2.422E-12 | 2.182E-04        | 2.9119E+03    | 2.266E-12 | 1.964E-04        |
| 1s 7d $^3D_3$   | 1s 7f $^3F_4^o$ | 8.4332E+03    | 6.104E-13 | 6.362E-06        | 8.7593E+03    | 5.382E-13 | 5.155E-06        |
| 1s 7d $^1D_2$   | 1s 7f $^3F_4^o$ | 9.2016E+03    | 3.828E-14 | 3.351E-07        | 9.0446E+03    | 4.045E-14 | 3.633E-07        |
| 1s 2p $^3P_0^o$ | 1s 7g $^3G_4$   | 1.3940E+00    | 1.685E-11 | 6.427E+03        |               |           |                  |
| 1s 3p $^3P_2^o$ | 1s 7g $^3G_4$   | 3.5149E+00    | 1.323E-11 | 7.934E+02        |               |           |                  |
| 1s 4p $^3P_0^o$ | 1s 7g $^3G_4$   | 7.5664E+00    | 2.232E-13 | 2.889E+00        |               |           |                  |
| 1s 4f $^3F_3^o$ | 1s 7g $^3G_4$   | 7.6554E+00    | 4.102E-07 | 5.187E+06        | 7.6229E+00    | 4.168E-07 | 5.271E+06        |
| 1s 4f $^3F_2^o$ | 1s 7g $^3G_4$   | 7.6569E+00    | 3.311E-08 | 4.186E+05        | 7.6244E+00    | 3.332E-08 | 4.212E+05        |
| 1s 4f $^3F_4^o$ | 1s 7g $^3G_4$   | 7.6914E+00    | 6.083E-13 | 7.620E+00        |               |           |                  |
| 1s 4f $^1F_3^o$ | 1s 7g $^3G_4$   | 7.6926E+00    | 1.492E-12 | 1.869E+01        |               |           |                  |
| 1s 5p $^3P_0^o$ | 1s 7g $^3G_4$   | 1.6215E+01    | 2.286E-14 | 6.444E-02        |               |           |                  |
| 1s 5f $^3F_3^o$ | 1s 7g $^3G_4$   | 1.6424E+01    | 3.500E-07 | 9.616E+05        | 1.6354E+01    | 3.528E-07 | 9.693E+05        |
| 1s 5f $^3F_2^o$ | 1s 7g $^3G_4$   | 1.6428E+01    | 2.827E-08 | 7.765E+04        | 1.6358E+01    | 2.820E-08 | 7.745E+04        |
| 1s 5f $^3F_4^o$ | 1s 7g $^3G_4$   | 1.6509E+01    | 5.308E-13 | 1.443E+00        |               |           |                  |
| 1s 5f $^1F_3^o$ | 1s 7g $^3G_4$   | 1.6512E+01    | 1.496E-12 | 4.068E+00        |               |           |                  |
| 1s 6p $^3P_2^o$ | 1s 7g $^3G_4$   | 4.2681E+01    | 1.962E-14 | 7.981E-03        |               |           |                  |
| 1s 6f $^3F_3^o$ | 1s 7g $^3G_4$   | 4.3526E+01    | 2.388E-07 | 9.340E+04        | 4.3346E+01    | 2.395E-07 | 9.368E+04        |
| 1s 6f $^3F_2^o$ | 1s 7g $^3G_4$   | 4.3540E+01    | 1.930E-08 | 7.546E+03        | 4.3346E+01    | 1.916E-08 | 7.494E+03        |
| 1s 6f $^3F_4^o$ | 1s 7g $^3G_4$   | 4.3873E+01    | 3.710E-13 | 1.429E-01        |               |           |                  |
| 1s 6f $^1F_3^o$ | 1s 7g $^3G_4$   | 4.3884E+01    | 1.132E-12 | 4.356E-01        |               |           |                  |
| 1s 6h $^3H_5^o$ | 1s 7g $^3G_4$   | 4.4083E+01    | 4.476E-09 | 1.707E+03        | 4.3896E+01    | 4.459E-09 | 1.700E+03        |
| 1s 6h $^3H_4^o$ | 1s 7g $^3G_4$   | 4.4088E+01    | 3.202E-10 | 1.221E+02        | 4.3896E+01    | 3.185E-10 | 1.214E+02        |
| 1s 6h $^3H_6^o$ | 1s 7g $^3G_4$   | 4.4223E+01    | 1.616E-09 | 6.123E+02        | 4.4034E+01    | 1.606E-09 | 6.089E+02        |
| 1s 6h $^1H_5^o$ | 1s 7g $^3G_4$   | 4.4227E+01    | 6.000E-11 | 2.273E+01        | 4.4034E+01    | 6.182E-11 | 2.342E+01        |
| 1s 7p $^3P_0^o$ | 1s 7g $^3G_4$   | 2.5209E+03    | 4.451E-21 | 5.191E-13        |               |           |                  |
| 1s 7f $^3F_3^o$ | 1s 7g $^3G_4$   | 8.7347E+03    | 1.399E-13 | 1.359E-06        | 8.7974E+03    | 1.354E-13 | 1.286E-06        |
| 1s 7f $^3F_2^o$ | 1s 7g $^3G_4$   | 9.1165E+03    | 9.944E-15 | 8.867E-08        | 8.7927E+03    | 1.085E-14 | 1.031E-07        |
| 1s 7f $^3F_4^o$ | 1s 7g $^3G_4$   | 4.7642E+06    | 1.343E-27 | 4.385E-26        |               |           |                  |
| 1s 2p $^3P_1^o$ | 1s 7g $^3G_3$   | 1.3356E+00    | 3.671E-14 | 1.961E+01        |               |           |                  |
| 1s 2p $^3P_2^o$ | 1s 7g $^3G_3$   | 1.3940E+00    | 1.616E-12 | 7.925E+02        |               |           |                  |
| 1s 2p $^1P_1^o$ | 1s 7g $^3G_3$   | 1.3995E+00    | 1.116E-11 | 5.428E+03        |               |           |                  |
| 1s 3p $^3P_0^o$ | 1s 7g $^3G_3$   | 3.4034E+00    | 3.734E-14 | 3.072E+00        |               |           |                  |
| 1s 3p $^3P_1^o$ | 1s 7g $^3G_3$   | 3.5149E+00    | 1.511E-12 | 1.166E+02        |               |           |                  |
| 1s 3p $^3P_2^o$ | 1s 7g $^3G_3$   | 3.5248E+00    | 7.982E-12 | 6.122E+02        |               |           |                  |
| 1s 4p $^3P_1^o$ | 1s 7g $^3G_3$   | 7.3482E+00    | 8.284E-16 | 1.462E-02        |               |           |                  |
| 1s 4p $^3P_2^o$ | 1s 7g $^3G_3$   | 7.5662E+00    | 2.075E-15 | 3.453E-02        |               |           |                  |
| 1s 4p $^1P_1^o$ | 1s 7g $^3G_3$   | 7.5852E+00    | 9.542E-14 | 1.580E+00        |               |           |                  |

(continued on next page)



Table 6 (continued)

| Lower   | Upper   | GRASP2K       |           |                        | FAC           |           |                        |
|---|---|---------------|-----------|------------------------|---------------|-----------|------------------------|
|   |   | $\lambda$ (Å) | <i>gf</i> | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | $A$ (s <sup>-1</sup> ) |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 7.6553E+00    | 4.932E-08 | 8.020E+05              | 7.6229E+00    | 5.002E-08 | 8.132E+05              |
| 1s4f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 7.6568E+00    | 2.955E-07 | 4.803E+06              | 7.6244E+00    | 2.999E-07 | 4.874E+06              |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 7.6913E+00    | 1.523E-19 | 2.453E-06              |               |           |                        |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 7.6924E+00    | 2.237E-13 | 3.603E+00              |               |           |                        |
| 1s5p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.5705E+01    | 1.628E-19 | 6.288E-07              |               |           |                        |
| 1s5p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6214E+01    | 8.575E-14 | 3.108E-01              |               |           |                        |
| 1s5p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6258E+01    | 3.715E-14 | 1.339E-01              |               |           |                        |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6423E+01    | 4.206E-08 | 1.486E+05              | 1.6354E+01    | 4.233E-08 | 1.495E+05              |
| 1s5f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6427E+01    | 2.522E-07 | 8.905E+05              | 1.6358E+01    | 2.538E-07 | 8.963E+05              |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6508E+01    | 1.692E-17 | 5.915E-05              |               |           |                        |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 1.6511E+01    | 1.720E-13 | 6.013E-01              |               |           |                        |
| 1s6p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.0673E+01    | 3.156E-18 | 1.818E-06              |               |           |                        |
| 1s6p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.2676E+01    | 7.118E-14 | 3.724E-02              |               |           |                        |
| 1s6p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.2852E+01    | 3.084E-14 | 1.601E-02              |               |           |                        |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.3521E+01    | 2.867E-08 | 1.442E+04              | 4.3346E+01    | 2.874E-08 | 1.445E+04              |
| 1s6f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.3535E+01    | 1.721E-07 | 8.651E+04              | 4.3346E+01    | 1.724E-07 | 8.672E+04              |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.3867E+01    | 3.588E-17 | 1.777E-05              |               |           |                        |
| 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.3878E+01    | 1.112E-13 | 5.505E-02              |               |           |                        |
| 1s6h <sup>3</sup> H <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.4077E+01    | 2.145E-10 | 1.052E+02              | 4.3896E+01    | 2.123E-10 | 1.041E+02              |
| 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.4083E+01    | 3.516E-09 | 1.724E+03              | 4.3896E+01    | 3.503E-09 | 1.718E+03              |
| 1s6h <sup>1</sup> H <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 4.4222E+01    | 1.299E-09 | 6.331E+02              | 4.4034E+01    | 1.297E-09 | 6.323E+02              |
| 1s7p <sup>3</sup> P <sub>1</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 8.8963E+02    | 4.277E-20 | 5.149E-11              |               |           |                        |
| 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 2.5035E+03    | 1.266E-18 | 1.925E-10              |               |           |                        |
| 1s7p <sup>1</sup> P <sub>1</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 2.9534E+03    | 5.714E-20 | 6.242E-12              |               |           |                        |
| 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 8.5297E+03    | 1.804E-14 | 2.362E-07              | 8.7975E+03    | 1.625E-14 | 1.984E-07              |
| 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 8.8934E+03    | 9.547E-14 | 1.150E-06              | 8.7928E+03    | 9.768E-14 | 1.193E-06              |
| 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>3</sub>              | 3.3768E+05    | 1.239E-26 | 1.035E-22              |               |           |                        |
| 1s2s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.3246E+00    | 2.065E-13 | 1.121E+02              |               |           |                        |
| 1s3s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.3838E+00    | 5.178E-13 | 4.309E+01              |               |           |                        |
| 1s3d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.5233E+00    | 4.933E-08 | 3.787E+06              | 3.5085E+00    | 4.924E-08 | 3.779E+06              |
| 1s3d <sup>3</sup> D <sub>1</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.5247E+00    | 2.810E-07 | 2.155E+07              | 3.5099E+00    | 2.827E-07 | 2.168E+07              |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.5600E+00    | 3.035E-07 | 2.282E+07              | 3.5449E+00    | 3.115E-07 | 2.342E+07              |
| 1s3d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 3.5614E+00    | 1.816E-06 | 1.364E+08              | 3.5463E+00    | 1.864E-06 | 1.400E+08              |
| 1s4s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.3110E+00    | 3.646E-13 | 6.500E+00              |               |           |                        |
| 1s4d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.5823E+00    | 3.022E-08 | 5.008E+05              | 7.5510E+00    | 3.040E-08 | 5.038E+05              |
| 1s4d <sup>3</sup> D <sub>1</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.5851E+00    | 1.684E-07 | 2.788E+06              | 7.5538E+00    | 1.701E-07 | 2.817E+06              |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.6541E+00    | 1.878E-07 | 3.055E+06              | 7.6222E+00    | 1.901E-07 | 3.091E+06              |
| 1s4d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.6570E+00    | 1.125E-06 | 1.828E+07              | 7.6252E+00    | 1.137E-06 | 1.848E+07              |
| 1s5s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.5619E+01    | 2.264E-13 | 8.845E-01              |               |           |                        |
| 1s5d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6251E+01    | 1.759E-08 | 6.347E+04              | 1.6186E+01    | 1.767E-08 | 6.374E+04              |
| 1s5d <sup>3</sup> D <sub>1</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6258E+01    | 9.706E-08 | 3.499E+05              | 1.6192E+01    | 9.776E-08 | 3.523E+05              |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6420E+01    | 1.111E-07 | 3.925E+05              | 1.6353E+01    | 1.117E-07 | 3.946E+05              |
| 1s5d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6427E+01    | 6.654E-07 | 2.349E+06              | 1.6360E+01    | 6.680E-07 | 2.357E+06              |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6508E+01    | 8.835E-15 | 3.089E-02              |               |           |                        |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6510E+01    | 1.556E-15 | 5.439E-03              |               |           |                        |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6559E+01    | 7.076E-10 | 2.459E+03              | 1.6489E+01    | 7.100E-10 | 2.467E+03              |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.6561E+01    | 1.182E-08 | 4.106E+04              | 1.6491E+01    | 1.168E-08 | 4.060E+04              |
| 1s6s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.0343E+01    | 1.294E-13 | 7.577E-02              |               |           |                        |
| 1s6d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.2826E+01    | 1.020E-08 | 5.300E+03              | 4.2671E+01    | 1.086E-08 | 5.638E+03              |
| 1s6d <sup>3</sup> D <sub>1</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.2851E+01    | 5.600E-08 | 2.906E+04              | 4.2665E+01    | 5.622E-08 | 2.918E+04              |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3507E+01    | 6.599E-08 | 3.322E+04              | 4.3345E+01    | 6.615E-08 | 3.327E+04              |
| 1s6d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3537E+01    | 3.957E-07 | 1.989E+05              | 4.3355E+01    | 3.952E-07 | 1.986E+05              |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3867E+01    | 2.568E-14 | 1.272E-02              |               |           |                        |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.3875E+01    | 3.279E-15 | 1.623E-03              |               |           |                        |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.4076E+01    | 1.668E-09 | 8.183E+02              | 4.3895E+01    | 1.679E-09 | 8.235E+02              |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 4.4083E+01    | 2.777E-08 | 1.362E+04              | 4.3895E+01    | 2.765E-08 | 1.355E+04              |
| 1s7s <sup>3</sup> S <sub>1</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 7.9654E+02    | 2.248E-16 | 3.376E-07              |               |           |                        |
| 1s7d <sup>3</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.8385E+03    | 3.075E-13 | 3.636E-05              | 2.9112E+03    | 2.970E-13 | 3.312E-05              |
| 1s7d <sup>3</sup> D <sub>1</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.9109E+03    | 1.557E-12 | 1.751E-04              | 2.8927E+03    | 1.569E-12 | 1.772E-04              |
| 1s7d <sup>3</sup> D <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 8.1837E+03    | 8.017E-14 | 1.141E-06              | 8.7525E+03    | 6.474E-14 | 7.985E-07              |
| 1s7d <sup>1</sup> D <sub>2</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 8.9054E+03    | 3.724E-13 | 4.474E-06              | 9.0373E+03    | 3.515E-13 | 4.066E-06              |
| 1s7g <sup>3</sup> G <sub>4</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 2.9370E+05    | 1.846E-23 | 2.039E-19              |               |           |                        |
| 1s7g <sup>3</sup> G <sub>3</sub>              | 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1.5307E+06    | 1.214E-26 | 4.936E-24              |               |           |                        |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 7.6514E+00    | 2.899E-07 | 3.003E+06              | 7.6190E+00    | 2.900E-07 | 3.003E+06              |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 7.6874E+00    | 2.475E-06 | 2.540E+07              | 7.6547E+00    | 2.516E-06 | 2.582E+07              |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 7.6885E+00    | 1.170E-07 | 1.200E+06              | 7.6558E+00    | 1.189E-07 | 1.220E+06              |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 1.6406E+01    | 2.441E-07 | 5.499E+05              | 1.6336E+01    | 2.453E-07 | 5.528E+05              |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 1.6491E+01    | 2.124E-06 | 4.737E+06              | 1.6420E+01    | 2.140E-06 | 4.772E+06              |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 1.6493E+01    | 1.005E-07 | 2.240E+05              | 1.6423E+01    | 1.012E-07 | 2.256E+05              |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 4.3397E+01    | 1.644E-07 | 5.294E+04              | 4.3219E+01    | 1.643E-07 | 5.291E+04              |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>5</sub>              | 4.3742E+01    | 1.459E-06 | 4.624E+05              | 4.3559E+01    | 1.462E-06 | 4.634E+05              |

(continued on next page)

Table 6 (continued)

| Lower           | Upper           | GRASP2K       |           |                  | FAC           |           |                  |
|-----------------|-----------------|---------------|-----------|------------------|---------------|-----------|------------------|
|                 |                 | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) | $\lambda$ (Å) | $gf$      | $A$ ( $s^{-1}$ ) |
| 1s 6f $^1F_3^0$ | 1s 7g $^3G_5$   | 4.3753E+01    | 6.906E-08 | 2.188E+04        | 4.3560E+01    | 6.976E-08 | 2.210E+04        |
| 1s 6h $^3H_5^0$ | 1s 7g $^3G_5$   | 4.3951E+01    | 2.044E-15 | 6.415E-04        |               |           |                  |
| 1s 6h $^3H_4^0$ | 1s 7g $^3G_5$   | 4.3956E+01    | 4.299E-19 | 1.349E-07        |               |           |                  |
| 1s 6h $^3H_6^0$ | 1s 7g $^3G_5$   | 4.4090E+01    | 1.830E-08 | 5.710E+03        | 4.3903E+01    | 1.822E-08 | 5.684E+03        |
| 1s 6h $^1H_5^0$ | 1s 7g $^3G_5$   | 4.4094E+01    | 8.725E-10 | 2.721E+02        | 4.3903E+01    | 8.677E-10 | 2.706E+02        |
| 1s 7f $^3F_3^0$ | 1s 7g $^3G_5$   | 5.4759E+03    | 3.951E-13 | 7.989E-06        | 5.5025E+03    | 3.830E-13 | 7.606E-06        |
| 1s 7f $^3F_4^0$ | 1s 7g $^3G_5$   | 1.4632E+04    | 1.821E-13 | 5.159E-07        | 1.4765E+04    | 1.751E-13 | 4.831E-07        |
| 1s 7f $^1F_3^0$ | 1s 7g $^3G_5$   | 1.5450E+04    | 7.324E-15 | 1.861E-08        | 1.4784E+04    | 8.325E-15 | 2.290E-08        |
| 1s 3d $^3D_3$   | 1s 7h $^3H_5^0$ | 3.5591E+00    | 6.235E-12 | 2.985E+02        |               |           |                  |
| 1s 4d $^3D_3$   | 1s 7h $^3H_5^0$ | 7.6503E+00    | 3.513E-12 | 3.640E+01        |               |           |                  |
| 1s 5d $^3D_3$   | 1s 7h $^3H_5^0$ | 1.6403E+01    | 6.894E-14 | 1.554E-01        |               |           |                  |
| 1s 5g $^3G_4$   | 1s 7h $^3H_5^0$ | 1.6491E+01    | 7.809E-07 | 1.741E+06        | 1.6420E+01    | 7.881E-07 | 1.757E+06        |
| 1s 5g $^3G_3$   | 1s 7h $^3H_5^0$ | 1.6493E+01    | 3.746E-08 | 8.351E+04        | 1.6423E+01    | 3.751E-08 | 8.363E+04        |
| 1s 5g $^3G_5$   | 1s 7h $^3H_5^0$ | 1.6542E+01    | 3.738E-13 | 8.285E-01        |               |           |                  |
| 1s 5g $^1G_4$   | 1s 7h $^3H_5^0$ | 1.6543E+01    | 7.520E-13 | 1.666E+00        |               |           |                  |
| 1s 6d $^3D_3$   | 1s 7h $^3H_5^0$ | 4.3385E+01    | 6.788E-14 | 2.187E-02        |               |           |                  |
| 1s 6g $^3G_4$   | 1s 7h $^3H_5^0$ | 4.3742E+01    | 8.186E-07 | 2.594E+05        | 4.3559E+01    | 8.213E-07 | 2.602E+05        |
| 1s 6g $^3G_3$   | 1s 7h $^3H_5^0$ | 4.3751E+01    | 3.929E-08 | 1.245E+04        | 4.3559E+01    | 3.911E-08 | 1.239E+04        |
| 1s 6g $^3G_5$   | 1s 7h $^3H_5^0$ | 4.3950E+01    | 3.908E-13 | 1.227E-01        |               |           |                  |
| 1s 6g $^1G_4$   | 1s 7h $^3H_5^0$ | 4.3957E+01    | 8.040E-13 | 2.523E-01        |               |           |                  |
| 1s 7d $^3D_3$   | 1s 7h $^3H_5^0$ | 5.3474E+03    | 4.485E-21 | 9.510E-14        |               |           |                  |
| 1s 7g $^3G_4$   | 1s 7h $^3H_5^0$ | 1.4659E+04    | 5.334E-14 | 1.505E-07        | 1.4689E+04    | 5.242E-14 | 1.460E-07        |
| 1s 7g $^3G_3$   | 1s 7h $^3H_5^0$ | 1.5275E+04    | 2.262E-15 | 5.879E-09        | 1.4689E+04    | 2.496E-15 | 6.956E-09        |
| 1s 7g $^3G_5$   | 1s 7h $^3H_5^0$ | 1.1751E+07    | 4.945E-29 | 2.170E-28        |               |           |                  |
| 1s 3d $^3D_2$   | 1s 7h $^3H_4^0$ | 3.5224E+00    | 9.274E-16 | 5.539E-02        |               |           |                  |
| 1s 3d $^3D_3$   | 1s 7h $^3H_4^0$ | 3.5591E+00    | 4.087E-13 | 2.391E+01        |               |           |                  |
| 1s 3d $^1D_2$   | 1s 7h $^3H_4^0$ | 3.5605E+00    | 4.517E-12 | 2.641E+02        |               |           |                  |
| 1s 4d $^3D_2$   | 1s 7h $^3H_4^0$ | 7.5785E+00    | 4.314E-16 | 5.566E-03        |               |           |                  |
| 1s 4d $^3D_3$   | 1s 7h $^3H_4^0$ | 7.6502E+00    | 2.093E-13 | 2.650E+00        |               |           |                  |
| 1s 4d $^1D_2$   | 1s 7h $^3H_4^0$ | 7.6531E+00    | 2.617E-12 | 3.312E+01        |               |           |                  |
| 1s 5d $^3D_2$   | 1s 7h $^3H_4^0$ | 1.6234E+01    | 1.476E-17 | 4.152E-05        |               |           |                  |
| 1s 5d $^3D_3$   | 1s 7h $^3H_4^0$ | 1.6402E+01    | 2.182E-15 | 6.010E-03        |               |           |                  |
| 1s 5d $^1D_2$   | 1s 7h $^3H_4^0$ | 1.6409E+01    | 4.943E-14 | 1.361E-01        |               |           |                  |
| 1s 5g $^3G_4$   | 1s 7h $^3H_4^0$ | 1.6490E+01    | 5.583E-08 | 1.522E+05        | 1.6420E+01    | 5.629E-08 | 1.534E+05        |
| 1s 5g $^3G_3$   | 1s 7h $^3H_4^0$ | 1.6492E+01    | 6.137E-07 | 1.672E+06        | 1.6423E+01    | 6.190E-07 | 1.686E+06        |
| 1s 5g $^3G_5$   | 1s 7h $^3H_4^0$ | 1.6541E+01    | 8.746E-16 | 2.369E-03        |               |           |                  |
| 1s 5g $^1G_4$   | 1s 7h $^3H_4^0$ | 1.6543E+01    | 1.942E-13 | 5.259E-01        |               |           |                  |
| 1s 6d $^3D_2$   | 1s 7h $^3H_4^0$ | 4.2704E+01    | 9.336E-18 | 3.794E-06        |               |           |                  |
| 1s 6d $^3D_3$   | 1s 7h $^3H_4^0$ | 4.3381E+01    | 8.044E-15 | 3.168E-03        |               |           |                  |
| 1s 6d $^1D_2$   | 1s 7h $^3H_4^0$ | 4.3411E+01    | 5.285E-14 | 2.079E-02        |               |           |                  |
| 1s 6g $^3G_4$   | 1s 7h $^3H_4^0$ | 4.3739E+01    | 5.849E-08 | 2.266E+04        | 4.3559E+01    | 5.866E-08 | 2.272E+04        |
| 1s 6g $^3G_3$   | 1s 7h $^3H_4^0$ | 4.3747E+01    | 6.433E-07 | 2.491E+05        | 4.3559E+01    | 6.453E-07 | 2.499E+05        |
| 1s 6g $^3G_5$   | 1s 7h $^3H_4^0$ | 4.3947E+01    | 9.550E-18 | 3.665E-06        |               |           |                  |
| 1s 6g $^1G_4$   | 1s 7h $^3H_4^0$ | 4.3954E+01    | 2.072E-13 | 7.949E-02        |               |           |                  |
| 1s 7d $^3D_2$   | 1s 7h $^3H_4^0$ | 2.3873E+03    | 4.238E-24 | 5.512E-16        |               |           |                  |
| 1s 7d $^3D_3$   | 1s 7h $^3H_4^0$ | 5.2970E+03    | 2.811E-21 | 7.426E-14        |               |           |                  |
| 1s 7d $^1D_2$   | 1s 7h $^3H_4^0$ | 5.5903E+03    | 3.729E-21 | 8.844E-14        |               |           |                  |
| 1s 7g $^3G_4$   | 1s 7h $^3H_4^0$ | 1.4287E+04    | 4.118E-15 | 1.495E-08        | 1.4689E+04    | 3.744E-15 | 1.275E-08        |
| 1s 7g $^3G_3$   | 1s 7h $^3H_4^0$ | 1.4871E+04    | 4.016E-14 | 1.346E-07        | 1.4689E+04    | 4.119E-14 | 1.402E-07        |
| 1s 7g $^3G_5$   | 1s 7h $^3H_4^0$ | 5.3648E+05    | 2.939E-30 | 7.568E-27        |               |           |                  |
| 1s 2p $^3P_2^0$ | 1s 7g $^1G_4$   | 1.3938E+00    | 1.901E-14 | 7.251E+00        |               |           |                  |
| 1s 3p $^3P_2^0$ | 1s 7g $^1G_4$   | 3.5141E+00    | 2.638E-15 | 1.583E-01        |               |           |                  |
| 1s 4p $^3P_2^0$ | 1s 7g $^1G_4$   | 7.5624E+00    | 3.399E-14 | 4.405E-01        |               |           |                  |
| 1s 4f $^3F_3^0$ | 1s 7g $^1G_4$   | 7.6513E+00    | 1.704E-08 | 2.158E+05        | 7.6190E+00    | 1.671E-08 | 2.116E+05        |
| 1s 4f $^3F_2^0$ | 1s 7g $^1G_4$   | 7.6528E+00    | 2.186E-07 | 2.766E+06        | 7.6205E+00    | 2.189E-07 | 2.770E+06        |
| 1s 4f $^3F_4^0$ | 1s 7g $^1G_4$   | 7.6873E+00    | 1.770E-07 | 2.220E+06        | 7.6547E+00    | 1.797E-07 | 2.254E+06        |
| 1s 4f $^1F_3^0$ | 1s 7g $^1G_4$   | 7.6884E+00    | 1.945E-06 | 2.439E+07        | 7.6558E+00    | 1.977E-06 | 2.478E+07        |
| 1s 5p $^3P_2^0$ | 1s 7g $^1G_4$   | 1.6196E+01    | 4.008E-14 | 1.132E-01        |               |           |                  |
| 1s 5f $^3F_3^0$ | 1s 7g $^1G_4$   | 1.6405E+01    | 1.439E-08 | 3.963E+04        | 1.6336E+01    | 1.419E-08 | 3.908E+04        |
| 1s 5f $^3F_2^0$ | 1s 7g $^1G_4$   | 1.6409E+01    | 1.841E-07 | 5.068E+05        | 1.6340E+01    | 1.852E-07 | 5.100E+05        |
| 1s 5f $^3F_4^0$ | 1s 7g $^1G_4$   | 1.6490E+01    | 1.518E-07 | 4.138E+05        | 1.6420E+01    | 1.528E-07 | 4.166E+05        |
| 1s 5f $^1F_3^0$ | 1s 7g $^1G_4$   | 1.6493E+01    | 1.670E-06 | 4.549E+06        | 1.6423E+01    | 1.681E-06 | 4.581E+06        |
| 1s 6p $^3P_2^0$ | 1s 7g $^1G_4$   | 4.2553E+01    | 3.141E-14 | 1.286E-02        |               |           |                  |
| 1s 6f $^3F_3^0$ | 1s 7g $^1G_4$   | 4.3393E+01    | 9.707E-09 | 3.821E+03        | 4.3219E+01    | 1.009E-08 | 3.971E+03        |
| 1s 6f $^3F_2^0$ | 1s 7g $^1G_4$   | 4.3407E+01    | 1.241E-07 | 4.880E+04        | 4.3218E+01    | 1.246E-07 | 4.903E+04        |
| 1s 6f $^3F_4^0$ | 1s 7g $^1G_4$   | 4.3738E+01    | 1.042E-07 | 4.037E+04        | 4.3559E+01    | 1.044E-07 | 4.045E+04        |
| 1s 6f $^1F_3^0$ | 1s 7g $^1G_4$   | 4.3749E+01    | 1.147E-06 | 4.441E+05        | 4.3560E+01    | 1.148E-06 | 4.449E+05        |
| 1s 6h $^3H_5^0$ | 1s 7g $^1G_4$   | 4.3947E+01    | 4.178E-15 | 1.603E-03        |               |           |                  |
| 1s 6h $^3H_4^0$ | 1s 7g $^1G_4$   | 4.3952E+01    | 1.102E-15 | 4.227E-04        |               |           |                  |
| 1s 6h $^3H_6^0$ | 1s 7g $^1G_4$   | 4.4086E+01    | 5.767E-10 | 2.199E+02        | 4.3903E+01    | 5.785E-10 | 2.205E+02        |
| 1s 6h $^1H_5^0$ | 1s 7g $^1G_4$   | 4.4090E+01    | 1.511E-08 | 5.759E+03        | 4.3903E+01    | 1.504E-08 | 5.734E+03        |

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Table 6 (continued)

| Lower   | Upper   | GRASP2K       |           |                             | FAC           |           |                             |
|---|---|---------------|-----------|-----------------------------|---------------|-----------|-----------------------------|
|   |   | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) | $\lambda$ (Å) | <i>gf</i> | <i>A</i> (s <sup>-1</sup> ) |
| 1s7p <sup>3</sup> P <sub>2</sub> <sup>o</sup> | 1s7g <sup>1</sup> G <sub>4</sub>              | 2.1414E+03    | 1.517E-18 | 2.452E-10                   |               |           |                             |
| 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>3</sup> G <sub>4</sub>              | 5.4114E+03    | 2.420E-14 | 6.124E-07                   | 5.5025E+03    | 2.355E-14 | 5.716E-07                   |
| 1s7f <sup>3</sup> F <sub>2</sub> <sup>o</sup> | 1s7g <sup>1</sup> G <sub>4</sub>              | 5.5556E+03    | 2.854E-13 | 6.854E-06                   | 5.5006E+03    | 2.907E-13 | 7.060E-06                   |
| 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7g <sup>1</sup> G <sub>4</sub>              | 1.4181E+04    | 1.429E-14 | 5.268E-08                   | 1.4765E+04    | 1.251E-14 | 4.217E-08                   |
| 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7g <sup>1</sup> G <sub>4</sub>              | 1.4947E+04    | 1.343E-13 | 4.455E-07                   | 1.4784E+04    | 1.370E-13 | 4.608E-07                   |
| 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7g <sup>1</sup> G <sub>4</sub>              | 4.7824E+05    | 1.517E-24 | 4.917E-21                   |               |           |                             |
| 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7g <sup>1</sup> G <sub>4</sub>              | 3.2051E+06    | 1.293E-27 | 9.331E-26                   |               |           |                             |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1.6478E+01    | 2.768E-07 | 5.230E+05                   | 1.6408E+01    | 2.770E-07 | 5.234E+05                   |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1.6529E+01    | 3.232E-06 | 6.069E+06                   | 1.6459E+01    | 3.261E-06 | 6.125E+06                   |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1.6531E+01    | 1.019E-07 | 1.913E+05                   | 1.6460E+01    | 1.028E-07 | 1.931E+05                   |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 4.3656E+01    | 2.869E-07 | 7.725E+04                   | 4.3473E+01    | 2.870E-07 | 7.727E+04                   |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 4.3863E+01    | 3.400E-06 | 9.068E+05                   | 4.3678E+01    | 3.410E-06 | 9.095E+05                   |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 4.3870E+01    | 1.073E-07 | 2.860E+04                   | 4.3678E+01    | 1.082E-07 | 2.887E+04                   |
| 1s7g <sup>3</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 8.8116E+03    | 8.646E-14 | 5.714E-07                   | 8.8256E+03    | 8.470E-14 | 5.532E-07                   |
| 1s7g <sup>3</sup> G <sub>5</sub>              | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 2.2048E+04    | 6.532E-14 | 6.895E-08                   | 2.2104E+04    | 6.405E-14 | 6.670E-08                   |
| 1s7g <sup>1</sup> G <sub>4</sub>              | 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 2.3159E+04    | 1.778E-15 | 1.701E-09                   | 2.2104E+04    | 2.033E-15 | 2.117E-09                   |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>6</sub>              | 7.6847E+00    | 1.806E-12 | 1.569E+01                   |               |           |                             |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>6</sub>              | 1.6478E+01    | 1.456E-12 | 2.751E+00                   |               |           |                             |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>6</sub>              | 4.3655E+01    | 6.343E-14 | 1.708E-02                   |               |           |                             |
| 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>6</sub>              | 4.3863E+01    | 2.235E-06 | 5.960E+05                   | 4.3678E+01    | 2.243E-06 | 5.983E+05                   |
| 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>6</sub>              | 4.3869E+01    | 7.139E-08 | 1.903E+04                   | 4.3678E+01    | 7.123E-08 | 1.899E+04                   |
| 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>6</sub>              | 4.4002E+01    | 4.282E-13 | 1.135E-01                   |               |           |                             |
| 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>6</sub>              | 4.4006E+01    | 9.095E-13 | 2.410E-01                   |               |           |                             |
| 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>6</sub>              | 8.7950E+03    | 4.030E-22 | 2.673E-15                   |               |           |                             |
| 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>6</sub>              | 2.2088E+04    | 1.687E-14 | 1.774E-08                   | 2.2113E+04    | 1.661E-14 | 1.728E-08                   |
| 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>6</sub>              | 2.2991E+04    | 4.777E-16 | 4.637E-10                   | 2.2113E+04    | 5.275E-16 | 5.488E-10                   |
| 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>6</sub>              | 2.7778E+08    | 1.588E-33 | 1.036E-35                   |               |           |                             |
| 1s4f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 7.6487E+00    | 4.069E-17 | 4.218E-04                   |               |           |                             |
| 1s4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 7.6846E+00    | 6.867E-14 | 7.052E-01                   |               |           |                             |
| 1s4f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 7.6858E+00    | 1.434E-12 | 1.472E+01                   |               |           |                             |
| 1s5f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 1.6393E+01    | 2.438E-17 | 5.502E-05                   |               |           |                             |
| 1s5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 1.6478E+01    | 5.569E-14 | 1.244E-01                   |               |           |                             |
| 1s5f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 1.6481E+01    | 1.157E-12 | 2.584E+00                   |               |           |                             |
| 1s6f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 4.3310E+01    | 6.496E-19 | 2.100E-07                   |               |           |                             |
| 1s6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 4.3653E+01    | 2.487E-15 | 7.915E-04                   |               |           |                             |
| 1s6f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 4.3664E+01    | 5.058E-14 | 1.609E-02                   |               |           |                             |
| 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 4.3861E+01    | 1.065E-07 | 3.356E+04                   | 4.3678E+01    | 1.068E-07 | 3.367E+04                   |
| 1s6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 4.3866E+01    | 1.845E-06 | 5.814E+05                   | 4.3678E+01    | 1.851E-06 | 5.836E+05                   |
| 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 4.4000E+01    | 6.477E-17 | 2.029E-05                   |               |           |                             |
| 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 4.4004E+01    | 2.541E-13 | 7.958E-02                   |               |           |                             |
| 1s7f <sup>3</sup> F <sub>3</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 4.3626E+03    | 1.645E-27 | 5.241E-20                   |               |           |                             |
| 1s7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 8.6997E+03    | 1.609E-23 | 1.289E-16                   |               |           |                             |
| 1s7f <sup>1</sup> F <sub>3</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 8.9822E+03    | 3.033E-22 | 2.280E-15                   |               |           |                             |
| 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 2.1496E+04    | 8.714E-16 | 1.144E-09                   | 2.2113E+04    | 7.913E-16 | 9.729E-10                   |
| 1s7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 2.2351E+04    | 1.344E-14 | 1.631E-08                   | 2.2113E+04    | 1.371E-14 | 1.686E-08                   |
| 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>5</sub>              | 8.0038E+05    | 8.707E-31 | 8.242E-28                   |               |           |                             |
| 1s3d <sup>3</sup> D <sub>3</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 3.5586E+00    | 2.702E-16 | 1.294E-02                   |               |           |                             |
| 1s4d <sup>3</sup> D <sub>3</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 7.6476E+00    | 2.941E-16 | 3.049E-03                   |               |           |                             |
| 1s5d <sup>3</sup> D <sub>3</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.6390E+01    | 1.850E-16 | 4.176E-04                   |               |           |                             |
| 1s5g <sup>3</sup> G <sub>4</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.6478E+01    | 1.027E-08 | 2.293E+04                   | 1.6408E+01    | 9.994E-09 | 2.231E+04                   |
| 1s5g <sup>3</sup> G <sub>3</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.6480E+01    | 2.227E-07 | 4.972E+05                   | 1.6410E+01    | 2.231E-07 | 4.981E+05                   |
| 1s5g <sup>3</sup> G <sub>5</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.6529E+01    | 1.539E-07 | 3.417E+05                   | 1.6459E+01    | 1.553E-07 | 3.447E+05                   |
| 1s5g <sup>1</sup> G <sub>4</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1.6530E+01    | 2.668E-06 | 5.920E+06                   | 1.6460E+01    | 2.692E-06 | 5.973E+06                   |
| 1s6d <sup>3</sup> D <sub>3</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3297E+01    | 1.613E-16 | 5.219E-05                   |               |           |                             |
| 1s6g <sup>3</sup> G <sub>4</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3653E+01    | 1.064E-08 | 3.387E+03                   | 4.3473E+01    | 1.104E-08 | 3.512E+03                   |
| 1s6g <sup>3</sup> G <sub>3</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3661E+01    | 2.309E-07 | 7.345E+04                   | 4.3473E+01    | 2.318E-07 | 7.376E+04                   |
| 1s6g <sup>3</sup> G <sub>5</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3860E+01    | 1.619E-07 | 5.104E+04                   | 4.3678E+01    | 1.624E-07 | 5.118E+04                   |
| 1s6g <sup>1</sup> G <sub>4</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.3867E+01    | 2.807E-06 | 8.845E+05                   | 4.3678E+01    | 2.815E-06 | 8.872E+05                   |
| 1s7d <sup>3</sup> D <sub>3</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.2781E+03    | 7.935E-22 | 2.629E-14                   |               |           |                             |
| 1s7g <sup>3</sup> G <sub>4</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 8.6987E+03    | 3.334E-15 | 2.672E-08                   | 8.8256E+03    | 3.259E-15 | 2.515E-08                   |
| 1s7g <sup>3</sup> G <sub>3</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 8.9120E+03    | 6.726E-14 | 5.135E-07                   | 8.8255E+03    | 6.841E-14 | 5.281E-07                   |
| 1s7g <sup>3</sup> G <sub>5</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.1355E+04    | 3.424E-15 | 4.553E-09                   | 2.2104E+04    | 3.050E-15 | 3.753E-09                   |
| 1s7g <sup>1</sup> G <sub>4</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 2.2395E+04    | 5.146E-14 | 6.221E-08                   | 2.2104E+04    | 5.287E-14 | 6.506E-08                   |
| 1s7i <sup>3</sup> I <sub>6</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 6.8074E+05    | 2.383E-25 | 3.119E-22                   |               |           |                             |
| 1s7i <sup>3</sup> I <sub>5</sub>              | 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 4.4823E+06    | 2.314E-28 | 6.985E-27                   |               |           |                             |
| 1s6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>7</sub>              | 4.3801E+01    | 4.717E-07 | 1.093E+05                   | 4.3617E+01    | 4.715E-07 | 1.092E+05                   |
| 1s6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>7</sub>              | 4.3940E+01    | 7.252E-06 | 1.670E+06                   | 4.3754E+01    | 7.280E-06 | 1.676E+06                   |
| 1s6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>7</sub>              | 4.3944E+01    | 1.639E-07 | 3.775E+04                   | 4.3754E+01    | 1.654E-07 | 3.810E+04                   |
| 1s7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>7</sub>              | 1.2900E+04    | 1.788E-14 | 4.778E-08                   | 1.2909E+04    | 1.756E-14 | 4.647E-08                   |
| 1s7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>7</sub>              | 3.1010E+04    | 1.983E-14 | 9.171E-09                   | 3.1022E+04    | 1.957E-14 | 8.967E-09                   |
| 1s7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s7i <sup>3</sup> I <sub>7</sub>              | 3.2494E+04    | 3.897E-16 | 1.641E-10                   | 3.1022E+04    | 4.448E-16 | 2.038E-10                   |

(continued on next page)

Table 6 (continued)

| Lower  | Upper                             | GRASP2K       |           |                        | FAC           |           |                        |
|--|-----------------------------------|---------------|-----------|------------------------|---------------|-----------|------------------------|
|  |                                   | $\lambda$ (Å) | $gf$      | $A$ (s <sup>-1</sup> ) | $\lambda$ (Å) | $gf$      | $A$ (s <sup>-1</sup> ) |
| 1s 4f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7i <sup>1</sup> I <sub>6</sub> | 7.6827E+00    | 9.016E-17 | 7.837E-04              |               |           |                        |
| 1s 5f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7i <sup>1</sup> I <sub>6</sub> | 1.6469E+01    | 7.167E-17 | 1.356E-04              |               |           |                        |
| 1s 6f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7i <sup>1</sup> I <sub>6</sub> | 4.3592E+01    | 1.033E-18 | 2.790E-07              |               |           |                        |
| 1s 6h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7i <sup>1</sup> I <sub>6</sub> | 4.3799E+01    | 1.213E-08 | 3.246E+03              | 4.3617E+01    | 1.257E-08 | 3.362E+03              |
| 1s 6h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7i <sup>1</sup> I <sub>6</sub> | 4.3805E+01    | 3.950E-07 | 1.056E+05              | 4.3617E+01    | 3.961E-07 | 1.059E+05              |
| 1s 6h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 7i <sup>1</sup> I <sub>6</sub> | 4.3938E+01    | 2.473E-07 | 6.572E+04              | 4.3754E+01    | 2.481E-07 | 6.595E+04              |
| 1s 6h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s 7i <sup>1</sup> I <sub>6</sub> | 4.3942E+01    | 6.182E-06 | 1.643E+06              | 4.3754E+01    | 6.204E-06 | 1.648E+06              |
| 1s 7f <sup>3</sup> F <sub>4</sub> <sup>o</sup> | 1s 7i <sup>1</sup> I <sub>6</sub> | 6.8024E+03    | 6.449E-27 | 7.151E-20              |               |           |                        |
| 1s 7h <sup>3</sup> H <sub>5</sub> <sup>o</sup> | 1s 7i <sup>1</sup> I <sub>6</sub> | 1.2726E+04    | 4.791E-16 | 1.518E-09              | 1.2909E+04    | 4.684E-16 | 1.430E-09              |
| 1s 7h <sup>3</sup> H <sub>4</sub> <sup>o</sup> | 1s 7i <sup>1</sup> I <sub>6</sub> | 1.3020E+04    | 1.456E-14 | 4.408E-08              | 1.2909E+04    | 1.475E-14 | 4.504E-08              |
| 1s 7h <sup>3</sup> H <sub>6</sub> <sup>o</sup> | 1s 7i <sup>1</sup> I <sub>6</sub> | 3.0020E+04    | 7.453E-16 | 4.243E-10              | 3.1022E+04    | 6.673E-16 | 3.527E-10              |
| 1s 7h <sup>1</sup> H <sub>5</sub> <sup>o</sup> | 1s 7i <sup>1</sup> I <sub>6</sub> | 3.1409E+04    | 1.627E-14 | 8.462E-09              | 3.1022E+04    | 1.668E-14 | 8.818E-09              |

**Table 7**

Calculated values using the GRASP2K code of the magnetic dipole  $A$ , electric quadrupole  $B$  and Landé  $g$ -factors for all levels of interest. For this calculation, the active set expanded to  $n = 10$  (GRASP3) has been considered.

| Configuration   | $A$ (MHz)  | $B$ (MHz)  | $g_j$        |
|-----------------|------------|------------|--------------|
| 1s 2s $^3S_1$   | 1.329E+07  | 1.941E+00  | 1.935167E+00 |
| 1s 2p $^3P_1^0$ | 1.218E+07  | 4.527E+03  | 1.285193E+00 |
| 1s 2p $^3P_2^0$ | 5.965E+06  | -6.466E+04 | 1.458966E+00 |
| 1s 2p $^1P_1^0$ | -5.636E+06 | -3.488E+04 | 1.150634E+00 |
| 1s 3s $^3S_1$   | 1.218E+07  | 1.709E+00  | 1.942586E+00 |
| 1s 3p $^3P_1^0$ | 1.184E+07  | 1.265E+03  | 1.291576E+00 |
| 1s 3p $^3P_2^0$ | 5.890E+06  | -1.976E+04 | 1.467393E+00 |
| 1s 3d $^3D_2$   | 5.879E+06  | -3.874E+03 | 1.067061E+00 |
| 1s 3d $^3D_1$   | -5.824E+06 | -1.941E+03 | 5.145892E-01 |
| 1s 3p $^1P_1^0$ | -5.774E+06 | -1.065E+04 | 1.165553E+00 |
| 1s 3d $^3D_3$   | 3.915E+06  | -5.068E+03 | 1.308971E+00 |
| 1s 3d $^1D_2$   | -3.892E+06 | -4.040E+03 | 1.074253E+00 |
| 1s 4s $^3S_1$   | 1.191E+07  | 8.684E-01  | 1.945151E+00 |
| 1s 4p $^3P_1^0$ | 1.175E+07  | 5.208E+02  | 1.293822E+00 |
| 1s 4p $^3P_2^0$ | 5.871E+06  | -8.406E+03 | 1.470347E+00 |
| 1s 4d $^3D_2$   | 5.867E+06  | -1.672E+03 | 1.070326E+00 |
| 1s 4d $^3D_1$   | -5.843E+06 | -8.397E+02 | 5.195030E-01 |
| 1s 4p $^1P_1^0$ | -5.809E+06 | -4.532E+03 | 1.170777E+00 |
| 1s 4d $^3D_3$   | 3.909E+06  | -2.169E+03 | 1.312098E+00 |
| 1s 4f $^3F_3^0$ | 3.908E+06  | -7.731E+02 | 1.025485E+00 |
| 1s 4f $^3F_2^0$ | -3.901E+06 | -6.174E+02 | 6.782567E-01 |
| 1s 4d $^1D_2$   | -3.900E+06 | -1.729E+03 | 1.078311E+00 |
| 1s 4f $^3F_4^0$ | 2.930E+06  | -8.773E+02 | 1.232907E+00 |
| 1s 4f $^1F_3^0$ | -2.927E+06 | -7.820E+02 | 1.044150E+00 |
| 1s 5s $^3S_1$   | 1.181E+07  | 4.676E-01  | 1.946327E+00 |
| 1s 5p $^3P_1^0$ | 1.172E+07  | 2.630E+02  | 1.294862E+00 |
| 1s 5p $^3P_2^0$ | 5.865E+06  | -4.316E+03 | 1.471711E+00 |
| 1s 5d $^3D_2$   | 5.862E+06  | -8.637E+02 | 1.071827E+00 |
| 1s 5p $^1P_1^0$ | -5.822E+06 | -2.327E+03 | 1.173184E+00 |
| 1s 5d $^3D_1$   | -5.851E+06 | -4.344E+02 | 5.217790E-01 |
| 1s 5d $^3D_3$   | 3.907E+06  | -1.116E+03 | 1.313549E+00 |
| 1s 5f $^3F_3^0$ | 3.906E+06  | -3.993E+02 | 1.026955E+00 |
| 1s 5f $^3F_2^0$ | -3.903E+06 | -3.188E+02 | 6.802985E-01 |
| 1s 5d $^1D_2$   | -3.902E+06 | -8.908E+02 | 1.080205E+00 |
| 1s 5f $^3F_4^0$ | 2.930E+06  | -4.520E+02 | 1.234400E+00 |
| 1s 5g $^3G_4$   | 2.930E+06  | -2.098E+02 | 1.011596E+00 |
| 1s 5g $^3G_3$   | -2.928E+06 | -1.874E+02 | 7.594756E-01 |
| 1s 5f $^1F_3^0$ | -2.928E+06 | -4.029E+02 | 1.046058E+00 |
| 1s 5g $^3G_5$   | 2.344E+06  | -2.262E+02 | 1.186952E+00 |
| 1s 5g $^1G_4$   | -2.343E+06 | -2.112E+02 | 1.029827E+00 |
| 1s 6s $^3S_1$   | 1.177E+07  | 2.710E-01  | 1.946963E+00 |
| 1s 6p $^3P_1^0$ | 1.171E+07  | 1.507E+02  | 1.295417E+00 |
| 1s 6p $^3P_2^0$ | 5.862E+06  | -2.497E+03 | 1.472450E+00 |
| 1s 6d $^3D_2$   | 5.860E+06  | -5.019E+02 | 1.072640E+00 |
| 1s 6p $^1P_1^0$ | -5.828E+06 | -1.346E+03 | 1.174496E+00 |
| 1s 6d $^3D_1$   | -5.854E+06 | -2.527E+02 | 5.230139E-01 |
| 1s 6d $^3D_3$   | 3.907E+06  | -6.475E+02 | 1.314338E+00 |
| 1s 6f $^3F_3^0$ | 3.906E+06  | -2.320E+02 | 1.027753E+00 |
| 1s 6f $^3F_2^0$ | -3.904E+06 | -1.853E+02 | 6.814050E-01 |
| 1s 6d $^1D_2$   | -3.903E+06 | -5.171E+02 | 1.081237E+00 |
| 1s 6f $^3F_4^0$ | 2.929E+06  | -2.624E+02 | 1.235214E+00 |
| 1s 6g $^3G_4$   | 2.929E+06  | -1.220E+02 | 1.012411E+00 |
| 1s 6g $^3G_3$   | -2.929E+06 | -1.090E+02 | 7.605229E-01 |
| 1s 6f $^1F_3^0$ | -2.928E+06 | -2.339E+02 | 1.047097E+00 |
| 1s 6g $^3G_5$   | 2.344E+06  | -1.314E+02 | 1.187784E+00 |
| 1s 6h $^3H_5^0$ | 2.343E+06  | -7.193E+01 | 1.005467E+00 |
| 1s 6h $^3H_4^0$ | -2.343E+06 | -6.707E+01 | 8.080359E-01 |
| 1s 6g $^1G_4$   | -2.343E+06 | -1.227E+02 | 1.030843E+00 |
| 1s 6h $^3H_6^0$ | 1.953E+06  | -7.560E+01 | 1.156123E+00 |
| 1s 6h $^1H_5^0$ | -1.952E+06 | -7.210E+01 | 1.021980E+00 |
| 1s 7s $^3S_1$   | 1.175E+07  | 1.638E-01  | 1.947346E+00 |
| 1s 7p $^3P_1^0$ | 1.170E+07  | 9.511E+01  | 1.295852E+00 |
| 1s 7p $^3P_2^0$ | 5.860E+06  | -1.576E+03 | 1.472878E+00 |
| 1s 7d $^3D_2$   | 5.859E+06  | -3.166E+02 | 1.073129E+00 |
| 1s 7d $^3D_1$   | -5.855E+06 | -1.596E+02 | 5.237575E-01 |
| 1s 7p $^1P_1^0$ | -5.830E+06 | -8.507E+02 | 1.175151E+00 |
| 1s 7d $^3D_3$   | 3.906E+06  | -4.081E+02 | 1.314814E+00 |
| 1s 7f $^3F_3^0$ | 3.906E+06  | -1.466E+02 | 1.028235E+00 |
| 1s 7f $^3F_2^0$ | -3.904E+06 | -1.171E+02 | 6.820742E-01 |
| 1s 7d $^1D_2$   | -3.904E+06 | -3.263E+02 | 1.081860E+00 |

(continued on next page)

Table 7 (continued)

| Configuration   | A (MHz)    | B (MHz)    | $g_j$        |
|-----------------|------------|------------|--------------|
| 1s 7f $^3F_4^o$ | 2.929E+06  | -1.654E+02 | 1.235703E+00 |
| 1s 7g $^3G_4$   | 2.929E+06  | -7.700E+01 | 1.012903E+00 |
| 1s 7g $^3G_3$   | -2.929E+06 | -6.881E+01 | 7.611546E-01 |
| 1s 7f $^1F_3^o$ | -2.928E+06 | -1.475E+02 | 1.047721E+00 |
| 1s 7g $^3G_5$   | 2.343E+06  | -8.289E+01 | 1.188286E+00 |
| 1s 7h $^3H_5^o$ | 2.343E+06  | -4.542E+01 | 1.005969E+00 |
| 1s 7h $^3H_4^o$ | -2.343E+06 | -4.235E+01 | 8.086497E-01 |
| 1s 7g $^1G_4$   | -2.343E+06 | -7.742E+01 | 1.031456E+00 |
| 1s 7h $^3H_6^o$ | 1.953E+06  | -4.771E+01 | 1.156632E+00 |
| 1s 7i $^3I_6$   | 1.953E+06  | -2.870E+01 | 1.002418E+00 |
| 1s 7i $^3I_5$   | -1.953E+06 | -2.743E+01 | 8.402692E-01 |
| 1s 7h $^1H_5^o$ | -1.952E+06 | -4.550E+01 | 1.022582E+00 |
| 1s 7i $^3I_7$   | 1.674E+06  | -2.974E+01 | 1.134057E+00 |
| 1s 7i $^1I_6$   | -1.674E+06 | -2.879E+01 | 1.017106E+00 |

**Table 8**

Calculated values using the GRASP2K code of normal, specific mass shifts and electron densities at the nucleus for the all singly excited levels up to  $n = 7$  with increasing the active set to  $n = 10$  (GRASP3).

| Index | Configuration  | $K_{NMS}$    | $K_{SMS}$     | Electron densities at the nucleus |
|-------|----------------|--------------|---------------|-----------------------------------|
| 1     | $1s^2 1S_0$    | 2.862115E+03 | 8.372810E+00  | 2.355815E+05                      |
| 2     | $1s 2s 3S_1$   | 1.819580E+03 | 6.544528E-01  | 1.364262E+05                      |
| 3     | $1s 2p 3P_1^0$ | 1.817000E+03 | -8.021940E+01 | 1.201622E+05                      |
| 4     | $1s 2p 3P_0^0$ | 1.815498E+03 | -1.953285E+02 | 1.201173E+05                      |
| 5     | $1s 2s 1S_0$   | 1.815192E+03 | 1.618605E+00  | 1.360149E+05                      |
| 6     | $1s 2p 3P_2^0$ | 1.803659E+03 | -2.058238E+02 | 1.196642E+05                      |
| 7     | $1s 2p 1P_1^0$ | 1.802099E+03 | 8.321168E+01  | 1.198328E+05                      |
| 8     | $1s 3s 3S_1$   | 1.613866E+03 | 2.454228E-01  | 1.247247E+05                      |
| 9     | $1s 3p 3P_1^0$ | 1.613208E+03 | -1.706693E+01 | 1.199436E+05                      |
| 10    | $1s 3s 1S_0$   | 1.612703E+03 | 5.420968E-01  | 1.246202E+05                      |
| 11    | $1s 3p 3P_0^0$ | 1.612808E+03 | -4.218003E+01 | 1.199297E+05                      |
| 12    | $1s 3p 3P_2^0$ | 1.609187E+03 | -4.894801E+01 | 1.197682E+05                      |
| 13    | $1s 3d 3D_2$   | 1.608843E+03 | 3.867396E-02  | 1.197815E+05                      |
| 14    | $1s 3d 3D_1$   | 1.608690E+03 | 1.545303E-01  | 1.197794E+05                      |
| 15    | $1s 3p 1P_1^0$ | 1.608726E+03 | 1.988737E+01  | 1.198104E+05                      |
| 16    | $1s 3d 3D_3$   | 1.607560E+03 | 6.261143E-02  | 1.197794E+05                      |
| 17    | $1s 3d 1D_2$   | 1.607466E+03 | 2.896360E-03  | 1.197827E+05                      |
| 18    | $1s 4s 3S_1$   | 1.542191E+03 | 1.159027E-01  | 1.218552E+05                      |
| 19    | $1s 4p 3P_1^0$ | 1.541967E+03 | -6.423856E+00 | 1.198675E+05                      |
| 20    | $1s 4s 1S_0$   | 1.541823E+03 | 2.449015E-01  | 1.218158E+05                      |
| 21    | $1s 4p 3P_0^0$ | 1.541804E+03 | -1.595949E+01 | 1.198612E+05                      |
| 22    | $1s 4p 3P_2^0$ | 1.540267E+03 | -1.916717E+01 | 1.197893E+05                      |
| 23    | $1s 4d 3D_2$   | 1.540095E+03 | 2.748062E-02  | 1.197824E+05                      |
| 24    | $1s 4d 3D_1$   | 1.540053E+03 | 8.509648E-02  | 1.197813E+05                      |
| 25    | $1s 4p 1P_1^0$ | 1.540076E+03 | 7.809108E+00  | 1.198064E+05                      |
| 26    | $1s 4d 3D_3$   | 1.539548E+03 | 4.557849E-02  | 1.197813E+05                      |
| 27    | $1s 4f 3F_3^0$ | 1.539594E+03 | 1.470809E-02  | 1.198033E+05                      |
| 28    | $1s 4f 3F_2^0$ | 1.539566E+03 | 2.242135E-02  | 1.198053E+05                      |
| 29    | $1s 4d 1D_2$   | 1.539534E+03 | 8.086057E-03  | 1.197830E+05                      |
| 30    | $1s 4f 3F_4^0$ | 1.539324E+03 | 6.452494E-03  | 1.198035E+05                      |
| 31    | $1s 4f 1F_3^0$ | 1.539303E+03 | 1.282208E-02  | 1.198050E+05                      |
| 32    | $1s 5s 3S_1$   | 1.509220E+03 | 6.414105E-02  | 1.208374E+05                      |
| 33    | $1s 5p 3P_1^0$ | 1.509162E+03 | -3.114675E+00 | 1.198376E+05                      |
| 34    | $1s 5s 1S_0$   | 1.509195E+03 | 1.322070E-01  | 1.208210E+05                      |
| 35    | $1s 5p 3P_0^0$ | 1.509081E+03 | -7.758204E+00 | 1.198342E+05                      |
| 36    | $1s 5p 3P_2^0$ | 1.508292E+03 | -9.475364E+00 | 1.197965E+05                      |
| 37    | $1s 5d 3D_2$   | 1.508180E+03 | 1.819042E-02  | 1.197829E+05                      |
| 38    | $1s 5p 1P_1^0$ | 1.508197E+03 | 3.868506E+00  | 1.198052E+05                      |
| 39    | $1s 5d 3D_1$   | 1.508177E+03 | 4.981599E-02  | 1.197822E+05                      |
| 40    | $1s 5d 3D_3$   | 1.507896E+03 | 2.909923E-02  | 1.197823E+05                      |
| 41    | $1s 5f 3F_3^0$ | 1.507945E+03 | 9.888449E-03  | 1.198037E+05                      |
| 42    | $1s 5f 3F_2^0$ | 1.507930E+03 | 1.398999E-02  | 1.198047E+05                      |
| 43    | $1s 5d 1D_2$   | 1.507911E+03 | 7.316622E-03  | 1.197832E+05                      |
| 44    | $1s 5f 3F_4^0$ | 1.507807E+03 | 5.878058E-03  | 1.198038E+05                      |
| 45    | $1s 5g 3G_4$   | 1.507772E+03 | 6.925163E-03  | 1.197834E+05                      |
| 46    | $1s 5g 3G_3$   | 1.507765E+03 | 9.936995E-03  | 1.197835E+05                      |
| 47    | $1s 5f 1F_3^0$ | 1.507796E+03 | 8.879435E-03  | 1.198046E+05                      |
| 48    | $1s 5g 3G_5$   | 1.507690E+03 | 3.848136E-03  | 1.197834E+05                      |
| 49    | $1s 5g 1G_4$   | 1.507684E+03 | 6.841721E-03  | 1.197835E+05                      |
| 50    | $1s 6s 3S_1$   | 1.491393E+03 | 3.966973E-02  | 1.203896E+05                      |
| 51    | $1s 6p 3P_1^0$ | 1.491425E+03 | -1.747137E+00 | 1.198237E+05                      |
| 52    | $1s 6s 1S_0$   | 1.491595E+03 | 8.044927E-02  | 1.203841E+05                      |
| 53    | $1s 6p 3P_0^0$ | 1.491378E+03 | -4.358955E+00 | 1.198217E+05                      |
| 54    | $1s 6p 3P_2^0$ | 1.490923E+03 | -5.374441E+00 | 1.197997E+05                      |
| 55    | $1s 6d 3D_2$   | 1.490835E+03 | 1.260114E-02  | 1.197831E+05                      |
| 56    | $1s 6p 1P_1^0$ | 1.490867E+03 | 2.197926E+00  | 1.198047E+05                      |
| 57    | $1s 6d 3D_1$   | 1.490852E+03 | 3.168686E-02  | 1.197827E+05                      |
| 58    | $1s 6d 3D_3$   | 1.490668E+03 | 1.933123E-02  | 1.197827E+05                      |
| 59    | $1s 6f 3F_3^0$ | 1.490720E+03 | 6.648316E-03  | 1.198039E+05                      |
| 60    | $1s 6f 3F_2^0$ | 1.490711E+03 | 9.068110E-03  | 1.198045E+05                      |
| 61    | $1s 6d 1D_2$   | 1.490698E+03 | 6.001879E-03  | 1.197833E+05                      |
| 62    | $1s 6f 3F_4^0$ | 1.490640E+03 | 4.399590E-03  | 1.198040E+05                      |
| 63    | $1s 6g 3G_4$   | 1.490603E+03 | 4.841594E-03  | 1.197834E+05                      |
| 64    | $1s 6g 3G_3$   | 1.490603E+03 | 6.624087E-03  | 1.197835E+05                      |
| 65    | $1s 6f 1F_3^0$ | 1.490634E+03 | 6.033506E-03  | 1.198044E+05                      |
| 66    | $1s 6g 3G_5$   | 1.490556E+03 | 2.987498E-03  | 1.197834E+05                      |
| 67    | $1s 6h 3H_3^0$ | 1.490594E+03 | 2.961360E-03  | 1.198041E+05                      |
| 68    | $1s 6h 3H_4^0$ | 1.490591E+03 | 3.804622E-03  | 1.198043E+05                      |
| 69    | $1s 6g 1G_4$   | 1.490556E+03 | 4.747536E-03  | 1.197835E+05                      |
| 70    | $1s 6h 3H_6^0$ | 1.490562E+03 | 1.899926E-03  | 1.198041E+05                      |
| 71    | $1s 6h 1H_5^0$ | 1.490560E+03 | 2.752518E-03  | 1.198043E+05                      |

(continued on next page)

Table 8 (continued)

| Index | Configuration   | $K_{NMS}$    | $K_{SMS}$     | Electron densities at the nucleus |
|-------|-----------------|--------------|---------------|-----------------------------------|
| 72    | 1s 7s $^3S_1$   | 1.480650E+03 | 2.694334E-02  | 1.201626E+05                      |
| 73    | 1s 7p $^3P_0^o$ | 1.481084E+03 | -1.087763E+00 | 1.198166E+05                      |
| 74    | 1s 7s $^1S_0$   | 1.481167E+03 | 5.410009E-02  | 1.201644E+05                      |
| 75    | 1s 7p $^3P_0^o$ | 1.481058E+03 | -2.715643E+00 | 1.198153E+05                      |
| 76    | 1s 7p $^3P_2^o$ | 1.480758E+03 | -3.364477E+00 | 1.198013E+05                      |
| 77    | 1s 7d $^3D_2$   | 1.480376E+03 | 9.571873E-03  | 1.197832E+05                      |
| 78    | 1s 7d $^3D_1$   | 1.480415E+03 | 2.200799E-02  | 1.197830E+05                      |
| 79    | 1s 7p $^1P_1^o$ | 1.480741E+03 | 1.381522E+00  | 1.198045E+05                      |
| 80    | 1s 7d $^3D_3$   | 1.480267E+03 | 1.390302E-02  | 1.197830E+05                      |
| 81    | 1s 7f $^3F_3^o$ | 1.480333E+03 | 4.632020E-03  | 1.198040E+05                      |
| 82    | 1s 7f $^3F_2^o$ | 1.480328E+03 | 6.156500E-03  | 1.198044E+05                      |
| 83    | 1s 7d $^1D_2$   | 1.480318E+03 | 5.311102E-03  | 1.197834E+05                      |
| 84    | 1s 7f $^3F_4^o$ | 1.480278E+03 | 3.356779E-03  | 1.198040E+05                      |
| 85    | 1s 7g $^3G_4$   | 1.480235E+03 | 3.714721E-03  | 1.197834E+05                      |
| 86    | 1s 7g $^3G_3$   | 1.480243E+03 | 4.889674E-03  | 1.197835E+05                      |
| 87    | 1s 7f $^1F_3^o$ | 1.480274E+03 | 4.340171E-03  | 1.198043E+05                      |
| 88    | 1s 7g $^3G_5$   | 1.480206E+03 | 2.491921E-03  | 1.197834E+05                      |
| 89    | 1s 7h $^3H_5^o$ | 1.480247E+03 | 2.300436E-03  | 1.198041E+05                      |
| 90    | 1s 7h $^3H_4^o$ | 1.480245E+03 | 2.822402E-03  | 1.198042E+05                      |
| 91    | 1s 7g $^1G_4$   | 1.480212E+03 | 3.650499E-03  | 1.197835E+05                      |
| 92    | 1s 7h $^3H_6^o$ | 1.480226E+03 | 1.590809E-03  | 1.198041E+05                      |
| 93    | 1s 7i $^3I_6$   | 1.480190E+03 | 1.649752E-03  | 1.197834E+05                      |
| 94    | 1s 7i $^3I_5$   | 1.480190E+03 | 2.164438E-03  | 1.197835E+05                      |
| 95    | 1s 7h $^1H_5^o$ | 1.480225E+03 | 2.112037E-03  | 1.198042E+05                      |
| 96    | 1s 7i $^3I_7$   | 1.480176E+03 | 1.080355E-03  | 1.197834E+05                      |
| 97    | 1s 7i $^1I_6$   | 1.480176E+03 | 1.594008E-03  | 1.197835E+05                      |