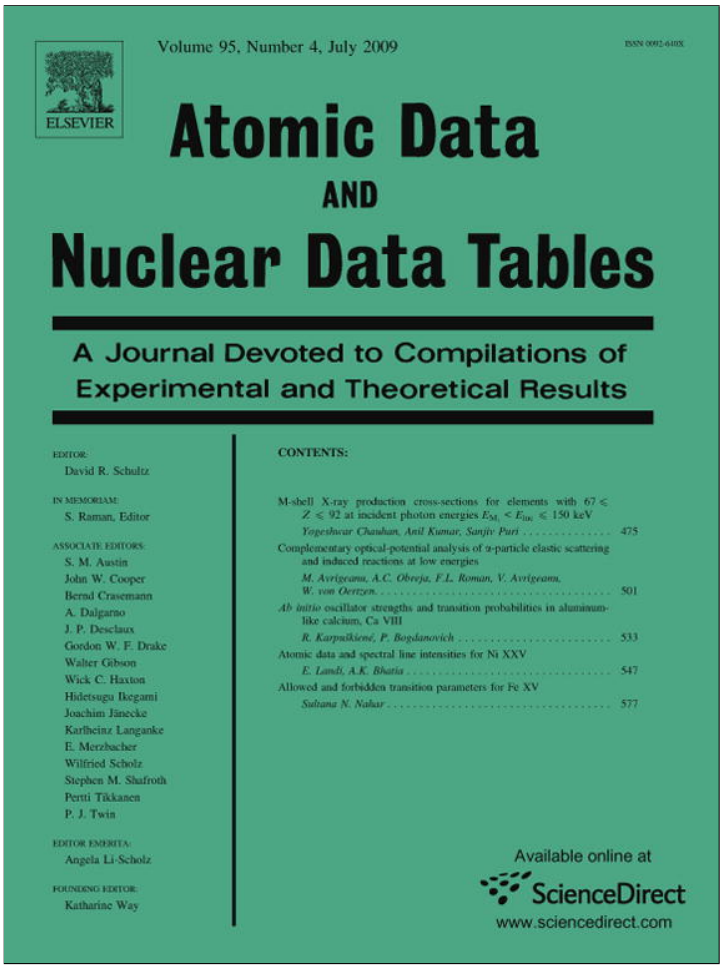

Atomic Data and Nuclear Data Tables 95 (2009) 577–605

Contents lists available at ScienceDirect

Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adt

Allowed and forbidden transition parameters for Fe XV

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ARTICLE INFO

Article history:
Available online 21 April 2009

ABSTRACT

A comprehensive set of fine structure energy levels, oscillator strengths (f), line strengths (S), and radiative decay rates (A) for bound–bound transitions in Fe XV is presented. The allowed electric dipole (E1) transitions were obtained from the relativistic Breit–Pauli R-matrix method which is based on the close coupling approximation. A total of 507 fine structure energy levels with $n \leqslant 10$, $l \leqslant 9$, and $0 \leqslant J \leqslant 10$ are found. They agree within 1% with the available observed energies. These energy levels yield a total of 27,812 E1, same-spin multiplets and intercombination transitions. The A values are in good agreement with those compiled by NIST and other existing values for most transitions. Forbidden transitions are obtained from a set of 20 configurations with orbitals ranging from 1s to 5f using the relativistic code SUPERSTRUCTURE (SS) in the Breit–Pauli approximation. From a set of 123 fine structure levels, a total of 6962 S and A values are presented for forbidden electric quadrupole (E2), electric octupole (E3), magnetic dipole (M1), and magnetic quadrupole (M2) transitions. The energies from SS calculations agree with observed energies to within 1–3%. A values for E2, M1 transitions agree very well with the available values for most transitions while those for M2 transitions show variable agreement. The large set of transition parameters presented should be applicable for both diagnostics and spectral modeling in the X-ray, ultraviolet, and optical regions of astrophysical plasmas.

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doi:10.1016/j.adt.2009.03.002

Contents

1. Introduction

Lines of the magnesium-like iron ion, Fe XV, with ground configuration $1s^22s^22p^63s^2$, are commonly seen in astrophysical spectra. For example, emission lines in an extreme ultraviolet wavelength range of about 200–400 Å arising from $n = 3$–3 transitions in Fe XV are widely detected in solar spectra (e.g., Ref. [1]). Soft X-ray emission lines of 50–80 Å due to $n = 3$–4 transitions in Fe XV are seen in solar flares and the corona of Capella [2], and X-ray lines of 15–17 Å due to M-shell transitions (mainly 2p–3d) are seen in various objects, such as IRAS 13349-2438 [3].

Accurate atomic transition parameters are needed to extract conditions such as temperature, density, plasma outflow velocities, etc., of the astronomical objects. Earlier calculations of transition rates for Fe XV were carried out by Shorer et al. [4], Cowan and Widing [5], Cheng and Johnson [6], Anderson and Anderson [7], and Kastner et al. [8], which are included in an evaluated compilation carried out by Shirai et al. [9]. Calculations by Anderson and Anderson included both allowed and forbidden transitions. Transitions have been reported more recently by Deb et al. [10], Aggarwal et al. [11], Deb and Msezane [12], and Berrington et al. [13]. Results from all of these works correspond to various approximations based on atomic structure calculations. The present work reports the first large-scale *ab initio* results for Fe XV from the relativistic Breit–Pauli R-matrix (BPRM) method aimed at improving astrophysical modeling.

2. Theory

The BPRM method is based on close coupling approximation where the atomic system is described as an N-electron target (core) interacting with a $(N + 1)$th electron. The wavefunction expansion, Ψ_E, of the $(N + 1)$ electron system with total orbital angular momentum L, spin multiplicity $(2S + 1)$, and total angular momentum symmetry $J\pi$, is written as

$$\Psi_E(\mathrm{e} + \mathrm{ion}) = A\sum_i \chi_i(\mathrm{ion})\theta_i + \sum_j c_j\Phi_j(\mathrm{e} + \mathrm{ion}), \tag{1}$$

where χ_i is the target ion wavefunction in a specific state $S_iL_i\pi_i$ or level $J_i\pi_i$, and θ_i is the wavefunction of the interacting $(N + 1)$th electron in a channel labeled as $S_iL_i(J_i)\pi_i\ k_i^2\ell_i(SL\pi$ or $J\pi)$ where k_i^2 is the incident kinetic energy. Φ_js are correlation wavefunctions of the $(N + 1)$ electron system that (a) compensate for the orthogonality conditions between the continuum and the bound orbitals and (b) represent additional short-range correlation.

The relativistic Hamiltonian for the $(N + 1)$ electron system in the Breit–Pauli approximation is given by (e.g., Ref. [15])

$$H_{N+1}^{\mathrm{BP}} = H_{N+1} + H_{N+1}^{\mathrm{mass}} + H_{N+1}^{\mathrm{Dar}} + H_{N+1}^{so} + \frac{1}{2}\sum_{i\neq j}^{N}[g_{ij}(so + so') + g_{ij}(ss') + g_{ij}(css') + g_{ij}(d) + g_{ij}(oo')], \tag{2}$$

where H_{N+1} is the nonrelativistic Hamiltonian,

$$H_{N+1} = \sum_{i=1}^{N+1}\left\{-\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N+1}\frac{2}{r_{ij}}\right\}. \tag{3}$$

H_{N+1}^{mass} is the mass correction, H_{N+1}^{Dar} is the Darwin, and H_{N+1}^{so} is the spin–orbit interaction term, respectively. The two-body interaction terms are with notation c for contraction, d for Darwin, o for orbit, s for spin, and a prime indicates 'other.' All terms improve the energies except the spin–orbit interaction term which splits the energies into fine structure components. The BPRM Hamiltonian used in the Iron Project [16] includes the first three one-body corrections. However, the atomic structure calculations for the forbidden transitions include the contribution of the full Breit interaction term consisting of the fine structure terms, that is spin-other-orbit (os') and spin-other-spin (ss') terms, and ignores the last three two-body interaction terms.

In the BPRM method, the set of $SL\pi$ are recoupled to obtain $(\mathrm{e} + \mathrm{ion})$ states with total $J\pi$, following the diagonalization of the $(N + 1)$-electron Hamiltonian,

$$H_{N+1}^{BP}\Psi = E\Psi. \tag{4}$$

Substitution of the wavefunction expansion results in a set of coupled equations that are solved using the R-matrix approach. At negative total energies ($E < 0$), the solutions of the close coupling equations occur at discrete eigenvalues of the $(\mathrm{e} + \mathrm{ion})$ Hamiltonian that correspond to pure bound states Ψ_B.

The oscillator strength (f) for an electric dipole (E1) transition is proportional to the generalized line strength as

$$S = \left|\left\langle \Psi_f \left| \sum_{j=1}^{N+1} r_j \right| \Psi_i \right\rangle\right|^2 \tag{5}$$

where Ψ_i and Ψ_f are the initial and final bound wavefunctions, respectively. The line strengths are energy independent quantities. This gives the oscillator strength, f_{ij}, and radiative decay rate or Einstein's A-coefficient (in atomic units, a.u.) as

$$f_{ij} = \frac{E_{ji}}{3g_i} S, \quad A_{ji}(\text{a.u.}) = \frac{1}{2}\alpha^3 \frac{g_i}{g_j} E_{ji}^2 f_{ij}. \tag{6}$$

E_{ji} is the energy difference between the initial and final states, α is the fine structure constant, and g_i, g_j are the statistical weight factors of the initial and final states, respectively.

The radiative decay rates for forbidden transitions are obtained from configuration interaction atomic structure calculations using the latest version of the program SUPERSTRUCTURE (SS) [17–19]. The transition rates for photo-excitations or de-excitations via various types of forbidden transitions can be obtained from the general line strength,

$$S^{X\lambda}(ij) = \left|\left\langle \Psi_j \middle| O^{X\lambda} \middle| \Psi_i \right\rangle\right|^2, \quad S(ji) = S(ij). \tag{7}$$

where X represents the electric (E) or magnetic (M) type and λ represents various multipoles, such as dipole (1), quadrupole (2), and octupole (3) [19]. The radiative decay rates for various higher orders of radiation are obtained from line strength $S^{X\lambda}(ij)$ as follows.

Electric quadrupole (E2) and magnetic dipole (M1)

$$g_j A_{ji}^{E2} = 2.6733 \times 10^3 \text{ s}^{-1} (E_j - E_i)^5 S^{E2}(i,j), \tag{8}$$

$$g_j A_{ji}^{M1} = 3.5644 \times 10^4 \text{ s}^{-1} (E_j - E_i)^3 S^{M1}(i,j), \tag{9}$$

and for electric octopole (E3) and magnetic quadrupole (M2)

$$g_j A_{ji}^{E3} = 1.2050 \times 10^{-3} \text{ s}^{-1} (E_j - E_i)^7 S^{E3}(i,j), \tag{10}$$

$$g_j A_{ji}^{M2} = 2.3727 \times 10^{-2} \text{ s}^{-1} (E_j - E_i)^5 S^{M2}(i,j). \tag{11}$$

The lifetime of a level can be obtained from the A values as,

$$\tau_k(s) = \frac{1}{\sum_i A_{ki}\ (s^{-1})}, \tag{12}$$

where the sum is the total radiative transition probability for the level k, and $A_{ji}\ (s^{-1}) = A_{ji}\ (\text{a.u.})/\tau_0$, $\tau_0 = 2.4191 \times 10^{-17}$ s is the atomic unit of time.

3. Calculations

3.1. BPRM calculations for E1 transitions

The BPRM calculation is initiated with the target (core) wavefunction which is obtained from an atomic structure calculation. Target Fe XVI wavefunctions were obtained from optimization of the 16 configurations, $2p^63s(1)$, $2p^63p(2)$, $2p^63d(3)$, $2p^64s(4)$, $2p^64p(5)$, $2p^64d(6)$, $2p^64f(7)$, $2p^53s^2(8)$, $2p^53s3p(9)$, $2p^53s3d(10)$, $2p^53s4s(11)$, $2p^53s4p(12)$, $2p^53s4d(13)$, $2p^53s4f(14)$, $2p^53p^2(15)$, and $2p^53p3d(16)$ using the code SUPERSTRUCTURE [17]. All configurations are treated as spectroscopic. The values of Thomas–Fermi–Amaldi scaling parameters, λ_{nl}, for individual orbitals are 1.38(1s), 1.15(2s), 1.08(2p), 1.05(3s), 1.01(3p), 1.0(3d), 1.0(4s), 1.0(4p), 1.0(4d), and 1.0(4f). The close coupling wavefunction expansion for Fe XV is formed from the first 12 levels of Fe XVI as given in Table A. The second bound-channel term of the wavefunction of Fe XV, Eq. (1), includes all possible $(N+1)$ configurations with filled 1s and 2s orbitals, and minimum and maximum occupancies, given within parentheses, in orbitals 2p(5–6), 3s(0–2), 3p(0–3), 3d(0–2), 4s(0–2), 4p(0–2), 4d(0–1), and 4f(0–1).

Computations were carried out using the BPRM package of codes [20,21]. The general steps have been described in earlier papers [19]. Calculations included bound levels of Fe XV with $0 \leqslant J \leqslant 10$ of even and odd parities, $n \leqslant 10$, $l \leqslant 9$, $0 \leqslant L \leqslant 12$, and $(2S+1) = 1,3$. The fine structure bound levels are obtained by scanning through the poles in the (e + ion) Hamiltonian with a fine mesh of effective quantum number ν, at $\Delta\nu = 0.001$ or smaller in code STGB.

Table A
Levels and energies (E_t) of the target Fe XVI in the wavefunction expansion of Fe XV. The present (SS) energies are compared with the observed energies in the NIST compilation [14].

Level		J_t	E_t (Ry) NIST	E_t (Ry) SS
1	$2p^63s(^2S)$	1/2	0.0	0.
2	$2p^63p(^2P^o)$	1/2	2.52596	2.5371040
3	$2p^63p(^2P^o)$	3/2	2.71688	2.7176403
4	$2p^63d(^2D)$	3/2	6.15544	6.1711038
5	$2p^63d(^2D)$	5/2	6.1819	6.2092417
6	$2p^64s(^2S)$	1/2	17.0182	17.0188128
7	$2p^64p(^2P^o)$	1/2	18.0252	18.0162598
8	$2p^64p(^2P^o)$	3/2	18.098	18.0840405
9	$2p^64d(^2D)$	3/2	19.3570	19.3520443
10	$2p^64d(^2D)$	5/2	19.3677	19.3690583
11	$2p^64f(^2F^o)$	5/2	19.9077	19.8951572
12	$2p^64f(^2F^o)$	7/2	19.9125	19.9015720

The energies were then identified through a theoretical spectroscopy procedure as described in Ref. [22]. The bound–bound transitions from the BPRM code have been processed for energies and transition wavelengths using code PBPRAD. For levels that have been measured, the oscillator strengths and A values, Eq. (6), were obtained from BPRM line strengths and the measured transition energies in order to improve the accuracy. This is a common practice of accuracy improvement, especially by the National Institute of Standards and Technology (NIST), since measured energies in general are more accurate than the calculated ones.

3.2. Atomic structure calculations for the forbidden transitions

Forbidden transitions of type E2, E3, M1, and M2 for Fe XV are obtained from an optimized set of 20 configurations with orbitals going up to 5g. All configurations are spectroscopic. The radiative decay rates were calculated from configuration interaction atomic structure calculations using the later version of SS that includes multipole transitions in the Breit–Pauli approximation [19]. The Thomas–Fermi–Amaldi λ_{nl} parameters for the orbitals are 1.38(1s), 1.25(2s), 1.15(2p), 1.15(3s), 1.(3p), 1.0(3d), 1.0(4s), 1.0(4p), 1.0(4d), 1.0(4f), 1.0(5s), 1.0(5p), 1.0(5d), 1.0(5f), and 1.0(5g). The transitions have been processed by replacing the calculated energies by the available observed energies using the code PRCSS.

4. Results and discussion

A comprehensive set of oscillator strengths, line strengths, and radiative decay rates for allowed and forbidden transitions in Fe XV are presented. They are discussed in separate sections below.

4.1. Energies and allowed E1 transitions in the BPRM approximation

The allowed E1 transitions of Fe XV correspond to a large number, 507 in total, of fine structure energy levels with $n \leqslant 10$, $0 \leqslant l \leqslant 9$, and $0 \leqslant J \leqslant 10$ of even and odd parities.

The BPRM method finds energy eigenvalues without any identification. These energies have been identified spectroscopically through a procedure [22] that analyzes the quantum defects of levels, matches possible components of the relevant LS terms, and con-

siders channel percentage contributions to the integrated wavefunctions in the outer region. Hund's rule is also used for levels arising from the same configuration such that the level with higher orbital angular momentum L and/or higher spin multiplicity will lie lower than those with lower L and lower spin. Spectroscopic identification is a major task compared to atomic structure calculations where the levels are identified automatically. Based on the identification criteria, a level may have one or more possible designations due to mixing of states and similar quantum defects. These could introduce some uncertainties in the identification. Hence levels have been specified with all possible identifications. The identified designation provides information on the configuration, *LS* term, and *J* value of the core and *nl* values of the outer or valence electron.

The complete set of 507 energy levels of Fe XV is available electronically. They are presented in two formats for various practical purposes: (i) in *LSJ* component format where fine structure levels are grouped as components of a *LS* term and (ii) in a $J\pi$ set where levels of the symmetry are listed in ascending order of energy positions. A partial set of energies in format (i), useful for spectroscopic diagnostics, is given in Table 1. It provides the check for completeness of the set of energy levels that belong to the *LS* term, and detects any missing level. Table B presents a partial set of energy levels in format (ii). The format is useful for modeling code applications.

The BPRM energies agree with those in the NIST table within 1% for all levels as shown in Table C. However, a large difference, 15%, is found for the NIST identified level, 3s6f(^{1}F^o). It appears that the level might have been misidentified by NIST. The BPRM energies show similar agreement with other calculated energies. Berrington et al. [13] compare their calculated energies, in the Breit–Pauli and Dirac–Fock approximations, with those in the compiled table by NIST [14] as well as other existing calculated energies, such as by Deb et al. [10], Aggarwal et al. [11], and Deb and Msezane [12]. They obtained very good agreement with NIST, as in the case of the present work, and with other calculations. However, coming from atomic structure calculations, their energies are relative to the zero ground state, that is, the ground state is not specified whereas present energies are absolute.

The complete set of fine structure E1 transitions among the 507 levels consists of 27,812 E1 transitions. A sample set of transitions is presented in Table D. The complete file containing *f*, *S*, and *A* values for E1 transitions is available electronically. In Table D, the top line specifies the nuclear charge ($Z = 26$) and number of electrons in the ion ($N_{elc} = 12$). This line is followed by sets of oscillator strengths belonging to various pairs of symmetries $J_i\pi_i$–$J_k\pi_k$. The transition symmetries are expressed in the form of the statistical weight factors, $g = 2J + 1$, and parity π (=0 for even and = 1 for odd parity). N_i, N_f are number of energies for the transitions symmetries and *NN* is the number of transitions. Identification of the transition level indices I_i and I_k can be found from the energy Table 2. The third column in Table D is the approximate transition wavelength (λ) in Å obtained using E (Å) = 911.2671/(E_{ik} (Ry). The fourth and fifth columns provide the energies E_i and E_k in Rydbergs of the transition levels. The sixth column is *f*, the oscillator strength in the length formulation. The sign of *f* indicates the upper and lower levels in transitions such that a negative value means that *i* is the lower level, while a positive value means *k* is the lower level. Column seven is the line strength *S*, and the last column is the transition probability or the radiative decay rate A_{ki} (s^{-1}). Calculated energies have been replaced by the observed energies wherever available for improved accuracy. Since the agreement of the calculated energies are within 1–3% with the observed values, accuracy improvement could be attained to about 10% depending on the values of the energy levels.

A set of transitions employing only the observed set of levels has been processed with complete spectroscopic notation and grouped as fine structure components of *LS* multiplets for direct comparison with experiment and other, such as, for diagnostic applications. The transitions are given in Table 2.

The present BPRM *A* values for Fe XV are compared with the existing values, all obtained from atomic structure calculations, in Table

Table B
Partial set of fine structure energy levels of Fe XV in $J\pi$ order. i_e is the energy index and I_J is the energy index of the level in its symmetry. There are 507 levels, $n \leqslant 10$, $l \leqslant 9$.

i_e	$J\pi$	I_J	E(Ry)	Config	$^{2S+1}L^{\pi}$	jjpiiii
1	0.0 e	1	−3.35800E+01	$2p^63s^2$	$^1S^e$	00001
2	0.0 e	2	−2.85268E+01	$3p^2$	$^3P^e$	00002
3	0.0 e	3	−2.75690E+01	$3p^2$	$^1S^e$	00003
4	0.0 e	4	−2.06333E+01	$2p^63d^2$	$^3P^e$	00004
5	0.0 e	5	−2.00290E+01	$3d^2$	$^1S^e$	00005
6	0.0 e	6	−1.72957E+01	3s4s	$^1S^e$	00006
7	0.0 e	7	−1.36853E+01	$2p^63p^2P^o4p$	$^3P^e$	00007
8	0.0 e	8	−1.31260E+01	$2p^63p^2P^o4p$	$^1S^e$	00008
9	0.0 e	9	−1.05409E+01	$2p^63s^2S^e5s$	$^1S^e$	00009
10	0.0 e	10	−8.45982E+00	$2p^63d^2D^e4d$	$^3P^e$	00010
11	0.0 e	11	−8.16289E+00	$2p^63d^2D^e4d$	$^1S^e$	00011
12	0.0 e	12	−7.50710E+00	$2p^63p^2P^o5p$	$^3P^e$	00012
13	0.0 e	13	−7.24559E+00	$2p^63p^2P^o5p$	$^1S^e$	00013
14	0.0 e	14	−6.99588E+00	$2p^63s^2S^e6s$	$^1S^e$	00014
15	0.0 e	15	−5.13427E+00	$2p^63s^2S^e7s$	$^1S^e$	00015
16	0.0 e	16	−4.31644E+00	$2p^63p^2P^o6p$	$^3P^e$	00016
17	0.0 e	17	−4.07372E+00	$2p^63p^2P^o6p$	$^1S^e$	00017
18	0.0 e	18	−3.86332E+00	$2p^63s^2S^e8s$	$^1S^e$	00018
19	0.0 e	19	−3.14757E+00	$2p^63p^2P^o7p$	$^3P^e$	00019
20	0.0 e	20	−3.03995E+00	$2p^63s^2S^e9s$	$^1S^e$	00020
21	0.0 e	21	−2.97675E+00	$2p^63p^2P^o7p$	$^1S^e$	00021
22	0.0 e	22	−2.44678E+00	$2p^63p^2P^o8p$	$^3P^e$	00022
23	0.0 e	23	−2.41103E+00	$2p^63s^2S^e10s$	$^1S^e$	00023
24	0.0 o	1	−3.14491E+01	3s3p	$^3P^o$	10001
25	0.0 o	2	−2.45048E+01	3p3d	$^3P^o$	10002

Table C
Comparison of calculated BPRM energies, E, for Fe XV with observed values (NIST). I_J is the calculated level index for its position in its $J\pi$ symmetry.

Level		J:I_J	E (Ry, NIST)	E (Ry, BPRM)
$2p^63s^2$	^{1}S	0.0:1	3.3580E+01	3.3505E+01
3s3p	$^3P^o$	2.0:1	3.1267E+01	3.1195E+01
3s3p	$^3P^o$	1.0:1	3.1396E+01	3.1320E+01
3s3p	$^3P^o$	0.0:1	3.1449E+01	3.1321E+01
3s3p	$^1P^o$	1.0:2	3.0373E+01	3.0282E+01
$3p^2$	^{3}P	2.0:1	2.8278E+01	2.8199E+01
$3p^2$	^{3}P	1.0:1	2.8435E+01	2.8350E+01
$3p^2$	^{3}P	0.0:2	2.8527E+01	2.8438E+01
$3p^2$	^{1}D	2.0:2	2.8481E+01	2.8398E+01
$3p^2$	^{1}S	0.0:3	2.7569E+01	2.7471E+01
3s3d	^{3}D	3.0:1	2.7371E+01	2.7267E+01
3s3d	^{3}D	2.0:3	2.7385E+01	2.7282E+01
3s3d	^{3}D	1.0:2	2.7395E+01	2.7292E+01
3s3d	^{1}D	2.0:4	2.6635E+01	2.6518E+01
3p3d	$^3F^o$	4.0:1	2.4926E+01	2.4825E+01
3p3d	$^3F^o$	3.0:1	2.5031E+01	2.4928E+01
3p3d	$^3F^o$	2.0:2	2.5121E+01	2.5018E+01
3p3d	$^1D^o$	2.0:3	2.4937E+01	2.4835E+01
3p3d	$^3D^o$	3.0:2	2.4514E+01	2.4405E+01
3p3d	$^3D^o$	2.0:4	2.4498E+01	2.4504E+01
3p3d	$^3D^o$	1.0:3	2.4623E+01	2.4511E+01
3p3d	$^3P^o$	2.0:5	2.4618E+01	2.4393E+01
3p3d	$^3P^o$	1.0:4	2.4502E+01	2.4394E+01
3p3d	$^3P^o$	0.0:2	2.4505E+01	2.4394E+01
3p3d	$^1F^o$	3.0:3	2.3898E+01	2.3779E+01
3p3d	$^1P^o$	1.0:5	2.3785E+01	2.3656E+01
$3d^2$	^{3}F	4.0:1	2.1059E+01	2.0928E+01
$3d^2$	^{3}F	3.0:2	2.1077E+01	2.0948E+01
$3d^2$	^{3}F	2.0:5	2.1093E+01	2.0964E+01
$3d^2$	^{1}D	2.0:6	2.0799E+01	2.0662E+01
$3d^2$	^{1}G	4.0:2	2.0758E+01	2.0625E+01
$3d^2$	^{3}P	2.0:7	2.0751E+01	2.0612E+01
$3d^2$	^{1}S	0.0:5	2.0029E+01	1.9861E+01
3s4s	^{3}S	1.0:4	1.7508E+01	1.7435E+01

Table D
Sample set of *f*-, *S* and *A*-values for allowed E1 transitions in Fe XV. See text for explanation.

	26			12								
I_i	I_k		λ(Å)	E_i(Ry)	E_k(Ry)		f			S		$A_{ki}(s^{-1})$
1	0	3	1	23	49	1127 = gi	Pi	gf	Pf	Ni	Nf	NN
1	1		417.27	−3.3580E+01	−3.1396E+01			−3.256E-03		4.473E-03		4.158E+07
1	2		284.17	−3.3580E+01	−3.0373E+01			−7.903E-01		7.393E-01		2.176E+10
1	3		101.74	−3.3580E+01	−2.4623E+01			−9.195E-07		3.080E-07		1.974E+05
1	4		100.38	−3.3580E+01	−2.4502E+01			−6.251E-08		2.066E-08		1.379E+04
1	5		93.03	−3.3580E+01	−2.3785E+01			−1.264E-03		3.871E-04		3.248E+08
1	6		52.90	−3.3580E+01	−1.6353E+01			−1.248E-01		2.174E-02		9.919E+10
1	7		52.91	−3.3580E+01	−1.6357E+01			−2.873E-01		5.004E-02		2.282E+11
1	8		48.43	−3.3580E+01	−1.4763E+01			−7.865E-04		1.254E-04		7.457E+08
1	9		47.75	−3.3580E+01	−1.4496E+01			−3.801E-03		5.975E-04		3.707E+09
1	10		43.06	−3.3580E+01	−1.2419E+01			−4.459E-04		6.321E-05		5.346E+08
1	11		42.50	−3.3580E+01	−1.2139E+01			−1.677E-03		2.346E-04		2.064E+09
1	12		42.37	−3.3580E+01	−1.2073E+01			−3.779E-03		5.272E-04		4.680E+09
1	13		38.82	−3.3580E+01	−1.0106E+01			−5.069E-02		6.479E-03		7.479E+10
1	14		38.80	−3.3580E+01	−1.0094E+01			−2.280E-03		2.913E-04		3.367E+09
1	15		38.96	−3.3580E+01	−1.0188E+01			−6.111E-02		7.838E-03		8.953E+10
1	16		38.54	−3.3580E+01	−9.9354E+00			−1.032E-03		1.310E-04		1.545E+09
1	17		38.25	−3.3580E+01	−9.7579E+00			−1.025E-02		1.291E-03		1.558E+10
1	18		35.54	−3.3580E+01	−7.9369E+00			−5.585E-06		6.534E-07		9.833E+06
1	19		35.51	−3.3580E+01	−7.9171E+00			−2.266E-07		2.649E-08		3.996E+05
1	20		35.46	−3.3580E+01	−7.8849E+00			−2.749E-04		3.210E-05		4.858E+08
1	21		35.45	−3.3580E+01	−7.8719E+00			−1.413E-07		1.649E-08		2.501E+05
1	22		35.17	−3.3580E+01	−7.6701E+00			−1.757E-04		2.034E-05		3.158E+08
1	23		34.19	−3.3580E+01	−6.9232E+00			−1.903E-02		2.142E-03		3.621E+10
1	24		34.12	−3.3580E+01	−6.8737E+00			−1.444E-02		1.622E-03		2.757E+10
1	25		34.08	−3.3580E+01	−6.8392E+00			−2.575E-02		2.889E-03		4.929E+10
...	...		...	...	...			...		...		...

E. The *A* values for E1 transitions using SS are also compared in Table E. The atomic structure calculations for the present forbidden transitions using SS also generated E1 transitions. This set is much smaller than the BPRM set. The NIST [14] table includes results from a number of authors and from the compiled table by Shirari et al. [9]. Recent calculations for the *A* values were carried out by Deb et al. [10] using CIV3 [23], Aggarwal et al. [11] and Deb and Msezane [12] using GRASP [24], and Berrington et al. [13] using AUTOSTRUCTURE, which is an adaptation of SS, as well as using Dirac–Fock GRASP code [24,25]. Comparison of the present BPRM *A* values with SS as well as the existing values show very good agreement for most of the E1 transitions. However, significant differences are found for a few

Table E
Comparison of present *A* values in units of s^{-1} for E1 transitions with those in the NIST compilation from Refs. [4](1), [5](2), [6](3), [7](4), [9](5), [8](6), and with Deb et al. [10](7), Berrington et al. [13](8) (a—Breit–Pauli atomic structure, b—Dirac atomic structure), Aggarwal et al. [11] and Deb et al. [10,12](9). The alphabetic letter is the NIST accuracy rating.

λ (Å)	A (Others)	A (Present)		C_i–C_j	$SL\pi_i$–$SL\pi_j$	g_i–g_j
		BPRM	SS			
52.911	2.94e+11[1]: C,2.77e+11[8a],2.95e+11[8b],2.29e+11[7]	2.28e+11	2.38e+11	$2p^63s^2$–3s4p	^1S–$^1P^o$	1–3
59.404	3.4e+11[2]: C,3.06e+11[8a],3.14e+11[8b],2.49e+11[7]	2.40e+11	2.23e+11	3s3p–3s4d	$^1P^o$–^1D	3–5
307.73	4.91e+09[3]: C,5.09e+09[8a],5.06e+09[8b],5.04e+09[9]	4.78e+09	4.91e+09	3s3p–$3p^2$	$^3P^o$–^3P	3–3
65.370	3.2e+10[2]: C,2.71e+10[8a],3.34e+10[8b]	3.70e+10	3.52e+10	3s3p–3s4s	$^3P^o$–^3S	1–3
65.612	9.8e+10[2]: C,8.24e+10[8a],1.02e+11[8b]	1.14e+11	1.06e+11	3s3p–3s4s	$^3P^o$–^3S	3–3
66.238	1.6e+11[2]: C,1.44e+11[8a],1.72e+11[8b]	1.95e+11	1.82e+11	3s3p–3s4s	$^3P^o$–^3S	5–3
224.754	1.38e+10[4]: C,1.42e+10[8a],1.42e+10[8b],1.36e+10[7]	1.35e+10	1.40e+10	3s3p–3s3d	$^3P^o$–^3D	1–3
227.206	1.8e+10[4]: C,1.86e+10[8a],1.85e+10[8b],1.77e+10[7]	1.76e+10	1.83e+10	3s3p–3s3d	$^3P^o$–^3D	3–5
227.734	9.8e+09[4]: C,1.02e+10[8a],1.02e+10[8b]	9.68e+09	1.0e+10	3s3p–3s3d	$^3P^o$–^3D	3–3
69.66	1.9e+11[5]: C,2.55e+11[8a],2.35e+11[8b]	2.18e+11	2.16e+11	3s3p–3s4s	$^1P^o$–^1S	3–1
243.794	4.2e+10[4]: D,4.40e+10[8a],4.41e+10[8b],4.36e+10[7]	4.09e+10	4.25e+10	3s3p–3s3d	$^1P^o$–^1D	3–5
63.96	1.6e+11[2]: E	1.91e+11	1.97e+11	$3p^2$–3s4f	^1D–$^1F^o$	5–7
194.067	3.8e+08[5]: E	3.57e+08	3.85e+08	$3p^2$–3p3d	^1D–$^1P^o$	5–3
231.68	1.5e+10[5]: E	1.43e+10	1.58e+10	$3p^2$–3p3d	^3P–$^3P^o$	3–3
231.87	2.1e+10[5]: E	2.04e+10	2.13e+10	$3p^2$–3p3d	^3P–$^3P^o$	3–1
242.100	2.3e+10[5]: D	2.36e+10	2.56e+10	$3p^2$–3p3d	^3P–$^3D^o$	5–7
68.849	9.2e+11[6]: C	9.15e+11	8.66e+11	3p3d–3p4f	$^3F^o$–^3G	9–11
69.945	7.4e+11[2]: C	7.25e+11	7.29e+11	3s3d–3s4f	^3D–$^3F^o$	3–5
69.987	7.9e+11[2]: C	7.67e+11	7.72e+11	3s3d–3s4f	^3D–$^3F^o$	5–7
70.054	8.8e+11[2]: C	8.63e+11	8.70e+11	3s3d–3s4f	^3D–$^3F^o$	7–9
70.224	4.13e+11[5]: C	4.23e+11	4.12e+11	3p3d–3p4f	$^3P^o$–^3D	1–3
73.199	8.8e+11[5]: C	6.97e+11	7.95e+11	3p3d–3p4f	$^1F^o$–^1G	7–9
73.473	6.2e+11[2]: C	6.01e+11	6.12e+11	3s3d–3s4f	^1D–$^1F^o$	5–7
312.556	1.1e+09[3]: E,1.14e+09[8a],1.09e+09[8b],1.08e+09[9]	1.16e+09	1.01e+09	3s3p–$3p^2$	$^3P^o$–^1D	3–5
238.114	3.2e+08[4]: E,2.88e+08[8a],3.27e+08[8b]	2.85e+08	2.81e+08	3s3p–$3p^2$	$^3P^o$–^1S	3–1
191.408	3.5e+08[4]: E,3.16e+08[8a],3.67e+08[8b]	3.44e+08	2.67e+08	3s3p–3s3d	$^3P^o$–^1D	3–5
196.741	1.6e+07[4]: E	1.45e+07	8.49e+06	3s3p–3s3d	$^3P^o$–^1D	5–5
304.998	3.0e+07[4]: E,1.17e+07[8a],1.73e+07[8b]	2.20e+07	1.17e+07	3s3p–3s3d	$^1P^o$–^3D	3–5
305.889	2.6e+07[4]: E,2.35e+07[8a],2.42e+07[8b]	2.63e+07	2.34e+07	3s3p–3s3d	$^1P^o$–^3D	3–3
38.95	1.69e+11[1]: C	8.95e+10	1.56e+11	$2p^63s^2$–3s5p	^1S–$^1P^o$	1–3

Table F
Comparison of the present (SS) *A* values for forbidden transitions with those in the NIST table. The alphabetic letter is the NIST accuracy (Ac) rating.

λ (Å)	*A*:Ac NIST	*A* (s^{-1}) SS	C_i–C_j	$SL\pi_i$–$SL\pi_j$	g_i–g_j
E2,M1,M2					
131.216	1.6e+06:D	1.73e+06	$2p^63s^2$–$3s3d$	^1S-^1D	1–5 E2
171.913	4.3e+04[1]:E	3.81e+04	$2p^63s^2$–$3p^2$	^1S–^3P	1–5 E2
178.702	4.1e+05[1]:E	1.59e+05	$2p^63s^2$–$3p^2$	^1S–^1D	1–5 E2
20080	4.4e−01:E	4.13e−01	$3p^2$–$3p^2$	^1D–^3P	5–3 M1
847.43	1.90e+02:E	1.70e+02	3s3p–3s3p	$^3P^o$–$^1P^o$	1–3 M1
975.84	3.0e+01:E	2.70e+01	$3p^2$–3s3d	^1S–^1D	1–5 E2
999.63	2.70e+02:E	2.70e+02	$3p^2$–$3p^2$	^1D–^1S	5–1 E2
1019.43	1.40e+02:E	1.24e+02	3s3p–3s3p	$^3P^o$–$^1P^o$	5–3 M1
1052.00	1.400e+03:E	1.25e+03	$3p^2$–$3p^2$	^3P–^1S	3–1 M1
1283.09	2.4e+01:E	2.13e+01	$3p^2$–$3p^2$	^3P–^1S	5–1 E2
224.278	1.2e+00:D	31.9	3s3p–3s3d	$^3P^o$–^3D	1–5 M2
226.372	1.98e+00:C	26.3	3s3p–3s3d	$^3P^o$–^3D	3–7 M2
246.423	4.2e+00:D	40.3	3s3p–$3p^2$	$^3P^o$–^1S	5–1 M2
303.494	6.4e+00:C	7.88e+00	3s3p–3s3d	$^1P^o$–^3D	3–7 M2
393.980	3.39e+00:C	3.38e+00	$2p^63s^2$–$3s3p$	^1S–$^3P^o$	1–5 M2

transitions, such as $3s2(^1S_0) - 3s5p(^1P^o_1)$, for which the BPRM *A* value is much lower than that from NIST as well as SS.

4.2. Energies and forbidden E2, E3, M1, M2 transitions from SUPERSTRUCTURE

Forbidden transitions of type E2, E3, M1, and M2 are presented for 123 levels of 20 configurations with orbitals going up to 5f. Of these, 101 levels lie below the ionization threshold. These are obtained from the code SS which lists the levels in energy order regardless of their symmetry. Table 3 lists these levels processed with spectroscopic identification. The calculated energies agree with the measured values in the NIST compilation within less than 1% to a maximum of 3%. They also show very good agreement with the 87-level calculations by Deb et al. [10], Aggarwal et al. [11], and Deb and Msezane [12], and 47-level calculations by Berrington et al. [13], all of which presented allowed transitions for a limited number of transitions. Small differences are expected since the set of configurations and relevant parameters are different for each calculation. The present calculations included higher levels than the earlier calculations.

The forbidden transitions with the observed levels have been reprocessed with calculated line strengths and observed energies to obtain the *A* values. The energies in Table 3 correspond to energies used to process the *A* values of the forbidden transitions. Hence they are combinations of observed (whenever available) and calculated energies, and calculated energies (when no observed values are available).

S and *A* values for a total of 6962 forbidden transitions of type E2, E3, M1, and M2 have been found for Fe XV. Table 4 presents a partial set of these transitions. The parity remains unchanged for the E2 and M1 transitions and hence are presented together. On the other hand, parity changes for E3 and M2 transitions which are presented together. The complete set of transitions processed from SS output with standard spectroscopic notation is available electronically.

Comparison of the present *A* values are made with those available in the NIST compilation, computed by Anderson and Anderson [7], in Table F. Good agreement is found between SS and NIST for E2, M1 transitions. Variable agreement is noted between SS and NIST for M2 transitions.

5. Conclusions

Photo-excitations and de-excitations of Fe XV are studied in detail and an extensive set of transition parameters for oscillator strengths, line strengths, and radiative decay rates is presented for both allowed and forbidden transitions. The allowed transitions are treated with a large-scale relativistic Breit–Pauli R-matrix method and the forbidden transitions are treated with relativistic atomic structure calculations using the code SUPERSTRUCTURE. Very good agreement, within 1%, is found for the BPRM calculated energies with the measured values while those from SS vary from less than 1–3%.

The BPRM E1 transition rates are in very good agreement with available results for most transitions. The advantage of the present BPRM method is its capability of including much more configuration interactions than that of the atomic structure calculations. However, the atomic structure calculations in the Breit–Pauli approximation can include two-body interaction terms and the Dirac–Fock method can make better optimization of the energies. For highly charged Fe XV, the 47-level calculations by Berrington et al. [13], the 87-level calculations by Aggarwal et al. [11] and Deb and Msezane [12], and the present calculations provide similar results for most of the transitions. Some differences in the results are expected from differences in the methodologies. The present forbidden transitions compare very well with those in the NIST compilation for most transitions. However, M2 transitions have variable agreement with others. The present results are expected to be accurate and complete enough for most astrophysical and laboratory applications. In addition to the present supplemental data files, all data are available electronically at the NORAD website: www.astronomy.ohio-state.edu/~nahar/nahar_radiativeatomicdata/index.html

Acknowledgements

This work was partially supported by the NASA APRA program. The computational work was carried out on the Cray X1 at the Ohio Supercomputer Center in Columbus, Ohio.

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.adt.2009.03.002.

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Explanation of Tables

Table 1. Partial set of 507 energy levels of Fe XV, grouped as fine structure components of *LS* terms.

The levels are designated as $C_t(S_tL_t\pi_t)J_tnlJ(SL)\pi$

The top line of each set provides the expected number of fine structure levels (Nlv) for the possible $^{(2S+1)}L^{\pi}$ terms with the given configurations. In the set, the spin multiplicity $(2S+1)$ and parity π are fixed, but L varies. Within parenthesis next to each L, all possible J values associated with the given LS term are specified. This line is followed by a set of the energy levels of the same configurations. Nlv(c) at the end specifies the total number of calculated J levels found for the set. If Nlv = Nlv(c), the calculated energy set for the given terms is complete

The levels are designated as $C_t(S_tL_t\pi_t)J_tnlJ(SL)\pi$

C_t	target configuration
$S_tL_t\pi_t$	$SL\pi$ symmetry of the target
J_t	total angular momentum of the target state
nl	configuration of the valence electron
J	total angular momentum of the level
E (Ry)	level energy in Rydberg
v	effective quantum number
$SL\pi$	symmetry of the level

Table 2. E1 transition probabilities for observed levels of Fe XV, grouped as fine structure components of *LS* multiplets.

The calculated transition energies have been replaced by the observed energies.

C_i–C_k	configurations of transition levels
T_i–T_k	LS term designation of the level
g_i	statistical weight factor $(2J+1)$ of the level
I	position of the level in its $SL\pi$ symmetry
E_ik (Å)	transition energy (in Angstroms)
f, S, A (s^{-1})	oscillator strength, line strength, radiative decay rate

Table 3. Fine structure energy levels of Fe XV for which forbidden (E2, E3, M1, M2) transitions are presented.

The indices (cf) correspond to configurations $2p^63s^2(1)$, $2p^63s3p(2)$, $2p^63p^2(3)$, $2p^63s3d(4)$, $2p^63p3d(5)$, $2p^63s4s(6)$, $2p^63s4p(7)$, $2p^63s4d(8)$, $2p^64s4f(9)$, $2p^63s5s(10)$, $2p^63s5p(11)$, $2p^63s5d(12)$, $2p^63p4s(13)$, $2p^63p4p(14)$, $2p^63p4d(15)$, $2p^63p4f(16)$, $2p^53s^23p(17)$, $2p^53s^23d(18)$, $2p^63d^2(19)$, $2p^63s5f(20)$

i_e	level index
SLp(cf)	LS term of the level and configuration number cf
$2J$	J is total angular momentum
E (Ry)	relative energy in Rydberg of the level

Table 4. Partial set of radiative decay rates for forbidden E2, M1, E3, M2 transitions in Fe XV.

The indices (cf) correspond to configurations $2p^63s^2(1)$, $2p^63s3p(2)$, $2p^63p^2(3)$, $2p^63s3d(4)$, $2p^63p3d(5)$, $2p^63s4s(6)$, $2p^63s4p(7)$, $2p^63s4d(8)$, $2p^64s4f(9)$, $2p^63s5s(10)$, $2p^63s5p(11)$, $2p^63s5d(12)$, $2p^63p4s(13)$, $2p^63p4p(14)$, $2p^63p4d(15)$, $2p^63p4f(16)$, $2p^53s^23p(17)$, $2p^53s^23d(18)$, $2p^63d^2(19)$, $2p^63s5f(20)$

N_{tr}	total number of transitions
i–j	energy indices of the levels as given in Table 3
N_i	LS term designation of the level
C_i	configuration number of the transition level
g_i	statistical weight factor $(2J+1)$ of the level
λ	transition energy. Note that for extremely low energy, λ = 10,000 Å
E_i, E_f	energies of the levels
$AE2$	radiative decay rate for E2 transition
$AE3$	radiative decay rate for E3 transition
$AM1$	radiative decay rate for M1 transition
$AM2$	radiative decay rate for M2 transition

Table 1
Partial set of 507 energy levels of Fe XV, grouped as fine structure components of *LS* terms. See page 583 for Explanation of Tables.

$C_t(S_tL_t\pi_t)$		J_t	nl	J	E (Ry)	v	$SL\pi$
Eqv electron/unidentified levels, parity: e							
$2p^63s^2$				0	−3.35050E+01	0.00	1 S e
Nlv(c) = 1: set complete							
Nlv = 3, $^3L^o$: P (2 1 0)							
$2p^63s$	(2Se)	1/2	3p	0	−3.13740E+01	2.68	3 P o
$2p^63s$	(2Se)	1/2	3p	1	−3.13214E+01	2.68	3 P o
$2p^63s$	(2Se)	1/2	3p	2	−3.11951E+01	2.69	3 P o
Nlv(c) = 3: set complete							
Nlv = 1, $^1L^o$: P(1)							
$2p^63s$	(2Se)	1/2	3p	1	−3.02823E+01	2.73	1 P o
Nlv(c) = 1: set complete							
Eqv electron/unidentified levels, parity: e							
$2p^63p^2$				0	−2.84377E+01	0.00	3 P e
$2p^63p^2$				1	−2.83502E+01	0.00	3 P e
$2p^63p^2$				2	−2.81990E+01	0.00	3 P e
Nlv(c) = 3: set complete							
Eqv electron/unidentified levels, parity: e							
$2p^63p^2$				2	−2.83981E+01	0.00	1 D e
Nlv(c) = 1: set complete							
Eqv electron/unidentified levels, parity: e							
$2p^63p^2$				0	−2.74705E+01	0.00	1 S e
Nlv(c) = 1: set complete							
Nlv = 3, $^3L^e$: D (3 2 1)							
$2p^63s$	(2Se)	1/2	3d	1	−2.72920E+01	2.87	3 D e
$2p^63s$	(2Se)	1/2	3d	2	−2.72822E+01	2.88	3 D e
$2p^63s$	(2Se)	1/2	3d	3	−2.72669E+01	2.87	3 D e
Nlv(c) = 3: set complete							
Nlv = 1, $^1L^e$: D (2)							
$2p^63s$	(2Se)	1/2	3d	2	−2.65180E+01	2.88	1 D e
Nlv(c) = 1: set complete							
Nlv=9, $^3L^o$: P (2 1 0) D (3 2 1) F (4 3 2)							
$2p^63p$	(2Po)	1/2	3d	2	−2.50182E+01	2.88	3 PDF o
$2p^63p$	(2Po)	1/2	3d	3	−2.49282E+01	2.88	3 DF o
$2p^63p$	(2Po)	1/2	3d	4	−2.48254E+01	2.86	3 F o
$2p^63p$	(2Po)	1/2	3d	1	−2.45113E+01	2.89	3 PD o
$2p^63p$	(2Po)	1/2	3d	2	−2.45045E+01	2.88	3 PDF o
$2p^63p$	(2Po)	1/2	3d	3	−2.44046E+01	2.88	3 DF o
$2p^63p$	(2Po)	1/2	3d	0	−2.43943E+01	2.88	3 P o
$2p^63p$	(2Po)	1/2	3d	1	−2.43941E+01	2.89	3 PD o
$2p^63p$	(2Po)	1/2	3d	2	−2.43929E+01	2.88	3 PDF o
Nlv(c) = 9: set complete							
Nlv = 3, $^1L^o$: P (1) D (2) F (3)							
$2p^63p$	(2Po)	1/2	3d	2	−2.48346E+01	2.88	1 D o
$2p^63p$	(2Po)	1/2	3d	3	−2.37794E+01	2.84	1 F o
$2p^63p$	(2Po)	3/2	3d	1	−2.36558E+01	2.85	1 P o
Nlv(c) = 3: set complete							
Eqv electron/unidentified levels, parity: e							
$2p^63d^2$				2	−2.09637E+01	0.00	3 F e
$2p^63d^2$				3	−2.09479E+01	0.00	3 F e
$2p^63d^2$				4	−2.09282E+01	0.00	3 F e
Nlv(c) = 3: set complete							
Eqv electron/unidentified levels, parity: e							
$2p^63d^2$				2	−2.06620E+01	0.00	1 D e
Nlv(c) = 1: set complete							
Eqv electron/unidentified levels, parity: e							
$2p^63d^2$				0	−2.06333E+01	0.00	3 P e
$2p^63d^2$				1	−2.06274E+01	0.00	3 P e
$2p^63d^2$				2	−2.06124E+01	0.00	3 P e
Nlv(c) = 3: set complete							
Eqv electron/unidentified levels, parity: e							
$2p^63d^2$				4	−2.06254E+01	0.00	1 G e
Nlv(c) = 1: set complete							
Eqv electron/unidentified levels, parity: e							
$2p^63d^2$				0	−1.98611E+01	0.00	1 S e
Nlv(c) = 1: set complete							
Nlv = 1, $^3L^e$: S (1)							
$2p^63s$	(2Se)	1/2	4s	1	−1.74351E+01	3.59	3 S e

Table 1. (*continued*)

$C_t(S_tL_t\pi_t)$		J_t	nl	J	E (Ry)	v	$SL\pi$
Nlv(c) = 1: set complete							
Nlv = 1, $^1L^e$: S (0)							
$2p^63s$	(2Se)	1/2	4s	0	−1.72217E+01	3.62	1 S e
Nlv(c) = 1: set complete							
Nlv = 3, $^3L^o$: P (2 1 0)							
$2p^63s$	(2Se)	1/2	4p	0	−1.63560E+01	3.71	3 P o
$2p^63s$	(2Se)	1/2	4p	1	−1.63526E+01	3.71	3 P o
$2p^63s$	(2Se)	1/2	4p	2	−1.62901E+01	3.72	3 P o
Nlv(c) = 3: set complete							
Nlv = 1, $^1L^o$: P (1)							
$2p^63s$	(2Se)	1/2	4p	1	−1.62877E+01	3.72	1 P o
Nlv(c) = 1: set complete							
Nlv = 3, $^3L^e$: D (3 2 1)							
$2p^63s$	(2Se)	1/2	4d	1	−1.49855E+01	3.88	3 D e
$2p^63s$	(2Se)	1/2	4d	2	−1.49789E+01	3.88	3 D e
$2p^63s$	(2Se)	1/2	4d	3	−1.49681E+01	3.88	3 D e
Nlv(c) = 3: set complete							
Nlv = 1, $^1L^e$: D (2)							
$2p^63s$	(2Se)	1/2	4d	2	−1.49577E+01	3.88	1 D e
Nlv(c) = 1: set complete							
Nlv = 3, $^3L^o$: P (2 1 0)							
$2p^63p$	(2Po)	1/2	4s	0	−1.47949E+01	3.60	3 P o
$2p^63p$	(2Po)	1/2	4s	1	−1.47629E+01	3.61	3 P o
$2p^63p$	(2Po)	3/2	4s	2	−1.46148E+01	3.60	3 P o
Nlv(c) = 3: set complete							
Nlv = 1, $^1L^o$: P (1)							
$2p^63p$	(2Po)	3/2	4s	1	−1.44962E+01	3.62	1 P o
Nlv(c) = 1: set complete							
Nlv = 3, $^3L^o$: F (4 3 2)							
$2p^63s$	(2Se)	1/2	4f	2	−1.42966E+01	3.97	3 F o
$2p^63s$	(2Se)	1/2	4f	3	−1.42947E+01	3.96	3 F o
$2p^63s$	(2Se)	1/2	4f	4	−1.42921E+01	3.97	3 F o
Nlv(c) = 3: set complete							
Nlv = 1, $^1L^o$: F (3)							
$2p^63s$	(2Se)	1/2	4f	3	−1.41619E+01	3.96	1 F o
Nlv(c) = 1: set complete							
Nlv = 7, $^3L^e$: S (1) P (2 1 0) D (3 2 1)							
$2p^63p$	(2Po)	1/2	4p	1	−1.38751E+01	3.70	3 SPD e
$2p^63p$	(2Po)	3/2	4p	1	−1.37468E+01	3.72	3 SPD e
$2p^63p$	(2Po)	1/2	4p	2	−1.37296E+01	3.72	3 PD e
$2p^63p$	(2Po)	1/2	4p	0	−1.36853E+01	3.72	3 P e
$2p^63p$	(2Po)	3/2	4p	1	−1.36147E+01	3.71	3 SPD e
$2p^63p$	(2Po)	3/2	4p	3	−1.35934E+01	3.71	3 D e
$2p^63p$	(2Po)	3/2	4p	2	−1.35481E+01	3.72	3 PD e
Nlv(c) = 7: set complete							
Nlv = 3, $^1L^e$: S (0) P (1) D (2)							
$2p^63p$	(2Po)	3/2	4p	1	−1.35203E+01	3.72	1 P e
$2p^63p$	(2Po)	3/2	4p	2	−1.33879E+01	3.74	1 D e
$2p^63p$	(2Po)	3/2	4p	0	−1.31260E+01	3.77	1 S e
Nlv(c) = 3: set complete							
Nlv = 9, $^3L^o$: P (2 1 0) D (3 2 1) F (4 3 2)							
$2p^63p$	(2Po)	1/2	4d	1	−1.24192E+01	3.88	3 PD o
$2p^63p$	(2Po)	1/2	4d	2	−1.24168E+01	3.88	3 PDF o
$2p^63p$	(2Po)	1/2	4d	2	−1.24112E+01	3.88	3 PDF o
$2p^63p$	(2Po)	1/2	4d	3	−1.23974E+01	3.88	3 DF o
$2p^63p$	(2Po)	3/2	4d	2	−1.22634E+01	3.88	3 PDF o
$2p^63p$	(2Po)	3/2	4d	3	−1.22502E+01	3.88	3 DF o
$2p^63p$	(2Po)	3/2	4d	4	−1.21875E+01	3.88	3 F o
$2p^63p$	(2Po)	2/2	4d	1	−1.21392E+01	3.89	3 PD o
$2p^63p$	(2Po)	3/2	4d	0	−1.21016E+01	3.90	3 P o
Nlv(c) = 9: set complete							
Nlv = 3, $^1L^o$: P (1) D (2) F (3)							
$2p^63p$	(2Po)	3/2	4d	3	−1.21875E+01	3.88	1 F o
$2p^63p$	(2Po)	1/2	4d	2	−1.21476E+01	3.89	1 D o
$2p^63p$	(2Po)	1/2	4d	1	−1.20731E+01	3.89	1 P o
Nlv(c) = 3: set complete							
Nlv = 9, $^3L^e$: D (3 2 1) F (4 3 2) G (5 4 3)							
$2p^63p$	(2Po)	1/2	4f	3	−1.18199E+01	3.96	3 DFG e
$2p^63p$	(2Po)	1/2	4f	4	−1.17585E+01	3.96	3 FG e
$2p^63p$	(2Po)	1/2	4f	3	−1.17572E+01	3.96	3 DFG e

(*continued on next page*)

Table 1. (*continued*)

$C_t(S_tL_t\pi_t)$		J_t	nl	J	E (Ry)	v	$SL\pi$
$2p^6 3p$	(2Po)	1/2	4f	2	−1.17244E+01	3.97	3 DF e
$2p^6 3p$	(2Po)	1/2	4f	5	−1.16235E+01	3.96	3 G e
$2p^6 3p$	(2Po)	3/2	4f	4	−1.16147E+01	3.96	3 FG e
$2p^6 3p$	(2Po)	3/2	4f	3	−1.15120E+01	3.96	3 DFG e
$2p^6 3p$	(2Po)	1/2	4f	2	−1.14848E+01	3.97	3 DF e
$2p^6 3p$	(2Po)	3/2	4f	1	−1.14563E+01	3.98	3 D e
Nlv(c) = 9: set complete							
Nlv = 3, $^1L^e$: D (2) F (3) G (4)							
$2p^6 3p$	(2Po)	3/2	4f	3	−1.16397E+01	3.96	1 F e
$2p^6 3p$	(2Po)	1/2	4f	4	−1.13759E+01	3.96	1 G e
$2p^6 3p$	(2Po)	3/2	4f	2	−1.13143E+01	3.97	1 D e
Nlv(c) = 3: set complete							
Nlv = 3, $^3L^e$: D (3 2 1)							
$2p^6 3d$	(2De)	3/2	4s	1	−1.10705E+01	3.51	3 D e
$2p^6 3d$	(2De)	3/2	4s	2	−1.10624E+01	3.51	3 D e
$2p^6 3d$	(2De)	5/2	4s	3	−1.10443E+01	3.61	3 D e
Nlv(c) = 3: set complete							
Nlv = 1, $^1L^e$: D (2)							
$2p^6 3d$	(2De)	3/2	4s	2	−1.09798E+01	3.53	1 D e
Nlv(c) = 1: set complete							
Nlv = 1, $^3L^e$: S (1)							
$2p^6 3s$	(2Se)	1/2	5s	1	−1.06187E+01	4.60	3 S e
Nlv(c) = 1: set complete							
Nlv = 1, $^1L^e$: S (0)							
$2p^6 3s$	(2Se)	1/2	5s	0	−1.05409E+01	4.62	1 S e
Nlv(c) = 1: set complete							
Nlv = 3, $^3L^o$: P (2 1 0)							
$2p^6 3s$	(2Se)	1/2	5p	2	−1.01371E+01	4.71	3 P o
$2p^6 3s$	(2Se)	1/2	5p	0	−1.01001E+01	4.72	3 P o
$2p^6 3s$	(2Se)	1/2	5p	1	−9.75794E+00	4.80	3 P o
Nlv(c) = 3: set complete							
Nlv = 9, $^3L^o$: P (2 1 0) D (3 2 1) F (4 3 2)							
$2p^6 3d$	(2De)	3/2	4p	1	−1.01063E+01	3.72	3 PD o
$2p^6 3d$	(2De)	3/2	4p	1	−1.00941E+01	3.72	3 PD o
$2p^6 3d$	(2De)	3/2	4p	2	−1.00838E+01	3.72	3 PDF o
$2p^6 3d$	(2De)	3/2	4p	2	−1.00669E+01	3.73	3 PDF o
$2p^6 3d$	(2De)	5/2	4p	3	−1.00645E+01	3.72	3 DF o
$2p^6 3d$	(2De)	5/2	4p	2	−1.00549E+01	3.73	3 PDF o
$2p^6 3d$	(2De)	3/2	4p	3	−1.00278E+01	3.73	3 DF o
$2p^6 3d$	(2De)	5/2	4p	4	−9.99826E+00	3.73	3 F o
$2p^6 3d$	(2De)	3/2	4p	0	−9.93217E+00	3.76	3 P o
Nlv(c) = 9: set complete							
Nlv = 1, $^1L^o$: P (1)							
$2p^6 3s$	(2Se)	1/2	5p	1	−1.00685E+01	4.73	1 P o
Nlv(c) = 1: set complete							
Nlv = 3, $^1L^o$: P (1) D (2) F (3)							
$2p^6 3d$	(2De)	3/2	4p	1	−9.93544E+00	3.76	1 P o
$2p^6 3d$	(2De)	3/2	4p	2	−9.93337E+00	3.76	1 D o
$2p^6 3d$	(2De)	3/2	4p	3	−9.85399E+00	3.78	1 F o
Nlv(c) = 3: set complete							
Nlv = 3, $^3L^e$: D (3 2 1)							
$2p^6 3s$	(2Se)	1/2	5d	1	−9.43488E+00	4.88	3 D e
$2p^6 3s$	(2Se)	1/2	5d	2	−9.43261E+00	4.88	3 D e
$2p^6 3s$	(2Se)	1/2	5d	3	−9.42836E+00	4.89	3 D e
Nlv(c) = 3: set complete							
Nlv = 1, $^1L^e$: D (2)							
$2p^6 3s$	(2Se)	1/2	5d	2	−9.41148E+00	4.89	1 D e
Nlv(c) = 1: set complete							
Nlv = 3, $^3L^o$: F (4 3 2)							
$2p^6 3s$	(2Se)	1/2	5f	2	−9.11279E+00	4.97	3 F o
$2p^6 3s$	(2Se)	1/2	5f	3	−9.11182E+00	4.97	3 F o
$2p^6 3s$	(2Se)	1/2	5f	4	−9.11052E+00	4.97	3 F o
Nlv(c) = 3: set complete							
Nlv = 1, $^1L^o$: F (3)							
$2p^6 3s$	(2Se)	1/2	5f	3	−9.06347E+00	4.98	1 F o
Nlv(c) = 1: set complete							
Nlv = 3, $^3L^e$: G (5 4 3)							
$2p^6 3s$	(2Se)	1/2	5g	3	−9.02326E+00	4.99	3 G e
$2p^6 3s$	(2Se)	1/2	5g	4	−9.02167E+00	4.99	3 G e
$2p^6 3s$	(2Se)	1/2	5g	5	−9.01982E+00	4.99	3 G e

Table 1. (*continued*)

$C_t(S_tL_t\pi_t)$		J_t	nl	J	E (Ry)	v	$SL\pi$
Nlv(c) = 3: set complete							
Nlv = 1, $^1L^e$: G (4)							
$2p^63s$	(2Se)	1/2	5g	4	−8.99516E+00	5.00	1 G e
Nlv(c) = 1: set complete							
Nlv=13, $^3L^e$: S (1) P (2 1 0) D (3 2 1) F (4 3 2) G (5 4 3)							
$2p^63d$	(2De)	3/2	4d	3	−8.87292E+00	4.04	3 DFG e
$2p^63d$	(2De)	3/2	4d	1	−8.83134E+00	4.05	3 SPD e
$2p^63d$	(2De)	3/2	4d	2	−8.81923E+00	4.05	3 PDF e
$2p^63d$	(2De)	3/2	4d	3	−8.80569E+00	4.05	3 DFG e
$2p^63d$	(2De)	5/2	4d	3	−8.79167E+00	5.06	3 DFG e
$2p^63d$	(2De)	3/2	4d	1	−8.77878E+00	4.06	3 SPD e
$2p^63d$	(2De)	3/2	4d	4	−8.77795E+00	4.06	3 FG e
$2p^63d$	(2De)	5/2	4d	5	−8.75900E+00	4.07	3 G e
$2p^63d$	(2De)	3/2	4d	1	−8.67371E+00	4.09	3 SPD e
$2p^63d$	(2De)	5/2	4d	2	−8.62585E+00	4.11	3 PDF e
$2p^63d$	(2De)	5/2	4d	4	−8.59901E+00	3.90	3 FG e
$2p^63d$	(2De)	3/2	4d	2	−8.48381E+00	4.15	3 PDF e
$2p^63d$	(2De)	3/2	4d	0	−8.45982E+00	4.00	3 P e
Nlv(c) = 13: set complete							
Nlv = 5, $^1L^e$: S (0) P (1) D (2) F (3) G (4)							
$2p^63d$	(2De)	3/2	4d	3	−8.61347E+00	3.90	1 F e
$2p^63d$	(2De)	3/2	4d	1	−8.45410E+00	4.00	1 P e
$2p^63d$	(2De)	5/2	4d	2	−8.44292E+00	4.16	1 D e
$2p^63d$	(2De)	5/2	4d	4	−8.41900E+00	4.17	1 G e
$2p^63d$	(2De)	3/2	4d	0	−8.16289E+00	4.00	1 S e
Nlv(c) = 5: set complete							
Nlv = 9, $^3L^o$: P (2 1 0) D (3 2 1) F (4 3 2)							
$2p^63p$	(2Po)	1/2	5d	4	−8.26285E+00	4.57	3 F o
$2p^63p$	(2Po)	1/2	5d	3	−8.16889E+00	4.95	3 DF o
$2p^63p$	(2Po)	3/2	5d	2	−8.07410E+00	4.88	3 PDF o
$2p^63p$	(2Po)	1/2	5d	3	−7.98156E+00	4.88	3 DF o
$2p^63p$	(2Po)	3/2	5d	2	−7.93125E+00	4.60	3 PDF o
$2p^63p$	(2Po)	3/2	5d	2	−7.91568E+00	4.60	3 PDF o
$2p^63p$	(2Po)	1/2	5d	1	−7.88490E+00	4.88	3 PD o
$2p^63p$	(2Po)	3/2	5d	1	−7.87187E+00	4.88	3 PD o
$2p^63p$	(2Po)	1/2	5d	0	−7.86951E+00	4.88	3 P o
Nlv(c) = 9: set complete							
Nlv = 9, $^3L^o$: F (4 3 2) G (5 4 3) H (6 5 4)							
$2p^63p$	(2Po)	3/2	5g	4	−8.24679E+00	5.00	3 FGH o
$2p^63p$	(2Po)	1/2	5g	5	−8.24598E+00	4.57	3 GH o
$2p^63p$	(2Po)	3/2	5g	6	−8.23032E+00	4.53	3 H o
$2p^63p$	(2Po)	1/2	5g	4	−8.16120E+00	4.88	3 FGH o
$2p^63p$	(2Po)	1/2	5g	4	−7.97148E+00	4.88	3 FGH o
$2p^63p$	(2Po)	3/2	5g	5	−7.96131E+00	4.59	3 GH o
$2p^63p$	(2Po)	3/2	5g	3	−7.91413E+00	4.88	3 FG o
$2p^63p$	(2Po)	3/2	5g	3	−7.87763E+00	4.88	3 FG o
$2p^63p$	(2Po)	3/2	5g	2	−7.87644E+00	4.98	3 F o
Nlv(c) = 9: set complete							

Table 2
E1 transition probabilities for observed levels of Fe XV, grouped as fine structure components of *LS* multiplets. See page 583 for Explanation of Tables.

C_i–C_k	T_i–T_k	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
$2p^63s^2$–3s3p	1Se–3Po	1:1–3:1	417.27	3.26E−03	4.47E−03	4.16E+07
$2p^63s^2$–3s3p	1Se–1Po	1:1–3:2	284.17	7.90E−01	7.39E−01	2.18E+10
$2p^63s^2$–3p3d	1Se–3Do	1:1–3:3	101.74	9.20E−07	3.08E−07	1.97E+05
$2p^63s^2$–3p3d	1Se–3Po	1:1–3:4	100.38	6.25E−08	2.07E−08	1.38E+04
$2p^63s^2$–3p3d	1Se–1Po	1:1–3:5	93.03	1.26E−03	3.87E−04	3.25E+08
$2p^63s^2$–3s4p	1Se–1Po	1:1–3:7	52.91	2.87E−01	5.00E−02	2.28E+11
$2p^63s^2$–3s5p	1Se–1Po	1:1–3:15	38.96	6.11E−02	7.84E−03	8.95E+10
3s3p–$3p^2$	3Po–3Pe	3:1–1:2	317.59	8.74E−02	2.74E−01	1.73E+10
3s3p–$3p^2$	3Po–3Pe	1:1–3:1	302.33	2.79E−01	2.77E−01	6.78E+09
3s3p–$3p^2$	3Po–3Pe	3:1–3:1	307.75	6.78E−02	2.06E−01	4.78E+09
3s3p–$3p^2$	3Po–3Pe	5:1–3:1	321.78	6.48E−02	3.43E−01	6.96E+09
3s3p–$3p^2$	3Po–3Pe	3:1–5:2	292.27	9.15E−02	2.64E−01	4.29E+09
3s3p–$3p^2$	3Po–3Pe	5:1–5:2	304.89	1.71E−01	8.60E−01	1.23E+10
LS	3Po–3Pe	9–9		2.44E−01	2.22E+00	1.72E+10
3s3p–$3p^2$	1Po–3Pe	3:2–1:2	493.54	6.82E−04	3.32E−03	5.60E+07
3s3p–$3p^2$	1Po–3Pe	3:2–3:1	470.16	2.78E−04	1.29E−03	8.39E+06
3s3p–$3p^2$	1Po–3Pe	3:2–5:2	434.97	2.40E−02	1.03E−01	5.07E+08
$3p^2$–3p3d	3Pe–3Do	1:2–3:3	233.45	6.19E−01	4.76E−01	2.52E+10
$3p^2$–3p3d	3Pe–3Do	3:1–3:3	239.08	3.94E−02	9.29E−02	4.59E+09
$3p^2$–3p3d	3Pe–3Do	3:1–5:4	231.47	3.40E−01	7.77E−01	2.54E+10
$3p^2$–3p3d	3Pe–3Do	5:2–3:3	249.33	1.20E−03	4.93E−03	2.15E+08
$3p^2$–3p3d	3Pe–3Do	5:2–5:4	241.07	1.05E−02	4.16E−02	1.20E+09
$3p^2$–3p3d	3Pe–3Do	5:2–7:2	242.10	2.90E−01	1.16E+00	2.36E+10
LS	3Pe–3Do	9–15		3.63E−01	2.55E+00	2.58E+10
$3p^2$–3p3d	3Pe–3Po	1:2–3:4	226.39	1.32E−03	9.81E−04	5.71E+07
$3p^2$–3p3d	3Pe–3Po	3:1–1:2	231.86	5.47E−02	1.25E−01	2.04E+10
$3p^2$–3p3d	3Pe–3Po	3:1–3:4	231.67	1.15E−01	2.64E−01	1.43E+10
$3p^2$–3p3d	3Pe–3Po	3:1–5:5	238.71	6.32E−02	1.49E−01	4.44E+09
$3p^2$–3p3d	3Pe–3Po	5:2–3:4	241.29	3.56E−02	1.42E−01	6.80E+09
$3p^2$–3p3d	3Pe–3Po	5:2–5:5	248.94	1.51E−01	6.21E−01	1.63E+10
LS	3Pe–3Po	9–9		1.81E−01	1.30E+00	2.06E+10
$3p^2$–3p3d	3Pe–1Po	1:2–3:5	192.17	3.50E−03	2.21E−03	2.10E+08
$3p^2$–3p3d	3Pe–1Po	3:1–3:5	195.97	4.29E−04	8.30E−04	7.44E+07
$3p^2$–3p3d	3Pe–1Po	5:2–3:5	202.81	3.37E−04	1.13E−03	9.12E+07
$3p^2$–3s4p	3Pe–1Po	1:2–3:7	74.88	5.10E−05	1.26E−05	2.02E+07
$3p^2$–3s4p	3Pe–1Po	3:1–3:7	75.45	5.52E−06	4.12E−06	6.47E+06
$3p^2$–3s4p	3Pe–1Po	5:2–3:7	76.44	3.66E−03	4.61E−03	6.97E+09
$3p^2$–3s5p	3Pe–1Po	1:2–3:15	49.69	2.50E−04	4.09E−05	2.25E+08
$3p^2$–3s5p	3Pe–1Po	3:1–3:15	49.94	1.09E−04	5.35E−05	2.90E+08
$3p^2$–3s5p	3Pe–1Po	5:2–3:15	50.37	2.38E−06	1.97E−06	1.04E+07
3s3p–$3p^2$	3Po–1Se	3:1–1:3	238.11	8.07E−04	1.90E−03	2.85E+08
3s3p–$3p^2$	1Po–1Se	3:2–1:3	324.97	1.03E−01	3.29E−01	1.94E+10
$3p^2$–3p3d	1Se–3Do	1:3–3:3	309.37	1.49E−03	1.51E−03	3.45E+07
$3p^2$–3p3d	1Se–3Po	1:3–3:4	297.08	4.11E−09	4.02E−09	1.04E+02
$3p^2$–3p3d	1Se–1Po	1:3–3:5	240.81	6.43E−01	5.10E−01	2.47E+10
$3p^2$–3s4p	1Se–1Po	1:3–3:7	81.28	1.61E−03	4.29E−04	5.40E+08
$3p^2$–3s5p	1Se–1Po	1:3–3:15	52.43	1.10E−03	1.90E−04	8.92E+08
3s3p–$3d^2$	3Po–1Se	3:1–1:5	80.17	2.06E−06	1.63E−06	6.43E+06
3s3p–$3d^2$	1Po–1Se	3:2–1:5	88.09	7.27E−04	6.32E−04	1.87E+09
3p3d–$3d^2$	3Do–1Se	3:3–1:5	198.34	1.32E−03	2.59E−03	6.71E+08
3p3d–$3d^2$	3Po–1Se	3:4–1:5	203.74	8.05E−06	1.62E−05	3.88E+06
3p3d–$3d^2$	1Po–1Se	3:5–1:5	242.62	1.65E−01	3.95E−01	5.60E+10
$3d^2$–3s4p	1Se–1Po	1:5–3:7	248.19	1.99E−03	1.62E−03	7.17E+07
$3d^2$–3s5p	1Se–1Po	1:5–3:15	92.60	6.84E−03	2.08E−03	1.77E+09
3s3p–3s4s	3Po–1Se	3:1–1:6	64.63	2.13E−04	1.36E−04	1.02E+09
3s3p–3s4s	1Po–1Se	3:2–1:6	69.68	5.31E−02	3.65E−02	2.19E+11
3p3d–3s4s	3Do–1Se	3:3–1:6	124.36	1.48E−07	1.82E−07	1.92E+05
3p3d–3s4s	3Po–1Se	3:4–1:6	126.46	2.02E−09	2.53E−09	2.53E+03
3p3d–3s4s	1Po–1Se	3:5–1:6	140.43	5.48E−08	7.60E−08	5.56E+04
3s4s–3s4p	1Se–1Po	1:6–3:7	971.09	2.70E−01	8.64E−01	6.37E+08
3s4s–3s5p	1Se–1Po	1:6–3:15	128.20	9.47E−02	4.00E−02	1.28E+10
3s3p–3s3d	3Po–3De	1:1–3:2	224.75	3.07E−01	2.27E−01	1.35E+10
3s3p–3s3d	3Po–3De	3:1–3:2	227.73	7.53E−02	1.69E−01	9.68E+09
3s3p–3s3d	3Po–3De	5:1–3:2	235.32	2.94E−03	1.14E−02	5.91E+08
3s3p–3s3d	3Po–3De	3:1–5:3	227.20	2.27E−01	5.09E−01	1.76E+10
3s3p–3s3d	3Po–3De	5:1–5:3	234.76	4.44E−02	1.72E−01	5.37E+09
3s3p–3s3d	3Po–3De	5:1–7:1	233.87	2.48E−01	9.55E−01	2.16E+10
LS	3Po–3De	9–15		2.99E−01	2.04E+00	2.25E+10
3s3p–3s4s	3Po–3Se	1:1–3:4	65.37	7.29E−02	1.57E−02	3.79E+10
3s3p–3s4s	3Po–3Se	3:1–3:4	65.61	7.36E−02	4.77E−02	1.14E+11
3s3p–3s4s	3Po–3Se	5:1–3:4	66.23	7.70E−02	8.39E−02	1.95E+11
LS	3Po–3Se	9–3		7.54E−02	1.47E−01	3.47E+11
3s3p–3s4d	3Po–3De	1:1–3:5	55.63	3.42E−01	6.27E−02	2.46E+11
3s3p–3s4d	3Po–3De	3:1–3:5	55.81	8.59E−02	4.73E−02	1.84E+11
3s3p–3s4d	3Po–3De	5:1–3:5	56.26	3.51E−03	3.25E−03	1.23E+10

Table 2. (*continued*)

C_i–C_k	T_i–T_k	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
3s3p–3s4d	3Po–3De	3:1–5:8	55.79	2.52E−01	1.39E−01	3.24E+11
3s3p–3s4d	3Po–3De	5:1–5:8	56.24	5.07E−02	4.70E−02	1.07E+11
3s3p–3s4d	3Po–3De	5:1–7:3	56.20	2.87E−01	2.66E−01	4.33E+11
LS	3Po–3De	9–15		3.40E−01	5.65E−01	4.33E+11
3s3p–3p4f	3Po–3De	1:1–3:10	45.74	1.03E−03	1.55E−04	1.09E+09
3s3p–3p4f	3Po–3De	3:1–3:10	45.86	3.07E−04	1.39E−04	9.74E+08
3s3p–3p4f	3Po–3De	5:1–3:10	46.16	1.67E−05	1.27E−05	8.71E+07
3s3p–3p4f	3Po–3De	3:1–5:14	45.98	6.69E−04	3.04E−04	1.27E+09
3s3p–3p4f	3Po–3De	5:1–5:14	46.29	1.87E−04	1.43E−04	5.82E+08
3s3p–3p4f	3Po–3De	5:1–7:8	46.31	6.52E−04	4.97E−04	1.45E+09
LS	3Po–3De	9–15		9.15E−04	1.25E−03	1.72E+09
3s3p–3s5s	3Po–3Se	1:1–3:12	43.27	1.35E−02	1.92E−03	1.60E+10
3s3p–3s5s	3Po–3Se	3:1–3:12	43.38	1.35E−02	5.80E−03	4.79E+10
3s3p–3s5s	3Po–3Se	5:1–3:12	43.65	1.39E−02	9.97E−03	8.10E+10
LS	3Po–3Se	9–3		1.37E−02	1.77E−02	1.45E+11
3s3p–3s5d	3Po–3De	1:1–3:13	41.56	9.51E−02	1.30E−02	1.22E+11
3s3p–3s5d	3Po–3De	3:1–3:13	41.66	2.38E−02	9.80E−03	9.15E+10
3s3p–3s5d	3Po–3De	5:1–3:13	41.91	9.77E−04	6.74E−04	6.18E+09
3s3p–3s5d	3Po–3De	3:1–5:18	41.66	7.15E−02	2.94E−02	1.65E+11
3s3p–3s5d	3Po–3De	5:1–5:18	41.91	1.44E−02	9.93E−03	5.47E+10
3s3p–3s5d	3Po–3De	5:1–7:10	41.90	8.16E−02	5.63E−02	2.21E+11
LS	3Po–3De	9–15		9.62E−02	1.19E−01	2.21E+11
3s3d–3p3d	3De–3Po	3:2–1:2	315.34	5.23E−02	1.63E−01	1.05E+10
3s3d–3p3d	3De–3Po	3:2–3:4	314.99	1.09E−01	3.38E−01	7.30E+09
3s3d–3p3d	3De–3Po	3:2–5:5	328.15	3.56E−02	1.15E−01	1.32E+09
3s3d–3p3d	3De–3Po	5:3–3:4	316.01	2.70E−02	1.40E−01	3.01E+09
3s3d–3p3d	3De–3Po	5:3–5:5	329.25	1.03E−01	5.59E−01	6.34E+09
3s3d–3p3d	3De–3Po	7:1–5:5	331.02	1.27E−02	9.70E−02	1.08E+09
LS	3De–3Po	15–9		8.86E−02	1.41E+00	9.47E+09
3p3d–3s4s	3Po–3Se	1:2–3:4	130.24	3.44E−05	1.47E−05	4.50E+06
3p3d–3s4s	3Po–3Se	3:4–3:4	130.30	2.82E−05	3.63E−05	1.11E+07
3p3d–3s4s	3Po–3Se	5:5–3:4	128.17	1.95E−05	4.11E−05	1.32E+07
LS	3Po–3Se	9–3		2.41E−05	9.21E−05	2.88E+07
3p3d–3s4d	3Po–3De	1:2–3:5	96.58	1.19E−04	3.78E−05	2.83E+07
3p3d–3s4d	3Po–3De	3:4–3:5	96.61	3.99E−05	3.80E−05	2.85E+07
3p3d–3s4d	3Po–3De	5:5–3:5	95.44	1.61E−05	2.53E−05	1.96E+07
3p3d–3s4d	3Po–3De	3:4–5:8	96.55	4.62E−05	4.41E−05	1.98E+07
3p3d–3s4d	3Po–3De	5:5–5:8	95.37	1.82E−05	2.86E−05	1.34E+07
3p3d–3s4d	3Po–3De	5:5–7:3	95.27	1.88E−05	2.95E−05	9.86E+06
LS	3Po–3De	9–15		7.14E−05	2.03E−04	3.10E+07
3p3d–3p4f	3Po–3De	1:2–3:10	70.21	9.48E−01	2.19E−01	4.28E+11
3p3d–3p4f	3Po–3De	3:4–3:10	70.23	3.21E−01	2.23E−01	4.35E+11
3p3d–3p4f	3Po–3De	5:5–3:10	69.61	2.77E−02	3.18E−02	6.37E+10
3p3d–3p4f	3Po–3De	3:4–5:14	70.52	5.61E−01	3.91E−01	4.52E+11
3p3d–3p4f	3Po–3De	5:5–5:14	69.89	2.46E−01	2.83E−01	3.36E+11
3p3d–3p4f	3Po–3De	5:5–7:8	69.95	4.79E−01	5.51E−01	4.66E+11
LS	3Po–3De	9–15		8.17E−01	1.70E+00	6.65E+11
3p3d–3s5s	3Po–3Se	1:2–3:12	64.56	1.94E−04	4.12E−05	1.03E+08
3p3d–3s5s	3Po–3Se	3:4–3:12	64.58	1.52E−04	9.68E−05	2.43E+08
3p3d–3s5s	3Po–3Se	5:5–3:12	64.05	9.02E−05	9.51E−05	2.44E+08
LS	3Po–3Se	9–3		1.22E−04	2.33E−04	5.92E+08
3p3d–3s5d	3Po–3De	1:2–3:13	60.82	3.65E−03	7.31E−04	2.20E+09
3p3d–3s5d	3Po–3De	3:4–3:13	60.83	6.90E−04	4.15E−04	1.24E+09
3p3d–3s5d	3Po–3De	5:5–3:13	60.36	1.69E−05	1.68E−05	5.15E+07
3p3d–3s5d	3Po–3De	3:4–5:18	60.84	2.07E−03	1.25E−03	2.24E+09
3p3d–3s5d	3Po–3De	5:5–5:18	60.37	2.05E−04	2.04E−04	3.75E+08
3p3d–3s5d	3Po–3De	5:5–7:10	60.36	1.36E−03	1.35E−03	1.78E+09
LS	3Po–3De	9–15		2.20E−03	3.97E−03	2.39E+09
3s3p–3s3d	1Po–3De	3:2–3:2	305.94	3.69E−04	1.11E−03	2.63E+07
3s3p–3s3d	1Po–3De	3:2–5:3	304.99	5.11E−04	1.54E−03	2.20E+07
3s3d–3p3d	3De–3Do	3:2–3:3	328.83	3.52E−02	1.14E−01	2.17E+09
3s3d–3p3d	3De–3Do	3:2–5:4	314.61	1.54E−02	4.77E−02	6.21E+08
3s3d–3p3d	3De–3Do	5:3–3:3	329.94	6.10E−02	3.32E−01	6.23E+09
3s3d–3p3d	3De–3Do	5:3–5:4	315.62	7.70E−03	4.00E−02	5.16E+08
3s3d–3p3d	3De–3Do	5:3–7:2	317.39	3.60E−02	1.88E−01	1.70E+09
3s3d–3p3d	3De–3Do	7:1–5:4	317.25	9.09E−02	6.65E−01	8.44E+09
3s3d–3p3d	3De–3Do	7:1–7:2	319.04	1.14E−01	8.36E−01	7.45E+09
LS	3De–3Do	15–15		1.41E−01	2.22E+00	9.16E+09
3s3d–3p3d	3De–1Po	3:2–3:5	252.45	4.40E−04	1.10E−03	4.61E+07
3s3d–3p3d	3De–1Po	5:3–3:5	253.10	7.93E−04	3.30E−03	1.38E+08
3s3d–3s4p	3De–1Po	3:2–3:7	82.56	5.08E−03	4.14E−03	4.97E+09
3s3d–3s4p	3De–1Po	5:3–3:7	82.63	9.06E−03	1.23E−02	1.47E+10
3s3d–3s5p	3De–1Po	3:2–3:15	52.96	1.63E−02	8.53E−03	3.88E+10
3s3d–3s5p	3De–1Po	5:3–3:15	52.99	2.23E−05	1.94E−05	8.83E+07
3s3p–3s4s	1Po–3Se	3:2–3:4	70.83	6.32E−04	4.42E−04	8.40E+08
3p3d–3s4s	3Do–3Se	3:3–3:4	128.07	7.78E−06	9.84E−06	3.16E+06

(*continued on next page*)

Table 2. (*continued*)

C_i–C_k	T_i–T_k	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
3p3d–3s4s	3Do–3Se	5:4–3:4	130.37	2.37E−05	5.08E−05	1.55E+07
LS	3Do–3Se	15–3		9.46E−06	6.06E−05	1.87E+07
3p3d–3s4s	1Po–3Se	3:5–3:4	145.18	2.79E−06	4.00E−06	8.83E+05
3s4s–3s4p	3Se–1Po	3:4–3:7	791.92	5.28E−02	4.13E−01	5.62E+08
3s4s–3s5p	3Se–1Po	3:4–3:15	124.49	1.93E−02	2.37E−02	8.29E+09
3s3p–3s4d	1Po–3De	3:2–3:5	59.54	5.16E−04	3.04E−04	9.71E+08
3s3p–3s4d	1Po–3De	3:2–5:8	59.52	1.30E−03	7.64E−04	1.47E+09
3p3d–3s4d	3Do–3De	3:3–3:5	95.38	7.84E−07	7.39E−07	5.75E+05
3p3d–3s4d	3Do–3De	5:4–3:5	96.65	1.40E−05	2.23E−05	1.67E+07
3p3d–3s4d	3Do–3De	3:3–5:8	95.32	4.16E−05	3.92E−05	1.83E+07
3p3d–3s4d	3Do–3De	5:4–5:8	96.58	6.55E−06	1.04E−05	4.68E+06
3p3d–3s4d	3Do–3De	7:2–5:8	96.42	6.14E−05	1.37E−04	6.17E+07
3p3d–3s4d	3Do–3De	5:4–7:3	96.47	6.65E−05	1.06E−04	3.41E+07
3p3d–3s4d	3Do–3De	7:2–7:3	96.31	1.09E−05	2.43E−05	7.87E+06
LS	3Do–3De	15–15		7.12E−05	3.40E−04	5.09E+07
3p3d–3s4d	1Po–3De	3:5–3:5	104.56	4.54E−06	4.69E−06	2.77E+06
3p3d–3s4d	1Po–3De	3:5–5:8	104.48	5.08E−06	5.24E−06	1.86E+06
3s4p–3s4d	1Po–3De	3:7–3:5	707.51	2.72E−02	1.90E−01	3.62E+08
3s4p–3s4d	1Po–3De	3:7–5:8	704.01	3.59E−02	2.50E−01	2.90E+08
3s4d–3s5p	3De–1Po	3:5–3:15	186.68	1.21E−02	2.23E−02	2.31E+09
3s4d–3s5p	3De–1Po	5:8–3:15	186.92	9.65E−03	2.97E−02	3.07E+09
3s3p–3p4f	1Po–3De	3:2–3:10	48.35	3.06E−07	1.46E−07	8.74E+05
3s3p–3p4f	1Po–3De	3:2–5:14	48.49	9.28E−05	4.45E−05	1.58E+08
3p3d–3p4f	3Do–3De	3:3–3:10	69.58	6.94E−04	4.77E−04	9.56E+08
3p3d–3p4f	3Do–3De	5:4–3:10	70.25	5.85E−04	6.76E−04	1.32E+09
3p3d–3p4f	3Do–3De	3:3–5:14	69.86	8.19E−02	5.65E−02	6.72E+10
3p3d–3p4f	3Do–3De	5:4–5:14	70.54	2.43E−05	2.83E−05	3.26E+07
3p3d–3p4f	3Do–3De	7:2–5:14	70.45	1.65E−02	2.68E−02	3.11E+10
3p3d–3p4f	3Do–3De	5:4–7:8	70.60	2.40E−01	2.79E−01	2.30E+11
3p3d–3p4f	3Do–3De	7:2–7:8	70.51	1.40E−01	2.28E−01	1.88E+11
LS	3Do–3De	15–15		1.70E−01	5.91E−01	2.27E+11
3p3d–3p4f	1Po–3De	3:5–3:10	74.34	1.25E−06	9.15E−07	1.50E+06
3p3d–3p4f	1Po–3De	3:5–5:14	74.66	1.43E−02	1.05E−02	1.03E+10
3s4p–3p4f	1Po–3De	3:7–3:10	188.63	9.77E−05	1.82E−04	1.83E+07
3s4p–3p4f	1Po–3De	3:7–5:14	190.72	1.34E−04	2.53E−04	1.48E+07
3p4f–3s5p	3De–1Po	3:10–3:15	680.76	6.48E−04	4.36E−03	9.33E+06
3p4f–3s5p	3De–1Po	5:14–3:15	654.88	7.10E−05	7.65E−04	1.84E+06
3s3p–3s5s	1Po–3Se	3:2–3:12	45.60	1.06E−04	4.75E−05	3.39E+08
3p3d–3s5s	3Do–3Se	3:3–3:12	64.02	4.16E−05	2.63E−05	6.77E+07
3p3d–3s5s	3Do–3Se	5:4–3:12	64.59	9.83E−05	1.04E−04	2.62E+08
LS	3Do–3Se	15–3		4.11E−05	1.30E−04	3.32E+08
3p3d–3s5s	1Po–3Se	3:5–3:12	68.03	1.24E−06	8.34E−07	1.79E+06
3s4p–3s5s	1Po–3Se	3:7–3:12	152.71	3.42E−02	5.16E−02	9.78E+09
3s5s–3s5p	3Se–1Po	3:12–3:15	4504.55	2.91E−02	1.29E+00	9.56E+06
3s3p–3s5d	1Po–3De	3:2–3:13	43.70	1.86E−04	8.03E−05	6.50E+08
3s3p–3s5d	1Po–3De	3:2–5:18	43.71	1.75E−04	7.54E−05	3.66E+08
3p3d–3s5d	3Do–3De	3:3–3:13	60.34	2.23E−04	1.33E−04	4.08E+08
3p3d–3s5d	3Do–3De	5:4–3:13	60.85	1.72E−05	1.72E−05	5.16E+07
3p3d–3s5d	3Do–3De	3:3–5:18	60.35	5.25E−04	3.13E−04	5.77E+08
3p3d–3s5d	3Do–3De	5:4–5:18	60.85	2.55E−04	2.55E−04	4.58E+08
3p3d–3s5d	3Do–3De	7:2–5:18	60.79	1.61E−08	2.25E−08	4.06E+04
3p3d–3s5d	3Do–3De	5:4–7:10	60.84	1.31E−03	1.31E−03	1.69E+09
3p3d–3s5d	3Do–3De	7:2–7:10	60.77	3.80E−06	5.32E−06	6.86E+06
LS	3Do–3De	15–15		6.79E−04	2.03E−03	1.23E+09
3p3d–3s5d	1Po–3De	3:5–3:13	63.89	4.62E−06	2.92E−06	7.56E+06
3p3d–3s5d	1Po–3De	3:5–5:18	63.90	2.07E−05	1.30E−05	2.02E+07
3s4p–3s5d	1Po–3De	3:7–3:13	133.31	1.63E−02	2.14E−02	6.11E+09
3s4p–3s5d	1Po–3De	3:7–5:18	133.35	2.80E−02	3.68E−02	6.29E+09
3s5p–3s5d	1Po–3De	3:15–3:13	1367.94	4.78E−02	6.45E−01	1.70E+08
3s5p–3s5d	1Po–3De	3:15–5:18	1371.69	9.48E−02	1.28E+00	2.02E+08
$3p^2$–3p3d	3Pe–3Fo	3:1–5:2	274.99	5.00E−04	1.36E−03	2.65E+07
$3p^2$–3p3d	3Pe–3Fo	5:2–5:2	288.65	1.63E−03	7.75E−03	1.30E+08
$3p^2$–3p3d	3Pe–3Fo	5:2–7:1	280.65	1.80E−03	8.32E−03	1.09E+08
LS	3Pe–3Fo	9–21		2.07E−03	1.74E−02	7.35E+07
$3p^2$–3p3d	3Pe–1Do	3:1–5:3	260.47	9.05E−03	2.33E−02	5.34E+08
$3p^2$–3p3d	3Pe–1Do	5:2–5:3	272.70	1.85E−02	8.29E−02	1.66E+09
$3p^2$–3s4f	3Pe–3Fo	3:1–5:8	64.77	2.66E−06	1.70E−06	2.54E+06
$3p^2$–3s4f	3Pe–3Fo	5:2–5:8	65.50	1.32E−06	1.42E−06	2.05E+06
$3p^2$–3s4f	3Pe–3Fo	5:2–7:4	65.50	3.12E−05	3.36E−05	3.46E+07
LS	3Pe–3Fo	9–21		1.90E−05	3.67E−05	1.27E+07
$3p^2$–3s5f	3Pe–3Fo	3:1–5:18	47.35	2.22E−07	1.04E−07	3.96E+05
$3p^2$–3s5f	3Pe–3Fo	5:2–5:18	47.74	9.56E−08	7.52E−08	2.80E+05
$3p^2$–3s5f	3Pe–3Fo	5:2–7:12	47.74	6.33E−06	4.97E−06	1.32E+07
LS	3Pe–3Fo	9–21		3.64E−06	5.15E−06	4.58E+06
3s3d–3p3d	3De–3Fo	3:2–5:2	400.84	1.23E−01	4.86E−01	3.06E+09
3s3d–3p3d	3De–3Fo	5:3–5:2	402.49	1.98E−02	1.31E−01	8.15E+08

Table 2. (*continued*)

C_i–C_k	T_i–T_k	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
3s3d–3p3d	3De–3Fo	5:3–7:1	387.10	1.27E−01	8.06E−01	4.02E+09
3s3d–3p3d	3De–3Fo	7:1–5:2	405.13	2.00E−04	1.87E−03	1.14E+07
3s3d–3p3d	3De–3Fo	7:1–7:1	389.55	2.00E−02	1.80E−01	8.81E+08
3s3d–3p3d	3De–3Fo	7:1–9:1	372.80	1.49E−01	1.28E+00	5.55E+09
LS	3De–3Fo	15–21		1.52E−01	2.88E+00	4.95E+09
3s3d–3p3d	3De–1Do	3:2–5:3	370.72	1.75E−02	6.39E−02	5.08E+08
3s3d–3p3d	3De–1Do	5:3–5:3	372.13	2.33E−03	1.43E−02	1.12E+08
3s3d–3p3d	3De–1Do	7:1–5:3	374.39	4.23E−03	3.65E−02	2.82E+08
3s3d–3s4f	3De–3Fo	3:2–5:8	69.94	8.93E−01	6.17E−01	7.31E+11
3s3d–3s4f	3De–3Fo	5:3–5:8	69.99	9.93E−02	1.14E−01	1.35E+11
3s3d–3s4f	3De–3Fo	5:3–7:4	69.99	7.95E−01	9.16E−01	7.73E+11
3s3d–3s4f	3De–3Fo	7:1–5:8	70.07	2.03E−03	3.28E−03	3.86E+09
3s3d–3s4f	3De–3Fo	7:1–7:4	70.07	7.11E−02	1.15E−01	9.65E+10
3s3d–3s4f	3De–3Fo	7:1–9:2	70.05	8.23E−01	1.33E+00	8.70E+11
LS	3De–3Fo	15–21		8.95E−01	3.10E+00	8.69E+11
3s3d–3s5f	3De–3Fo	3:2–5:18	50.06	1.71E−01	8.44E−02	2.73E+11
3s3d–3s5f	3De–3Fo	5:3–5:18	50.08	1.90E−02	1.56E−02	5.04E+10
3s3d–3s5f	3De–3Fo	5:3–7:12	50.08	1.52E−01	1.25E−01	2.88E+11
3s3d–3s5f	3De–3Fo	7:1–5:18	50.13	3.87E−04	4.48E−04	1.44E+09
3s3d–3s5f	3De–3Fo	7:1–7:12	50.13	1.35E−02	1.56E−02	3.60E+10
3s3d–3s5f	3De–3Fo	7:1–9:5	50.12	1.57E−01	1.81E−01	3.24E+11
LS	3De–3Fo	15–21		1.71E−01	4.22E−01	3.26E+11
3p3d–3s4s	3Fo–3Se	5:2–3:4	119.70	3.62E−09	7.13E−09	2.81E+03
3p3d–3s4s	1Do–3Se	5:3–3:4	122.67	5.75E−07	1.16E−06	4.25E+05
3s4s–3s4f	3Se–3Fo	3:4–5:8	290.01	1.30E−11	3.72E−11	6.18E−01
3s4s–3s5f	3Se–3Fo	3:4–5:18	109.56	2.54E−11	2.75E−11	8.47E+00
3p3d–3s4d	3Fo–3De	5:2–3:5	90.66	2.99E−03	4.47E−03	4.05E+09
3p3d–3s4d	3Fo–3De	5:2–5:8	90.60	5.00E−04	7.45E−04	4.06E+08
3p3d–3s4d	3Fo–3De	7:1–5:8	91.42	2.95E−03	6.21E−03	3.30E+09
3p3d–3s4d	3Fo–3De	5:2–7:3	90.50	9.79E−06	1.46E−05	5.69E+06
3p3d–3s4d	3Fo–3De	7:1–7:3	91.32	3.68E−04	7.74E−04	2.94E+08
3p3d–3s4d	3Fo–3De	9:1–7:3	92.29	3.13E−03	8.57E−03	3.15E+09
LS	3Fo–3De	21–15		3.28E−03	2.08E−02	3.65E+09
3p3d–3s4d	1Do–3De	5:3–3:5	92.35	3.20E−04	4.87E−04	4.18E+08
3p3d–3s4d	1Do–3De	5:3–5:8	92.29	4.92E−05	7.47E−05	3.85E+07
3p3d–3s4d	1Do–3De	5:3–7:3	92.19	1.42E−05	2.15E−05	7.96E+06
3s4d–3s4f	3De–3Fo	3:5–5:8	1295.33	1.38E−01	1.76E+00	3.29E+08
3s4d–3s4f	3De–3Fo	5:8–5:8	1307.23	1.47E−02	3.16E−01	5.74E+07
3s4d–3s4f	3De–3Fo	5:8–7:4	1305.35	1.19E−01	2.56E+00	3.33E+08
3s4d–3s4f	3De–3Fo	7:3–5:8	1327.41	3.03E−04	9.27E−03	1.61E+06
3s4d–3s4f	3De–3Fo	7:3–7:4	1325.48	1.07E−02	3.26E−01	4.06E+07
3s4d–3s4f	3De–3Fo	7:3–9:2	1321.06	1.25E−01	3.81E+00	3.72E+08
LS	3De–3Fo	15–21		1.36E−01	8.78E+00	3.76E+08
3s4d–3s5f	3De–3Fo	3:5–5:18	155.02	6.53E−01	9.99E−01	1.09E+11
3s4d–3s5f	3De–3Fo	5:8–5:18	155.19	7.08E−02	1.81E−01	1.96E+10
3s4d–3s5f	3De–3Fo	5:8–7:12	155.19	5.70E−01	1.46E+00	1.13E+11
3s4d–3s5f	3De–3Fo	7:3–5:18	155.47	1.50E−03	5.36E−03	5.78E+08
3s4d–3s5f	3De–3Fo	7:3–7:12	155.47	5.24E−02	1.88E−01	1.45E+10
3s4d–3s5f	3De–3Fo	7:3–9:5	155.42	6.07E−01	2.18E+00	1.30E+11
LS	3De–3Fo	15–21		6.53E−01	5.01E+00	1.28E+11
3p3d–3p4f	3Fo–3De	5:2–3:10	67.03	3.98E−03	4.39E−03	9.84E+09
3p3d–3p4f	3Fo–3De	5:2–5:14	67.29	1.69E−05	1.87E−05	2.48E+07
3p3d–3p4f	3Fo–3De	7:1–5:14	67.74	6.96E−03	1.09E−02	1.42E+10
3p3d–3p4f	3Fo–3De	5:2–7:8	67.35	4.96E−04	5.50E−04	5.21E+08
3p3d–3p4f	3Fo–3De	7:1–7:8	67.80	1.39E−03	2.18E−03	2.02E+09
3p3d–3p4f	3Fo–3De	9:1–7:8	68.34	9.12E−03	1.85E−02	1.67E+10
LS	3Fo–3De	21–15		7.76E−03	3.65E−02	1.56E+10
3p3d–3p4f	1Do–3De	5:3–3:10	67.95	9.44E−04	1.06E−03	2.27E+09
3p3d–3p4f	1Do–3De	5:3–5:14	68.22	8.25E−03	9.26E−03	1.18E+10
3p3d–3p4f	1Do–3De	5:3–7:8	68.28	2.72E−03	3.06E−03	2.78E+09
3s4f–3p4f	3Fo–3De	5:8–3:10	320.94	9.22E−02	4.87E−01	9.95E+09
3s4f–3p4f	3Fo–3De	5:8–5:14	327.03	5.36E−02	2.89E−01	3.34E+09
3s4f–3p4f	3Fo–3De	7:4–5:14	327.15	6.62E−02	4.99E−01	5.78E+09
3s4f–3p4f	3Fo–3De	5:8–7:8	328.42	5.22E−03	2.82E−02	2.31E+08
3s4f–3p4f	3Fo–3De	7:4–7:8	328.54	4.90E−02	3.71E−01	3.03E+09
3s4f–3p4f	3Fo–3De	9:2–7:8	328.81	6.96E−02	6.79E−01	5.52E+09
LS	3Fo–3De	21–15		1.04E−01	2.35E+00	9.11E+09
3p4f–3s5f	3De–3Fo	3:10–5:18	390.17	6.40E−03	2.47E−02	1.68E+08
3p4f–3s5f	3De–3Fo	5:14–5:18	381.53	4.88E−04	3.06E−03	2.23E+07
3p4f–3s5f	3De–3Fo	5:14–7:12	381.53	5.14E−03	3.23E−02	1.68E+08
3p4f–3s5f	3De–3Fo	7:8–5:18	379.66	2.43E−06	2.12E−05	1.57E+05
3p4f–3s5f	3De–3Fo	7:8–7:12	379.66	2.98E−04	2.61E−03	1.38E+07
3p4f–3s5f	3De–3Fo	7:8–9:5	379.37	4.75E−03	4.15E−02	1.71E+08
LS	3De–3Fo	15–21		5.51E−03	1.04E−01	1.79E+08
3p3d–3s5s	3Fo–3Se	5:2–3:12	61.86	1.68E−07	1.71E−07	4.88E+05
3p3d–3s5s	1Do–3Se	5:3–3:12	62.65	4.76E−06	4.90E−06	1.35E+07

(*continued on next page*)

Table 2. (*continued*)

C_i–C_k	T_i–T_k	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
3s4f–3s5s	3Fo–3Se	5:8–3:12	229.21	1.27E−10	4.81E−10	2.70E+01
3s5s–3s5f	3Se–3Fo	3:12–5:18	759.86	5.09E−13	3.82E−12	3.53E−03
3p3d–3s5d	3Fo–3De	5:2–3:13	58.42	1.59E−05	1.53E−05	5.19E+07
3p3d–3s5d	3Fo–3De	5:2–5:18	58.42	1.92E−05	1.85E−05	3.76E+07
3p3d–3s5d	3Fo–3De	7:1–5:18	58.76	2.52E−05	3.41E−05	6.81E+07
3p3d–3s5d	3Fo–3De	5:2–7:10	58.41	2.08E−06	2.00E−06	2.90E+06
3p3d–3s5d	3Fo–3De	7:1–7:10	58.75	1.62E−06	2.19E−06	3.12E+06
3p3d–3s5d	3Fo–3De	9:1–7:10	59.15	3.21E−05	5.62E−05	7.86E+07
LS	3Fo–3De	21–15		3.15E−05	1.28E−04	8.52E+07
3p3d–3s5d	1Do–3De	5:3–3:13	59.12	7.80E−06	7.59E−06	2.48E+07
3p3d–3s5d	1Do–3De	5:3–5:18	59.12	7.80E−05	7.59E−05	1.49E+08
3p3d–3s5d	1Do–3De	5:3–7:10	59.11	6.69E−05	6.51E−05	9.13E+07
3s4f–3s5d	3Fo–3De	5:8–3:13	188.12	1.65E−02	5.10E−02	5.17E+09
3s4f–3s5d	3Fo–3De	5:8–5:18	188.19	2.96E−03	9.17E−03	5.57E+08
3s4f–3s5d	3Fo–3De	7:4–5:18	188.23	1.73E−02	7.49E−02	4.55E+09
3s4f–3s5d	3Fo–3De	5:8–7:10	188.05	8.48E−05	2.63E−04	1.14E+07
3s4f–3s5d	3Fo–3De	7:4–7:10	188.08	2.15E−03	9.32E−03	4.05E+08
3s4f–3s5d	3Fo–3De	9:2–7:10	188.17	1.97E−02	1.10E−01	4.78E+09
LS	3Fo–3De	21–15		1.96E−02	2.55E−01	5.17E+09
3s5d–3s5f	3De–3Fo	3:13–5:18	2754.82	2.56E−01	6.96E+00	1.35E+08
3s5d–3s5f	3De–3Fo	5:18–5:18	2739.75	2.81E−02	1.27E+00	2.50E+07
3s5d–3s5f	3De–3Fo	5:18–7:12	2739.75	2.26E−01	1.02E+01	1.43E+08
3s5d–3s5f	3De–3Fo	7:10–5:18	2770.15	5.76E−04	3.68E−02	7.01E+05
3s5d–3s5f	3De–3Fo	7:10–7:12	2770.15	2.02E−02	1.29E+00	1.75E+07
3s5d–3s5f	3De–3Fo	7:10–9:5	2754.82	2.35E−01	1.49E+01	1.61E+08
LS	3De–3Fo	15–21		2.55E−01	3.47E+01	1.61E+08
3s3p–$3p^2$	3Po–1De	3:1–5:1	312.56	2.84E−02	8.76E−02	1.16E+09
3s3p–$3p^2$	3Po–1De	5:1–5:1	327.04	3.29E−02	1.77E−01	2.05E+09
3s3p–3s3d	3Po–1De	3:1–5:4	191.41	3.15E−03	5.95E−03	3.44E+08
3s3p–3s3d	3Po–1De	5:1–5:4	196.75	8.43E−05	2.73E−04	1.45E+07
3s3p–$3d^2$	3Po–3Fe	3:1–5:5	88.44	8.37E−08	7.31E−08	4.28E+04
3s3p–$3d^2$	3Po–3Fe	5:1–5:5	89.56	2.03E−08	3.00E−08	1.69E+04
3s3p–$3d^2$	3Po–3Fe	5:1–7:2	89.43	2.64E−07	3.88E−07	1.57E+05
LS	3Po–3Fe	9–21		1.86E−07	4.91E−07	6.68E+04
3s3p–$3d^2$	3Po–1De	3:1–5:6	85.99	3.38E−05	2.87E−05	1.83E+07
3s3p–$3d^2$	3Po–1De	5:1–5:6	87.05	3.12E−06	4.47E−06	2.75E+06
3s3p–$3d^2$	3Po–3Pe	3:1–5:7	85.61	3.49E−05	2.95E−05	1.91E+07
3s3p–$3d^2$	3Po–3Pe	5:1–5:7	86.66	7.88E−05	1.12E−04	7.00E+07
LS	3Po–3Pe	9–9		5.54E−05	1.42E−04	4.98E+07
3s3p–3s4d	3Po–1De	3:1–5:9	55.69	3.11E−03	1.71E−03	4.02E+09
3s3p–3s4d	3Po–1De	5:1–5:9	56.13	1.38E−03	1.28E−03	2.92E+09
3s3p–3p4f	3Po–3Fe	3:1–5:13	46.50	7.38E−05	3.39E−05	1.37E+08
3s3p–3p4f	3Po–3Fe	5:1–5:13	46.81	1.86E−05	1.44E−05	5.68E+07
LS	3Po–3Fe	9–21		3.49E−05	4.83E−05	4.59E+07
3s3p–3p4f	3Po–1De	3:1–5:15	45.53	1.32E−06	5.92E−07	2.54E+06
3s3p–3p4f	3Po–1De	5:1–5:15	45.83	1.43E−06	1.08E−06	4.55E+06
3s3p–$3p^2$	1Po–1De	3:2–5:1	481.49	8.89E−02	4.23E−01	1.53E+09
3s3p–3s3d	1Po–1De	3:2–5:4	243.79	6.07E−01	1.46E+00	4.09E+10
3s3p–$3d^2$	1Po–3Fe	3:2–5:5	98.19	1.15E−07	1.11E−07	4.76E+04
3s3p–$3d^2$	1Po–1De	3:2–5:6	95.18	1.09E−03	1.02E−03	4.81E+08
3s3p–$3d^2$	1Po–3Pe	3:2–5:7	94.71	1.48E−04	1.39E−04	6.61E+07
3s3p–3s4d	1Po–1De	3:2–5:9	59.40	2.12E−01	1.24E−01	2.40E+11
3s3p–3p4f	1Po–3Fe	3:2–5:13	49.06	2.93E−04	1.42E−04	4.87E+08
3s3p–3p4f	1Po–1De	3:2–5:15	47.98	7.81E−03	3.70E−03	1.36E+10
$3p^2$–3p3d	1De–3Do	5:1–3:3	236.25	1.24E−04	4.83E−04	2.48E+07
$3p^2$–3p3d	1De–3Do	5:1–5:4	228.82	1.63E−03	6.12E−03	2.07E+08
$3p^2$–3p3d	1De–3Do	5:1–7:2	229.75	8.16E−02	3.09E−01	7.37E+09
3s3d–3p3d	1De–3Do	5:4–3:3	452.94	7.58E−04	5.65E−03	4.11E+07
3s3d–3p3d	1De–3Do	5:4–5:4	426.38	1.24E−03	8.68E−03	4.54E+07
3s3d–3p3d	1De–3Do	5:4–7:2	429.62	8.31E−04	5.87E−03	2.14E+07
3p3d–$3d^2$	3Do–3Fe	3:3–5:5	258.09	2.39E−01	6.09E−01	1.43E+10
3p3d–$3d^2$	3Do–3Fe	5:4–5:5	267.59	9.92E−03	4.37E−02	9.24E+08
3p3d–$3d^2$	3Do–3Fe	7:2–5:5	266.33	2.19E−04	1.35E−03	2.89E+07
3p3d–$3d^2$	3Do–3Fe	5:4–7:2	266.37	1.26E−01	5.50E−01	8.43E+09
3p3d–$3d^2$	3Do–3Fe	7:2–7:2	265.13	1.47E−02	8.97E−02	1.39E+09
3p3d–$3d^2$	3Do–3Fe	7:2–9:1	263.71	2.86E−01	1.74E+00	2.13E+10
LS	3Do–3Fe	15–21		2.34E−01	3.03E+00	1.61E+10
3p3d–$3d^2$	3Do–1De	3:3–5:6	238.25	4.28E−03	1.01E−02	3.02E+08
3p3d–$3d^2$	3Do–1De	5:4–5:6	246.32	5.66E−05	2.30E−04	6.23E+06
3p3d–$3d^2$	3Do–1De	7:2–5:6	245.25	8.53E−03	4.82E−02	1.32E+09
3p3d–$3d^2$	3Do–3Pe	3:3–5:7	235.35	1.31E−02	3.06E−02	9.50E+08
3p3d–$3d^2$	3Do–3Pe	5:4–5:7	243.22	6.95E−02	2.78E−01	7.84E+09
3p3d–$3d^2$	3Do–3Pe	7:2–5:7	242.18	5.76E−02	3.21E−01	9.17E+09
LS	3Do–3Pe	15–9		5.27E−02	6.30E−01	9.99E+09
3p3d–3s4d	3Do–1De	3:3–5:9	95.02	5.58E−06	5.24E−06	2.48E+06
3p3d–3s4d	3Do–1De	5:4–5:9	96.28	8.71E−07	1.38E−06	6.26E+05

Table 2. (*continued*)

C_i–C_k	T_i–T_k	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
3p3d–3s4d	3Do–1De	7:2–5:9	96.12	4.25E−05	9.42E−05	4.30E+07
3p3d–3p4f	3Do–3Fe	3:3–5:13	71.06	7.99E−01	5.61E−01	6.33E+11
3p3d–3p4f	3Do–3Fe	5:4–5:13	71.76	4.71E−02	5.57E−02	6.10E+10
3p3d–3p4f	3Do–3Fe	7:2–5:13	71.67	1.95E−04	3.22E−04	3.55E+08
3p3d–3p4f	3Do–3Fe	7:2–9:4	71.06	5.41E−01	8.87E−01	5.56E+11
LS	3Do–3Fe	15–21		4.28E−01	1.50E+00	4.03E+11
3p3d–3p4f	3Do–1De	3:3–5:15	68.82	1.89E−02	1.29E−02	1.60E+10
3p3d–3p4f	3Do–1De	5:4–5:15	69.47	1.04E−02	1.19E−02	1.44E+10
3p3d–3p4f	3Do–1De	7:2–5:15	69.39	2.46E−04	3.93E−04	4.76E+08
$3p^2$–3p3d	1De–3Po	5:1–3:4	229.02	7.43E−03	2.80E−02	1.58E+09
$3p^2$–3p3d	1De–3Po	5:1–5:5	235.90	2.27E−02	8.81E−02	2.72E+09
3s3d–3p3d	1De–3Po	5:4–3:4	427.08	1.15E−05	8.07E−05	7.00E+05
3s3d–3p3d	1De–3Po	5:4–5:5	451.64	1.24E−04	9.19E−04	4.04E+06
3p3d–$3d^2$	3Po–3Fe	3:4–5:5	267.31	6.67E−02	1.76E−01	3.74E+09
3p3d–$3d^2$	3Po–3Fe	5:5–5:5	258.52	1.47E−02	6.24E−02	1.46E+09
3p3d–$3d^2$	3Po–3Fe	5:5–7:2	257.38	1.53E−01	6.48E−01	1.10E+10
LS	3Po–3Fe	9–21		1.15E−01	8.86E−01	4.91E+09
3p3d–$3d^2$	3Po–1De	3:4–5:6	246.09	1.40E−02	3.41E−02	9.26E+08
3p3d–$3d^2$	3Po–1De	5:5–5:6	238.61	8.63E−03	3.39E−02	1.01E+09
3p3d–$3d^2$	3Po–3Pe	3:4–5:7	242.99	9.59E−02	2.30E−01	6.50E+09
3p3d–$3d^2$	3Po–3Pe	5:5–5:7	235.70	1.68E−01	6.53E−01	2.02E+10
LS	3Po–3Pe	9–9		1.25E−01	8.83E−01	1.48E+10
3p3d–3s4d	3Po–1De	3:4–5:9	96.24	2.80E−07	2.66E−07	1.21E+05
3p3d–3s4d	3Po–1De	5:5–5:9	95.08	1.60E−06	2.51E−06	1.18E+06
3p3d–3p4f	3Po–3Fe	3:4–5:13	71.74	4.46E−02	3.16E−02	3.47E+10
3p3d–3p4f	3Po–3Fe	5:5–5:13	71.09	9.13E−03	1.07E−02	1.21E+10
LS	3Po–3Fe	9–21		1.99E−02	4.23E−02	1.11E+10
3p3d–3p4f	3Po–1De	3:4–5:15	69.46	5.91E−03	4.06E−03	4.91E+09
3p3d–3p4f	3Po–1De	5:5–5:15	68.85	8.15E−03	9.24E−03	1.15E+10
$3p^2$–3p3d	1De–1Po	5:1–3:5	194.06	1.21E−03	3.86E−03	3.57E+08
3s3d–3p3d	1De–1Po	5:4–3:5	319.70	1.11E−01	5.84E−01	1.21E+10
3p3d–$3d^2$	1Po–3Fe	3:5–5:5	338.47	6.16E−04	2.06E−03	2.15E+07
3p3d–$3d^2$	1Po–1De	3:5–5:6	305.15	1.64E−01	4.95E−01	7.06E+09
3p3d–$3d^2$	1Po–3Pe	3:5–5:7	300.40	2.21E−02	6.55E−02	9.79E+08
3p3d–3s4d	1Po–1De	3:5–5:9	104.12	3.78E−04	3.88E−04	1.39E+08
3p3d–3p4f	1Po–3Fe	3:5–5:13	76.03	9.75E−03	7.32E−03	6.75E+09
3p3d–3p4f	1Po–1De	3:5–5:15	73.47	8.58E−01	6.23E−01	6.36E+11
$3p^2$–3s4p	1De–1Po	5:1–3:7	75.17	1.74E−02	2.15E−02	3.42E+10
3s3d–3s4p	1De–1Po	5:4–3:7	88.66	1.25E−02	1.82E−02	1.76E+10
$3d^2$–3s4p	3Fe–1Po	5:5–3:7	192.44	1.78E−07	5.64E−07	5.35E+04
$3d^2$–3s4p	1De–1Po	5:6–3:7	205.18	3.84E−05	1.30E−04	1.02E+07
$3d^2$–3s4p	3Pe–1Po	5:7–3:7	207.38	5.39E−06	1.84E−05	1.39E+06
3s4p–3s4d	1Po–1De	3:7–5:9	688.22	3.22E−01	2.19E+00	2.72E+09
3s4p–3p4f	1Po–3Fe	3:7–5:13	199.95	3.26E−07	6.44E−07	3.27E+04
3s4p–3p4f	1Po–1De	3:7–5:15	183.14	4.39E−04	7.94E−04	5.24E+07
$3p^2$–3s5p	1De–1Po	5:1–3:15	49.82	1.95E−04	1.60E−04	8.75E+08
3s3d–3s5p	1De–1Po	5:4–3:15	55.40	1.43E−04	1.31E−04	5.19E+08
$3d^2$–3s5p	3Fe–1Po	5:5–3:15	83.57	7.85E−03	1.08E−02	1.25E+10
$3d^2$–3s5p	1De–1Po	5:6–3:15	85.88	2.14E−03	3.03E−03	3.23E+09
$3d^2$–3s5p	3Pe–1Po	5:7–3:15	86.26	1.08E−05	1.53E−05	1.61E+07
3s4d–3s5p	1De–1Po	5:9–3:15	188.07	5.18E−02	1.60E−01	1.63E+10
3p4f–3s5p	3Fe–1Po	5:13–3:15	565.30	9.86E−05	9.18E−04	3.43E+06
3p4f–3s5p	1De–1Po	5:15–3:15	763.40	1.52E−03	1.91E−02	2.90E+07
$3p^2$–3p3d	1De–3Fo	5:1–5:2	271.26	2.16E−02	9.66E−02	1.96E+09
$3p^2$–3p3d	1De–3Fo	5:1–7:1	264.18	2.16E−03	9.37E−03	1.47E+08
$3p^2$–3p3d	1De–1Do	5:1–5:3	257.12	1.42E−01	6.01E−01	1.43E+10
$3p^2$–3s4f	1De–3Fo	5:1–5:8	64.56	4.75E−08	5.05E−08	7.60E+04
$3p^2$–3s4f	1De–3Fo	5:1–7:4	64.56	2.84E−05	3.02E−05	3.24E+07
$3p^2$–3s5f	1De–3Fo	5:1–5:18	47.24	8.95E−07	6.96E−07	2.67E+06
$3p^2$–3s5f	1De–3Fo	5:1–7:12	47.24	3.68E−05	2.86E−05	7.86E+07
3s3d–3p3d	1De–3Fo	5:4–5:2	601.85	3.91E−03	3.87E−02	7.20E+07
3s3d–3p3d	1De–3Fo	5:4–7:1	568.09	7.76E−04	7.26E−03	1.15E+07
3s3d–3p3d	1De–1Do	5:4–5:3	536.42	3.15E−02	2.78E−01	7.31E+08
3s3d–3s4f	1De–3Fo	5:4–5:8	74.27	1.81E−05	2.22E−05	2.19E+07
3s3d–3s4f	1De–3Fo	5:4–7:4	74.26	1.23E−05	1.51E−05	1.06E+07
3s3d–3s5f	1De–3Fo	5:4–5:18	52.24	4.25E−06	3.66E−06	1.04E+07
3s3d–3s5f	1De–3Fo	5:4–7:12	52.24	1.25E−08	1.07E−08	2.17E+04
3p3d–$3d^2$	3Fo–3Fe	5:2–5:5	226.20	1.17E−01	4.37E−01	1.53E+10
3p3d–$3d^2$	3Fo–3Fe	7:1–5:5	231.37	1.08E−02	5.75E−02	1.88E+09
3p3d–$3d^2$	3Fo–3Fe	5:2–7:2	225.33	6.89E−03	2.56E−02	6.47E+08
3p3d–$3d^2$	3Fo–3Fe	7:1–7:2	230.46	1.22E−01	6.46E−01	1.53E+10
3p3d–$3d^2$	3Fo–3Fe	9:1–7:2	236.75	8.11E−03	5.69E−02	1.24E+09
3p3d–$3d^2$	3Fo–3Fe	7:1–9:1	229.39	2.10E−03	1.11E−02	2.07E+08
3p3d–$3d^2$	3Fo–3Fe	9:1–9:1	235.63	1.22E−01	8.54E−01	1.47E+10
LS	3Fo–3Fe	21–21		1.30E−01	2.09E+00	1.61E+10
3p3d–$3d^2$	1Do–3Fe	5:3–7:2	236.12	8.76E−05	3.40E−04	7.48E+06

(*continued on next page*)

Table 2. (*continued*)

C_i–C_k	T_i–T_k	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
$3d^2$–3s4f	3Fe–3Fo	5:5–5:8	135.47	7.24E−05	1.61E−04	2.63E+07
$3d^2$–3s4f	3Fe–3Fo	5:5–7:4	135.45	9.59E−06	2.14E−05	2.49E+06
$3d^2$–3s4f	3Fe–3Fo	7:2–5:8	135.78	6.04E−06	1.89E−05	3.06E+06
$3d^2$–3s4f	3Fe–3Fo	7:2–7:4	135.76	6.75E−05	2.11E−04	2.44E+07
$3d^2$–3s4f	3Fe–3Fo	7:2–9:2	135.71	7.05E−06	2.21E−05	1.99E+06
$3d^2$–3s4f	3Fe–3Fo	9:1–7:4	136.13	4.58E−06	1.85E−05	2.12E+06
$3d^2$–3s4f	3Fe–3Fo	9:1–9:2	136.09	7.44E−05	3.00E−04	2.68E+07
LS	3Fe–3Fo	21–21		8.02E−05	7.53E−04	2.90E+07
$3d^2$–3s5f	3Fe–3Fo	5:5–5:18	76.57	2.90E−04	3.66E−04	3.30E+08
$3d^2$–3s5f	3Fe–3Fo	5:5–7:12	76.57	3.97E−05	5.00E−05	3.22E+07
$3d^2$–3s5f	3Fe–3Fo	7:2–5:18	76.67	2.57E−05	4.55E−05	4.09E+07
$3d^2$–3s5f	3Fe–3Fo	7:2–7:12	76.67	2.72E−04	4.80E−04	3.08E+08
$3d^2$–3s5f	3Fe–3Fo	7:2–9:5	76.65	2.79E−05	4.93E−05	2.47E+07
$3d^2$–3s5f	3Fe–3Fo	9:1–7:12	76.78	2.02E−05	4.59E−05	2.93E+07
$3d^2$–3s5f	3Fe–3Fo	9:1–9:5	76.77	3.01E−04	6.84E−04	3.40E+08
LS	3Fe–3Fo	21–21		3.25E−04	1.72E−03	3.69E+08
3p3d–$3d^2$	3Fo–1De	5:2–5:6	210.81	2.44E−02	8.48E−02	3.67E+09
3p3d–$3d^2$	3Fo–1De	7:1–5:6	215.30	5.86E−04	2.91E−03	1.18E+08
3p3d–$3d^2$	1Do–1De	5:3–5:6	220.22	2.03E−01	7.36E−01	2.79E+10
$3d^2$–3s4f	1De–3Fo	5:6–5:8	141.66	3.51E−08	8.19E−08	1.17E+04
$3d^2$–3s4f	1De–3Fo	5:6–7:4	141.64	8.05E−08	1.88E−07	1.91E+04
$3d^2$–3s5f	1De–3Fo	5:6–5:18	78.51	4.00E−07	5.17E−07	4.33E+05
$3d^2$–3s5f	1De–3Fo	5:6–7:12	78.51	2.67E−06	3.45E−06	2.07E+06
3p3d–$3d^2$	3Fo–3Pe	5:2–5:7	208.54	6.55E−04	2.25E−03	1.00E+08
3p3d–$3d^2$	3Fo–3Pe	7:1–5:7	212.92	4.69E−04	2.30E−03	9.66E+07
LS	3Fo–3Pe	21–9		3.12E−04	4.55E−03	1.09E+08
3p3d–$3d^2$	1Do–3Pe	5:3–5:7	217.74	5.24E−03	1.88E−02	7.37E+08
$3d^2$–3s4f	3Pe–3Fo	5:7–5:8	142.71	1.24E−08	2.91E−08	4.05E+03
$3d^2$–3s4f	3Pe–3Fo	5:7–7:4	142.68	1.20E−08	2.81E−08	2.80E+03
LS	3Pe–3Fo	9–21		1.36E−08	5.72E−08	1.91E+03
$3d^2$–3s5f	3Pe–3Fo	5:7–5:18	78.83	3.40E−08	4.41E−08	3.65E+04
$3d^2$–3s5f	3Pe–3Fo	5:7–7:12	78.83	3.44E−07	4.46E−07	2.64E+05
LS	3Pe–3Fo	9–21		2.10E−07	4.90E−07	9.68E+04
3p3d–3s4d	3Fo–1De	5:2–5:9	90.33	1.74E−05	2.59E−05	1.42E+07
3p3d–3s4d	3Fo–1De	7:1–5:9	91.14	2.26E−04	4.75E−04	2.54E+08
3p3d–3s4d	1Do–1De	5:3–5:9	92.02	1.56E−06	2.36E−06	1.23E+06
3s4d–3s4f	1De–3Fo	5:9–5:8	1365.40	4.34E−04	9.76E−03	1.55E+06
3s4d–3s4f	1De–3Fo	5:9–7:4	1363.36	2.96E−03	6.65E−02	7.60E+06
3s4d–3s5f	1De–3Fo	5:9–5:18	155.98	2.14E−03	5.49E−03	5.86E+08
3s4d–3s5f	1De–3Fo	5:9–7:12	155.98	1.33E−02	3.42E−02	2.61E+09
3p3d–3p4f	3Fo–3Fe	5:2–5:13	68.41	6.06E−02	6.83E−02	8.64E+10
3p3d–3p4f	3Fo–3Fe	7:1–5:13	68.87	2.68E−03	4.25E−03	5.27E+09
3p3d–3p4f	3Fo–3Fe	7:1–9:4	68.31	1.38E−01	2.16E−01	1.53E+11
3p3d–3p4f	3Fo–3Fe	9:1–9:4	68.85	1.10E−01	2.25E−01	1.55E+11
LS	3Fo–3Fe	21–21		1.08E−01	5.14E−01	1.54E+11
3p3d–3p4f	1Do–3Fe	5:3–5:13	69.37	7.15E−05	8.16E−05	9.91E+07
3s4f–3p4f	3Fo–3Fe	5:8–5:13	355.13	8.28E−02	4.84E−01	4.38E+09
3s4f–3p4f	3Fo–3Fe	7:4–5:13	355.27	3.18E−02	2.60E−01	2.35E+09
3s4f–3p4f	3Fo–3Fe	7:4–9:4	340.75	6.05E−02	4.75E−01	2.70E+09
3s4f–3p4f	3Fo–3Fe	9:2–9:4	341.04	6.66E−02	6.73E−01	3.82E+09
LS	3Fo–3Fe	21–21		7.90E−02	1.89E+00	4.39E+09
3p4f–3s5f	3Fe–3Fo	5:13–5:18	349.29	2.38E−04	1.37E−03	1.30E+07
3p4f–3s5f	3Fe–3Fo	5:13–7:12	349.29	3.29E−04	1.89E−03	1.29E+07
3p4f–3s5f	3Fe–3Fo	9:4–7:12	364.56	4.71E−04	5.08E−03	3.04E+07
3p4f–3s5f	3Fe–3Fo	9:4–9:5	364.29	4.53E−06	4.88E−05	2.27E+05
LS	3Fe–3Fo	21–21		3.39E−04	8.39E−03	1.76E+07
3p3d–3p4f	3Fo–1De	5:2–5:15	66.32	3.74E−03	4.08E−03	5.67E+09
3p3d–3p4f	3Fo–1De	7:1–5:15	66.76	4.28E−05	6.58E−05	8.96E+07
3p3d–3p4f	1Do–1De	5:3–5:15	67.23	8.08E−02	8.94E−02	1.19E+11
3s4f–3p4f	3Fo–1De	5:8–5:15	305.35	6.45E−04	3.24E−03	4.61E+07
3s4f–3p4f	3Fo–1De	7:4–5:15	305.46	6.88E−03	4.84E−02	6.88E+08
3p4f–3s5f	1De–3Fo	5:15–5:18	415.98	4.65E−05	3.19E−04	1.79E+06
3p4f–3s5f	1De–3Fo	5:15–7:12	415.98	1.66E−04	1.14E−03	4.57E+06
$3p^2$–3p3d	1De–1Fo	5:1–7:3	198.84	1.72E−01	5.62E−01	2.07E+10
$3p^2$–3s4f	1De–1Fo	5:1–7:5	63.96	1.64E−01	1.72E−01	1.91E+11
$3p^2$–3s5f!$3p5d^3$	1De–1Fo	5:1–7:14	44.98	4.51E−07	3.34E−07	1.06E+06
$3p^2$–3s6f	1De–1Fo	5:1–7:25	39.50	1.88E−05	1.22E−05	5.74E+07
$3p^2$–3p3d	3Pe–1Fo	5:2–7:3	208.03	4.96E−02	1.70E−01	5.46E+09
$3p^2$–3s4f	3Pe–1Fo	5:2–7:5	64.88	4.08E−02	4.36E−02	4.62E+10
$3p^2$–3s5f!$3p5d^3$	3Pe–1Fo	5:2–7:14	45.44	3.10E−06	2.32E−06	7.15E+06
$3p^2$–3s6f	3Pe–1Fo	5:2–7:25	39.85	6.70E−07	4.39E−07	2.01E+06
3s3d–3p3d	3De–1Fo	5:3–7:3	261.29	3.79E−04	1.63E−03	2.64E+07
3s3d–3p3d	3De–1Fo	7:1–7:3	262.40	1.40E−03	8.49E−03	1.36E+08
3s3d–3s4f	3De–1Fo	5:3–7:5	69.28	5.02E−07	5.73E−07	4.99E+05
3s3d–3s4f	3De–1Fo	7:1–7:5	69.36	5.17E−06	8.27E−06	7.17E+06
3s3d–3s5f!$3p5d^3$	3De–1Fo	5:3–7:14	47.55	6.72E−05	5.26E−05	1.42E+08

Table 2. (*continued*)

C_i–C_k	T_i–T_k	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
3s3d–3s5f!3p5d^3	3De–1Fo	7:1–7:14	47.59	2.22E−07	2.44E−07	6.55E+05
3s3d–3s6f	3De–1Fo	5:3–7:25	41.46	5.50E−04	3.75E−04	1.52E+09
3s3d–3s6f	3De–1Fo	7:1–7:25	41.49	4.69E−05	4.48E−05	1.82E+08
3s3d–3p3d	1De–1Fo	5:4–7:3	332.87	3.90E−01	2.14E+00	1.68E+10
3s3d–3s4f	1De–1Fo	5:4–7:5	73.47	6.89E−01	8.33E−01	6.08E+11
3s3d–3s5f!3p5d^3	1De–1Fo	5:4–7:14	49.49	5.74E−06	4.68E−06	1.12E+07
3s3d–3s6f	1De–1Fo	5:4–7:25	42.93	8.52E−04	6.02E−04	2.20E+09
3p3d–3d^2	1Fo–3Fe	7:3–5:5	324.86	1.93E−04	1.45E−03	1.71E+07
3p3d–3d^2	1Fo–3Fe	7:3–7:2	323.08	5.48E−04	4.08E−03	3.50E+07
3p3d–3d^2	1Fo–3Fe	7:3–9:1	320.98	2.51E−04	1.86E−03	1.26E+07
3d^2–3s4f	3Fe–1Fo	5:5–7:5	132.83	7.82E−07	1.71E−06	2.11E+05
3d^2–3s4f	3Fe–1Fo	7:2–7:5	133.13	1.41E−07	4.32E−07	5.30E+04
3d^2–3s4f	3Fe–1Fo	9:1–7:5	133.49	1.83E−08	7.24E−08	8.81E+03
3d^2–3s5f!3p5d^3	3Fe–1Fo	5:5–7:14	70.80	6.29E−02	7.33E−02	5.98E+10
3d^2–3s5f!3p5d^3	3Fe–1Fo	7:2–7:14	70.89	3.19E−01	5.20E−01	4.23E+11
3d^2–3s5f!3p5d^3	3Fe–1Fo	9:1–7:14	70.99	2.24E−02	4.72E−02	3.82E+10
3d^2–3s6f	3Fe–1Fo	5:5–7:25	58.10	7.77E−05	7.43E−05	1.10E+08
3d^2–3s6f	3Fe–1Fo	7:2–7:25	58.16	1.26E−04	1.68E−04	2.48E+08
3d^2–3s6f	3Fe–1Fo	9:1–7:25	58.23	1.02E−05	1.76E−05	2.59E+07
3p3d–3d^2	1Fo–1De	7:3–5:6	294.04	2.47E−02	1.67E−01	2.66E+09
3d^2–3s4f	1De–1Fo	5:6–7:5	138.78	1.97E−04	4.49E−04	4.86E+07
3d^2–3s5f!3p5d^3	1De–1Fo	5:6–7:14	72.46	1.20E−03	1.43E−03	1.09E+09
3d^2–3s6f	1De–1Fo	5:6–7:25	59.21	2.64E−03	2.57E−03	3.58E+09
3p3d–3d^2	1Fo–3Pe	7:3–5:7	289.63	5.18E−03	3.46E−02	5.76E+08
3d^2–3s4f	3Pe–1Fo	5:7–7:5	139.79	2.22E−05	5.11E−05	5.41E+06
3d^2–3s5f!3p5d^3	3Pe–1Fo	5:7–7:14	72.73	7.21E−04	8.63E−04	6.49E+08
3d^2–3s6f	3Pe–1Fo	5:7–7:25	59.39	3.02E−04	2.95E−04	4.08E+08
3p3d–3s4d	1Fo–3De	7:3–5:8	103.15	2.65E−04	6.30E−04	2.32E+08
3p3d–3s4d	1Fo–3De	7:3–7:3	103.02	1.17E−06	2.79E−06	7.37E+05
3s4d–3s4f	3De–1Fo	5:8–7:5	1097.25	4.33E−03	7.81E−02	1.71E+07
3s4d–3s4f	3De–1Fo	7:3–7:5	1111.44	5.42E−07	1.39E−05	2.92E+03
3s4d–3s5f!3p5d^3	3De–1Fo	5:8–7:14	133.21	2.54E−04	5.56E−04	6.81E+07
3s4d–3s5f!3p5d^3	3De–1Fo	7:3–7:14	133.42	3.18E−05	9.78E−05	1.19E+07
3s4d–3s6f	3De–1Fo	5:8–7:25	94.39	1.23E−03	1.91E−03	6.58E+08
3s4d–3s6f	3De–1Fo	7:3–7:25	94.49	4.65E−05	1.01E−04	3.47E+07
3p3d–3s4d	1Fo–1De	7:3–5:9	102.80	6.76E−03	1.60E−02	5.97E+09
3s4d–3s4f	1De–1Fo	5:9–7:5	1137.95	1.54E−01	2.88E+00	5.66E+08
3s4d–3s5f!3p5d^3	1De–1Fo	5:9–7:14	133.79	1.51E−05	3.33E−05	4.03E+06
3s4d–3s6f	1De–1Fo	5:9–7:25	94.68	4.47E−03	6.97E−03	2.38E+09
3p3d–3p4f	1Fo–3Fe	7:3–5:13	75.32	8.68E−05	1.51E−04	1.43E+08
3p3d–3p4f	1Fo–3Fe	7:3–9:4	74.65	1.15E−04	1.97E−04	1.07E+08
3s4f–3p4f	1Fo–3Fe	7:5–5:13	374.61	3.80E−03	3.28E−02	2.53E+08
3s4f–3p4f	1Fo–3Fe	7:5–9:4	358.50	2.29E−05	1.89E−04	9.24E+05
3p4f–3s5f!3p5d^3	3Fe–1Fo	5:13–7:14	254.71	2.43E−03	1.02E−02	1.78E+08
3p4f–3s5f!3p5d^3	3Fe–1Fo	9:4–7:14	262.74	2.22E−05	1.73E−04	2.75E+06
3p4f–3s6f	3Fe–1Fo	5:13–7:25	142.57	2.67E−02	6.26E−02	6.25E+09
3p4f–3s6f	3Fe–1Fo	9:4–7:25	145.05	1.16E−03	4.98E−03	4.72E+08
3p3d–3p4f	1Fo–3De	7:3–5:14	73.98	2.90E−05	4.94E−05	4.94E+07
3p3d–3p4f	1Fo–3De	7:3–7:8	74.05	7.21E−03	1.23E−02	8.77E+09
3s4f–3p4f	1Fo–3De	7:5–5:14	343.47	2.61E−03	2.07E−02	2.07E+08
3s4f–3p4f	1Fo–3De	7:5–7:8	345.01	6.17E−03	4.91E−02	3.46E+08
3p4f–3s5f!3p5d^3	3De–1Fo	5:14–7:14	271.44	3.72E−02	1.66E−01	2.40E+09
3p4f–3s5f!3p5d^3	3De–1Fo	7:8–7:14	270.49	2.73E−03	1.70E−02	2.49E+08
3p4f–3s6f	3De–1Fo	5:14–7:25	147.67	1.95E−01	4.74E−01	4.26E+10
3p4f–3s6f	3De–1Fo	7:8–7:25	147.38	8.04E−02	2.73E−01	2.47E+10
3p3d–3p4f	1Fo–1De	7:3–5:15	72.81	2.87E−03	4.82E−03	5.06E+09
3s4f–3p4f	1Fo–1De	7:5–5:15	319.64	1.03E−01	7.61E−01	9.44E+09
3p4f–3s5f!3p5d^3	1De–1Fo	5:15–7:14	288.44	6.53E−04	3.10E−03	3.74E+07
3p4f–3s6f	1De–1Fo	5:15–7:25	152.56	1.27E+00	3.18E+00	2.59E+11
3p3d–3s5d	1Fo–3De	7:3–5:18	63.40	2.59E−09	3.79E−09	6.03E+03
3p3d–3s5d	1Fo–3De	7:3–7:10	63.38	1.29E−07	1.89E−07	2.15E+05
3s4f–3s5d	1Fo–3De	7:5–5:18	193.52	3.00E−04	1.34E−03	7.48E+07
3s4f–3s5d	1Fo–3De	7:5–7:10	193.37	9.27E−08	4.13E−07	1.65E+04
3s5d–3s5f!3p5d^3	3De–1Fo	5:18–7:14	700.28	3.90E−07	4.49E−06	3.79E+03
3s5d–3s5f!3p5d^3	3De–1Fo	7:10–7:14	702.25	5.88E−08	9.52E−07	7.95E+02
3s5d–3s6f	3De–1Fo	5:18–7:25	221.44	1.44E−02	5.25E−02	1.40E+09
3s5d–3s6f	3De–1Fo	7:10–7:25	221.63	1.19E−03	6.07E−03	1.61E+08
3s3p–3p4f	3Po–3*Ge*	5:1–7:5	47.03	6.99E−06	5.41E−06	1.51E+07
3s3p–3p4f	3Po–1Fe	5:1–7:6	46.89	1.08E−04	8.36E−05	2.35E+08
3p3d–3p4f	3Fo–3*Ge*	5:2–7:5	68.87	7.68E−01	8.71E−01	7.71E+11
3p3d–3p4f	3Fo–3*Ge*	7:1–7:5	69.35	2.37E−02	3.79E−02	3.29E+10
3p3d–3p4f	3Fo–3*Ge*	9:1–7:5	69.91	5.00E−06	1.04E−05	8.77E+06
3p3d–3p4f	3Fo–3*Ge*	7:1–9:3	69.03	6.52E−01	1.04E+00	7.10E+11
3p3d–3p4f	3Fo–3*Ge*	9:1–9:3	69.59	2.93E−04	6.04E−04	4.04E+08
3p3d–3p4f	3Fo–3*Ge*	9:1–11:1	68.85	8.01E−01	1.63E+00	9.22E+11
LS	3Fo–3*Ge*	21–27		7.52E−01	3.58E+00	8.21E+11

(*continued on next page*)

Table 2. (*continued*)

C_i–C_k	T_i–T_k	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
3p3d–3p4f	3Fo–1Fe	5:2–7:6	68.57	4.14E−02	4.68E−02	4.20E+10
3p3d–3p4f	3Fo–1Fe	7:1–7:6	69.03	7.72E−03	1.23E−02	1.08E+10
3p3d–3p4f	3Fo–1Fe	9:1–7:6	69.59	6.46E−05	1.33E−04	1.14E+08
3p3d–3p4f	1Do–3*Ge*	5:3–7:5	69.85	6.31E−02	7.25E−02	6.16E+10
3p3d–3p4f	1Do–1Fe	5:3–7:6	69.53	5.14E−01	5.89E−01	5.07E+11
3p3d–3p4f	3Do–3*Ge*	5:4–7:5	72.28	3.44E−03	4.10E−03	3.14E+09
3p3d–3p4f	3Do–3*Ge*	7:2–7:5	72.19	4.41E−03	7.34E−03	5.65E+09
3p3d–3p4f	3Do–3*Ge*	7:2–9:3	71.85	1.60E−01	2.65E−01	1.61E+11
LS	3Do–3*Ge*	15–27		7.79E−02	2.76E−01	5.58E+10
3p3d–3p4f	3Do–1Fe	5:4–7:6	71.94	2.52E−01	2.98E−01	2.32E+11
3p3d–3p4f	3Do–1Fe	7:2–7:6	71.85	1.72E−03	2.85E−03	2.23E+09
3p3d–3p4f	3Po–3*Ge*	5:5–7:5	71.60	6.14E−03	7.24E−03	5.71E+09
3p3d–3p4f	3Po–1Fe	5:5–7:6	71.27	4.87E−02	5.71E−02	4.57E+10
3s4f–3p4f	3Fo–3*Ge*	5:8–7:5	368.13	3.65E−02	2.21E−01	1.28E+09
3s4f–3p4f	3Fo–3*Ge*	7:4–7:5	368.28	1.39E−02	1.18E−01	6.84E+08
3s4f–3p4f	3Fo–3*Ge*	9:2–7:5	368.62	7.62E−05	8.33E−04	4.81E+06
3s4f–3p4f	3Fo–3*Ge*	7:4–9:3	359.62	2.55E−02	2.12E−01	1.02E+09
3s4f–3p4f	3Fo–3*Ge*	9:2–9:3	359.94	5.87E−02	6.26E−01	3.02E+09
3s4f–3p4f	3Fo–3*Ge*	9:2–11:1	341.04	7.89E−02	7.97E−01	3.70E+09
LS	3Fo–3*Ge*	21–27		8.08E−02	1.97E+00	3.36E+09
3s4f–3p4f	3Fo–1Fe	5:8–7:6	359.47	1.00E−03	5.93E−03	3.69E+07
3s4f–3p4f	3Fo–1Fe	7:4–7:6	359.62	3.79E−02	3.14E−01	1.96E+09
3s4f–3p4f	3Fo–1Fe	9:2–7:6	359.94	3.13E−02	3.33E−01	2.07E+09
3p4f–3s5f	3*Ge*–3Fo	7:5–5:18	337.56	6.20E−04	4.82E−03	5.08E+07
3p4f–3s5f	3*Ge*–3Fo	7:5–7:12	337.56	5.05E−05	3.93E−04	2.96E+06
3p4f–3s5f	3*Ge*–3Fo	7:5–9:5	337.33	7.09E−05	5.52E−04	3.23E+06
3p4f–3s5f	3*Ge*–3Fo	9:3–7:12	345.18	6.35E−04	6.49E−03	4.57E+07
3p4f–3s5f	3*Ge*–3Fo	9:3–9:5	344.94	1.38E−04	1.41E−03	7.75E+06
3p4f–3s5f	3*Ge*–3Fo	11:1–9:5	364.29	1.26E−03	1.66E−02	7.74E+07
LS	3*Ge*–3Fo	27–21		9.63E−04	3.03E−02	6.61E+07
3p4f–3s5f	1Fe–3Fo	7:6–5:18	345.18	7.75E−05	6.16E−04	6.07E+06
3p4f–3s5f	1Fe–3Fo	7:6–7:12	345.18	2.77E−04	2.20E−03	1.55E+07
3p4f–3s5f	1Fe–3Fo	7:6–9:5	344.94	6.64E−04	5.28E−03	2.90E+07
3p3d–3p4f	1Fo–3*Ge*	7:3–7:5	75.89	2.50E−02	4.37E−02	2.90E+10
3p3d–3p4f	1Fo–3*Ge*	7:3–9:3	75.52	1.51E−02	2.63E−02	1.37E+10
3s4f–3p4f	1Fo–3*Ge*	7:5–7:5	389.10	4.48E−02	4.02E−01	1.97E+09
3s4f–3p4f	1Fo–3*Ge*	7:5–9:3	379.44	2.89E−03	2.53E−02	1.04E+08
3p4f–3s5f!3p5d^3	3*Ge*–1Fo	7:5–7:14	248.42	5.08E−04	2.91E−03	5.49E+07
3p4f–3s5f!3p5d^3	3*Ge*–1Fo	9:3–7:14	252.52	2.32E−02	1.74E−01	3.12E+09
3p4f–3s6f	3*Ge*–1Fo	7:5–7:25	140.58	4.34E−03	1.40E−02	1.46E+09
3p4f–3s6f	3*Ge*–1Fo	9:3–7:25	141.88	3.41E−04	1.43E−03	1.45E+08
3p3d–3p4f	1Fo–1Fe	7:3–7:6	75.52	2.55E−02	4.44E−02	2.98E+10
3s4f–3p4f	1Fo–1Fe	7:5–7:6	379.44	4.20E−02	3.67E−01	1.95E+09
3p4f–3s5f!3p5d^3	1Fe–1Fo	7:6–7:14	252.52	4.72E−02	2.75E−01	4.94E+09
3p4f–3s6f	1Fe–1Fo	7:6–7:25	141.88	1.94E−02	6.34E−02	6.43E+09
3s3d–3s6f	3De–3Fo	7:1–9:13	43.39	1.40E−05	1.40E−05	3.87E+07
3d^2–3s6f	3Fe–3Fo	7:2–9:13	61.96	1.59E−03	2.27E−03	2.15E+09
3d^2–3s6f	3Fe–3Fo	9:1–9:13	62.03	7.44E−05	1.37E−04	1.29E+08
LS	3Fe–3Fo	21–21		5.62E−04	2.41E−03	9.76E+08
3s4d–3s6f	3De–3Fo	7:3–9:13	104.94	5.49E−05	1.33E−04	2.59E+07
3p4f–3s6f	3*Ge*–3Fo	7:5–9:13	165.03	4.50E−02	1.71E−01	8.56E+09
3p4f–3s6f	3*Ge*–3Fo	9:3–9:13	166.83	4.96E−03	2.45E−02	1.19E+09
3p4f–3s6f	3*Ge*–3Fo	11:1–9:13	171.23	1.31E−03	8.15E−03	3.65E+08
LS	3*Ge*–3Fo	27–21		1.39E−02	2.04E−01	4.34E+09
3p4f–3s6f	1Fe–3Fo	7:6–9:13	166.83	1.98E−02	7.59E−02	3.68E+09
3p4f–3s6f	3De–3Fo	7:8–9:13	174.49	2.01E−03	8.09E−03	3.43E+08
3s5d–3s6f	3De–3Fo	7:10–9:13	289.18	7.72E−05	5.15E−04	4.79E+06
3p3d–3d^2	3Fo–1*Ge*	7:1–9:2	213.25	1.34E−03	6.59E−03	1.53E+08
3p3d–3d^2	3Fo–1*Ge*	9:1–9:2	218.62	1.50E−04	9.71E−04	2.09E+07
3p3d–3p4f	3Fo–1*Ge*	7:1–9:5	67.09	1.65E−02	2.55E−02	1.90E+10
3p3d–3p4f	3Fo–1*Ge*	9:1–9:5	67.61	3.96E−05	7.94E−05	5.78E+07
3p3d–3d^2	3Do–1*Ge*	7:2–9:2	242.60	9.35E−04	5.23E−03	8.24E+07
3p3d–3p4f	3Do–1*Ge*	7:2–9:5	69.74	2.28E−03	3.67E−03	2.43E+09
3p3d–3d^2	1Fo–1*Ge*	7:3–9:2	290.23	3.63E−01	2.43E+00	2.24E+10
3p3d–3p4f	1Fo–1*Ge*	7:3–9:5	73.20	7.20E−01	1.21E+00	6.97E+11
3d^2–3s4f	1*Ge*–3Fo	9:2–7:4	142.54	5.54E−08	2.34E−07	2.34E+04
3d^2–3s4f	1*Ge*–3Fo	9:2–9:2	142.49	4.93E−10	2.08E−09	1.62E+02
3s4f–3p4f	3Fo–1*Ge*	7:4–9:5	312.43	1.23E−03	8.84E−03	6.52E+07
3s4f–3p4f	3Fo–1*Ge*	9:2–9:5	312.68	4.62E−03	4.28E−02	3.15E+08
3d^2–3s4f	1*Ge*–1Fo	9:2–7:5	139.65	4.79E−06	1.98E−05	2.11E+06
3s4f–3p4f	1Fo–1*Ge*	7:5–9:5	327.29	6.20E−02	4.67E−01	3.00E+09
3d^2–3s5f	1*Ge*–3Fo	9:2–7:12	78.78	2.48E−07	5.79E−07	3.43E+05
3d^2–3s5f	1*Ge*–3Fo	9:2–9:5	78.77	1.20E−07	2.81E−07	1.29E+05
3p4f–3s5f	1*Ge*–3Fo	9:5–7:12	403.71	4.39E−05	5.25E−04	2.31E+06
3p4f–3s5f	1*Ge*–3Fo	9:5–9:5	403.38	9.15E−06	1.09E−04	3.75E+05
3d^2–3s5f!3p5d^3	1*Ge*–1Fo	9:2–7:14	72.69	1.60E−05	3.46E−05	2.60E+07

Table 2. (*continued*)

C_i–C_k	T_i–T_k	g_i:I–g_j:K	E_{ik} (Å)	f	S	A (s^{-1})
3p4f–3s5f!3p5d^3	1*Ge*–1Fo	9:5–7:14	282.48	1.05E−03	8.82E−03	1.13E+08
3d^2–3s6f	1*Ge*–1Fo	9:2–7:25	59.37	4.37E−05	7.69E−05	1.06E+08
3p4f–3s6f	1*Ge*–1Fo	9:5–7:25	150.87	6.73E−05	3.01E−04	2.53E+07
3d^2–3s6f	1*Ge*–3Fo	9:2–9:13	63.33	1.53E−04	2.87E−04	2.55E+08
3p4f–3s6f	3Fe–3Fo	9:4–9:13	171.23	5.75E−02	2.92E−01	1.31E+10
3p4f–3s6f	1*Ge*–3Fo	9:5–9:13	179.40	3.71E−02	1.97E−01	7.68E+09

Table 3
Fine structure energy levels of Fe XV for which forbidden (E2, E3, M1, M2) transitions are presented. See page 583 for Explanation of Tables.

i_e	SLp(cf)	2J	E (Ry)
1	1Se(1)	0	0.00000E+00
2	3Po(2)	0	2.13090E+00
3	3Po(2)	2	2.18390E+00
4	3Po(2)	4	2.31300E+00
5	1Po(2)	2	3.20680E+00
6	3Pe(3)	0	5.05320E+00
7	1De(3)	4	5.09950E+00
8	3Pe(3)	2	5.14500E+00
9	3Pe(3)	4	5.30180E+00
10	1Se(3)	0	6.01100E+00
11	3De(4)	2	6.18540E+00
12	3De(4)	4	6.19470E+00
13	3De(4)	6	6.20950E+00
14	1De(4)	4	6.94470E+00
15	3Fo(5)	4	8.45880E+00
16	3Fo(5)	6	8.54880E+00
17	3Fo(5)	8	8.65390E+00
18	1Do(5)	4	8.64350E+00
19	3Do(5)	2	8.95660E+00
20	3Po(5)	4	8.96240E+00
21	3Po(5)	0	9.07520E+00
22	3Po(5)	2	9.07840E+00
23	3Do(5)	6	9.06580E+00
24	3Do(5)	4	9.08190E+00
25	1Fo(5)	6	9.68240E+00
26	1Po(5)	2	9.79510E+00
27	3Fe(19)	4	1.24870E+01
28	3Fe(19)	6	1.25030E+01
29	3Fe(19)	8	1.25210E+01
30	3Pe(19)	4	1.28290E+01
31	3Pe(19)	0	1.29746E+01
32	3Pe(19)	2	1.29836E+01
33	1De(19)	4	1.27810E+01
34	1Ge(19)	8	1.28220E+01
35	1Se(19)	0	1.35510E+01
36	3Se(6)	2	1.60720E+01
37	1Se(6)	0	1.62840E+01
38	3Po(7)	0	1.72016E+01
39	3Po(7)	2	1.72077E+01
40	3Po(7)	4	1.72589E+01
41	1Po(7)	2	1.72230E+01
42	3De(8)	2	1.85110E+01
43	3De(8)	4	1.85170E+01
44	3De(8)	6	1.85280E+01
45	1De(8)	4	1.85470E+01
46	3Po(13)	0	1.88070E+01
47	3Po(13)	2	1.88400E+01
48	3Po(13)	4	1.89794E+01
49	1Po(13)	2	1.91124E+01
50	3Fo(9)	4	1.92140E+01
51	3Fo(9)	6	1.92150E+01
52	3Fo(9)	8	1.92180E+01
53	1Fo(9)	6	1.93480E+01
54	1Pe(14)	2	1.97201E+01
55	3De(14)	2	1.98396E+01
56	3De(14)	4	1.98639E+01
57	3Pe(14)	0	1.98988E+01
58	3Pe(14)	2	1.99625E+01
59	3De(14)	6	1.99898E+01
60	3Pe(14)	4	2.00312E+01
61	3Se(14)	2	2.00710E+01
62	1De(14)	4	2.02511E+01
63	1Se(14)	0	2.05245E+01
64	1Do(15)	4	2.11549E+01
65	3Do(15)	2	2.11744E+01
66	3Do(15)	4	2.11774E+01
67	3Do(15)	6	2.12018E+01
68	3Fo(15)	4	2.13085E+01
69	3Fo(15)	6	2.13334E+01
70	3Fo(15)	8	2.13847E+01
71	3Po(15)	4	2.14277E+01
72	3Po(15)	2	2.14441E+01
73	1Fo(15)	6	2.14621E+01
74	3Po(15)	0	2.14681E+01
75	1Po(15)	2	2.15607E+01
76	3Ge(16)	6	2.16900E+01
77	1Fe(16)	6	2.17490E+01
78	3Ge(16)	8	2.17490E+01
79	3Fe(16)	4	2.17800E+01
80	3Fe(16)	6	2.19173E+01
81	3Fe(16)	8	2.18900E+01
82	3Ge(16)	10	2.18900E+01
83	3De(16)	6	2.19890E+01
84	3De(16)	4	2.20010E+01
85	3De(16)	2	2.20540E+01
86	1Ge(16)	8	2.21320E+01
87	1De(16)	4	2.21980E+01
88	3Se(10)	2	2.31900E+01
89	1Se(10)	0	2.30314E+01
90	3Po(11)	0	2.34461E+01
91	3Po(11)	2	2.34522E+01
92	3Po(11)	4	2.34727E+01
93	1Po(11)	2	2.33920E+01
94	3De(12)	2	2.40580E+01
95	3De(12)	4	2.40570E+01
96	3De(12)	6	2.40600E+01
97	1De(12)	4	2.41384E+01
98	3Fo(20)	4	2.43890E+01
99	3Fo(20)	6	2.43890E+01
100	3Fo(20)	8	2.43910E+01
101	1Fo(20)	6	2.53580E+01
102	3Se(17)	2	5.38742E+01
103	3De(17)	4	5.40548E+01
104	3De(17)	6	5.41476E+01
105	3Pe(17)	2	5.42275E+01
106	3Pe(17)	4	5.43337E+01
107	3Pe(17)	0	5.47663E+01
108	1Pe(17)	2	5.49536E+01
109	3De(17)	2	5.51546E+01
110	1De(17)	4	5.51773E+01
111	1Se(17)	0	5.61908E+01
112	3Po(18)	0	5.78646E+01
113	3Po(18)	2	5.79289E+01
114	3Fo(18)	8	5.80344E+01
115	3Po(18)	4	5.80450E+01
116	3Fo(18)	6	5.80719E+01
117	3Do(18)	4	5.81797E+01
118	3Do(18)	6	5.82470E+01
119	3Do(18)	2	5.85566E+01
120	3Fo(18)	4	5.89991E+01
121	1Do(18)	4	5.90576E+01
122	1Fo(18)	6	5.90879E+01
123	1Po(18)	2	5.95062E+01

Table 3. (*continued*)

Table 4
Partial set of radiative decay rates for forbidden E2, M1, E3, M2 transitions in Fe XV. See page 583 for Explanation of Tables.

i–j	T_iC_i–T_jC_j	g_i–g_j	λ (Å)	E_i (Ry)	E_j (Ry)	AE2	AM1
E2 and M1, N_{tr} = 5066							
2–3	3Po 2–3Po 2	1–3	17193	2.13E+00	2.18E+00	0.00E+00	3.52E+00
2–4	3Po 2–3Po 2	1–5	5004	2.13E+00	2.31E+00	9.18E−03	0.00E+00
3–4	3Po 2–3Po 2	3–5	7058	2.18E+00	2.31E+00	3.69E−03	3.81E+01
2–5	3Po 2–1Po 2	1–3	846.98	2.13E+00	3.21E+00	0.00E+00	1.70E+02
3–5	3Po 2–1Po 2	3–3	890.87	2.18E+00	3.21E+00	2.19E+00	1.12E+02
4–5	3Po 2–1Po 2	5–3	1019	2.31E+00	3.21E+00	6.04E−01	1.24E+02
1–7	1Se 1–1De 3	1–5	178.70	0.00E+00	5.10E+00	1.59E+05	0.00E+00
6–7	3Pe 3–1De 3	1–5	19681	5.05E+00	5.10E+00	3.34E−06	0.00E+00
1–8	1Se 1–3Pe 3	1–3	177.12	0.00E+00	5.14E+00	0.00E+00	8.42E+01
6–8	3Pe 3–3Pe 3	1–3	9926	5.05E+00	5.14E+00	0.00E+00	1.79E+01
7–8	1De 3–3Pe 3	5–3	20027	5.10E+00	5.14E+00	4.35E−06	4.13E−01
1–9	1Se 1–3Pe 3	1–5	171.88	0.00E+00	5.30E+00	3.81E+04	0.00E+00
6–9	3Pe 3–3Pe 3	1–5	3665	5.05E+00	5.30E+00	2.51E−02	0.00E+00
7–9	1De 3–3Pe 3	5–5	4504	5.10E+00	5.30E+00	2.45E−02	5.55E+01
8–9	3Pe 3–3Pe 3	3–5	5811	5.14E+00	5.30E+00	7.26E−03	5.86E+01
7–10	1De 3–1Se 3	5–1	999	5.10E+00	6.01E+00	2.70E+02	0.00E+00
8–10	3Pe 3–1Se 3	3–1	1052	5.14E+00	6.01E+00	0.00E+00	1.25E+03
9–10	3Pe 3–1Se 3	5–1	1284	5.30E+00	6.01E+00	2.13E+01	0.00E+00
1–11	1Se 1–3De 4	1–3	147.33	0.00E+00	6.19E+00	0.00E+00	1.39E+00
6–11	3Pe 3–3De 4	1–3	804.86	5.05E+00	6.19E+00	0.00E+00	2.26E−04
7–11	1De 3–3De 4	5–3	839.18	5.10E+00	6.19E+00	8.04E−02	3.23E+00
8–11	3Pe 3–3De 4	3–3	875.88	5.14E+00	6.19E+00	8.17E−01	1.29E−04
9–11	3Pe 3–3De 4	5–3	1031	5.30E+00	6.19E+00	9.29E−02	5.47E−01
10–11	1Se 3–3De 4	1–3	5225	6.01E+00	6.19E+00	0.00E+00	9.56E−07
1–12	1Se 1–3De 4	1–5	147.10	0.00E+00	6.19E+00	1.76E+02	0.00E+00
6–12	3Pe 3–3De 4	1–5	798.31	5.05E+00	6.19E+00	5.08E−01	0.00E+00
7–12	1De 3–3De 4	5–5	832.06	5.10E+00	6.19E+00	3.22E−02	4.83E−01
8–12	3Pe 3–3De 4	3–5	868.12	5.14E+00	6.19E+00	1.02E−01	3.50E−02
9–12	3Pe 3–3De 4	5–5	1020	5.30E+00	6.19E+00	2.88E−01	2.40E−06
10–12	1Se 3–3De 4	1–5	4960	6.01E+00	6.19E+00	1.83E−05	0.00E+00
11–12	3De 4–3De 4	3–5	97988	6.19E+00	6.19E+00	2.61E−09	2.58E−02
7–13	1De 3–3De 4	5–7	820.96	5.10E+00	6.21E+00	1.15E−01	1.50E+00
8–13	3Pe 3–3De 4	3–7	856.05	5.14E+00	6.21E+00	4.18E−01	0.00E+00
9–13	3Pe 3–3De 4	5–7	1003	5.30E+00	6.21E+00	3.43E−01	2.51E−01
11–13	3De 4–3De 4	3–7	37812	6.19E+00	6.21E+00	2.49E−08	0.00E+00
12–13	3De 4–3De 4	5–7	61571	6.19E+00	6.21E+00	2.18E−08	7.70E−02
1–14	1Se 1–1De 4	1–5	131.22	0.00E+00	6.94E+00	1.73E+06	0.00E+00
6–14	3Pe 3–1De 4	1–5	481.77	5.05E+00	6.94E+00	2.29E+01	0.00E+00
7–14	1De 3–1De 4	5–5	493.86	5.10E+00	6.94E+00	1.37E+02	2.08E+01
8–14	3Pe 3–1De 4	3–5	506.34	5.14E+00	6.94E+00	5.73E−01	4.16E+01
9–14	3Pe 3–1De 4	5–5	554.67	5.30E+00	6.94E+00	4.77E+00	8.46E+01
10–14	1Se 3–1De 4	1–5	975.97	6.01E+00	6.94E+00	2.70E+01	0.00E+00
11–14	3De 4–1De 4	3–5	1200	6.19E+00	6.94E+00	3.21E−03	5.37E+00
12–14	3De 4–1De 4	5–5	1215	6.19E+00	6.94E+00	2.45E−03	1.07E+00
13–14	3De 4–1De 4	7–5	1239	6.21E+00	6.94E+00	5.07E−03	5.18E+00
2–15	3Po 2–3Fo 5	1–5	144.01	2.13E+00	8.46E+00	4.41E+05	0.00E+00
3–15	3Po 2–3Fo 5	3–5	145.22	2.18E+00	8.46E+00	4.39E+05	1.85E+00
4–15	3Po 2–3Fo 5	5–5	148.27	2.31E+00	8.46E+00	3.32E+04	6.80E−01
5–15	1Po 2–3Fo 5	3–5	173.51	3.21E+00	8.46E+00	3.63E+04	6.05E−01
3–16	3Po 2–3Fo 5	3–7	143.17	2.18E+00	8.55E+00	7.65E+05	0.00E+00
4–16	3Po 2–3Fo 5	5–7	146.13	2.31E+00	8.55E+00	2.51E+05	8.20E−01
5–16	1Po 2–3Fo 5	3–7	170.59	3.21E+00	8.55E+00	5.62E+02	0.00E+00
15–16	3Fo 5–3Fo 5	5–7	10125	8.46E+00	8.55E+00	2.86E−04	2.20E+01
4–17	3Po 2–3Fo 5	5–9	143.71	2.31E+00	8.65E+00	1.03E+06	0.00E+00
15–17	3Fo 5–3Fo 5	5–9	4670	8.46E+00	8.65E+00	3.45E−04	0.00E+00
16–17	3Fo 5–3Fo 5	7–9	8670	8.55E+00	8.65E+00	5.80E−04	3.07E+01
2–18	3Po 2–1Do 5	1–5	139.92	2.13E+00	8.64E+00	1.17E+05	0.00E+00
3–18	3Po 2–1Do 5	3–5	141.07	2.18E+00	8.64E+00	1.79E+03	3.57E+00
4–18	3Po 2–1Do 5	5–5	143.95	2.31E+00	8.64E+00	1.36E+04	2.81E+00
5–18	1Po 2–1Do 5	3–5	167.61	3.21E+00	8.64E+00	4.80E+05	7.88E−01
15–18	3Fo 5–1Do 5	5–5	4933	8.46E+00	8.64E+00	5.59E−03	1.44E+01
16–18	3Fo 5–1Do 5	7–5	9622	8.55E+00	8.64E+00	2.80E−05	4.35E+00
17–18	3Fo 5–1Do 5	9–5	87623	8.65E+00	8.64E+00	9.11E−10	0.00E+00
2–19	3Po 2–3Do 5	1–3	133.51	2.13E+00	8.96E+00	0.00E+00	2.67E−01
3–19	3Po 2–3Do 5	3–3	134.55	2.18E+00	8.96E+00	1.03E+06	2.72E+00
4–19	3Po 2–3Do 5	5–3	137.16	2.31E+00	8.96E+00	7.04E+02	1.04E+01
5–19	1Po 2–3Do 5	3–3	158.49	3.21E+00	8.96E+00	9.06E+02	9.18E+00
15–19	3Fo 5–3Do 5	5–3	1830	8.46E+00	8.96E+00	1.61E−01	8.17E+00
16–19	3Fo 5–3Do 5	7–3	2234	8.55E+00	8.96E+00	6.43E−01	0.00E+00
18–19	1Do 5–3Do 5	5–3	2910	8.64E+00	8.96E+00	5.82E−03	2.38E+01
2–20	3Po 2–3Po 5	1–5	133.39	2.13E+00	8.96E+00	4.62E+05	0.00E+00
3–20	3Po 2–3Po 5	3–5	134.43	2.18E+00	8.96E+00	5.41E+05	2.05E+00
4–20	3Po 2–3Po 5	5–5	137.04	2.31E+00	8.96E+00	6.38E+03	6.75E−01
5–20	1Po 2–3Po 5	3–5	158.33	3.21E+00	8.96E+00	2.72E+04	2.28E+01

(*continued on next page*)

Table 4. (*continued*)

i–*j*	T_iC_i–T_jC_j	g_i–g_j	λ (Å)	E_i (Ry)	E_j (Ry)	AE2	AM1
15–20	3Fo 5–3Po 5	5–5	1809	8.46E+00	8.96E+00	9.43E−03	7.41E+00
16–20	3Fo 5–3Po 5	7–5	2203	8.55E+00	8.96E+00	2.27E−01	1.17E+00
17–20	3Fo 5–3Po 5	9–5	2953	8.65E+00	8.96E+00	3.13E−01	0.00E+00
18–20	1Do 5–3Po 5	5–5	2857	8.64E+00	8.96E+00	1.24E−02	3.64E+01
19–20	3Do 5–3Po 5	3–5	157108	8.96E+00	8.96E+00	2.95E−11	4.44E−03
3–21	3Po 2–3Po 5	3–1	132.23	2.18E+00	9.08E+00	0.00E+00	1.29E+01
4–21	3Po 2–3Po 5	5–1	134.76	2.31E+00	9.08E+00	1.04E+06	0.00E+00
5–21	1Po 2–3Po 5	3–1	155.28	3.21E+00	9.08E+00	0.00E+00	6.02E+00
15–21	3Fo 5–3Po 5	5–1	1478	8.46E+00	9.08E+00	1.49E+01	0.00E+00
18–21	1Do 5–3Po 5	5–1	2110	8.64E+00	9.08E+00	3.41E−01	0.00E+00
19–21	3Do 5–3Po 5	3–1	7683	8.96E+00	9.08E+00	0.00E+00	3.15E+01
20–21	3Po 5–3Po 5	5–1	8078	8.96E+00	9.08E+00	5.61E−04	0.00E+00
2–22	3Po 2–3Po 5	1–3	131.16	2.13E+00	9.08E+00	0.00E+00	7.81E−01
3–22	3Po 2–3Po 5	3–3	132.17	2.18E+00	9.08E+00	2.36E+02	6.47E−01
4–22	3Po 2–3Po 5	5–3	134.70	2.31E+00	9.08E+00	1.03E+06	5.56E+00
5–22	1Po 2–3Po 5	3–3	155.20	3.21E+00	9.08E+00	3.99E+01	1.81E+01
15–22	3Fo 5–3Po 5	5–3	1470	8.46E+00	9.08E+00	6.86E+00	2.73E+01
16–22	3Fo 5–3Po 5	7–3	1720	8.55E+00	9.08E+00	2.90E+00	0.00E+00
18–22	1Do 5–3Po 5	5–3	2095	8.64E+00	9.08E+00	1.11E−01	1.71E+01
19–22	3Do 5–3Po 5	3–3	7481	8.96E+00	9.08E+00	3.83E−04	2.50E+01
20–22	3Po 5–3Po 5	5–3	7855	8.96E+00	9.08E+00	6.51E−06	1.33E+00
21–22	3Po 5–3Po 5	1–3	284808	9.08E+00	9.08E+00	0.00E+00	5.70E−04
3–23	3Po 2–3Do 5	3–7	132.42	2.18E+00	9.07E+00	2.65E+05	0.00E+00
4–23	3Po 2–3Do 5	5–7	134.95	2.31E+00	9.07E+00	7.63E+05	1.04E+00
5–23	1Po 2–3Do 5	3–7	155.53	3.21E+00	9.07E+00	1.34E+02	0.00E+00
15–23	3Fo 5–3Do 5	5–7	1501	8.46E+00	9.07E+00	9.71E−02	1.21E+01
16–23	3Fo 5–3Do 5	7–7	1762	8.55E+00	9.07E+00	3.42E−01	2.69E+01
17–23	3Fo 5–3Do 5	9–7	2212	8.65E+00	9.07E+00	9.44E−02	1.94E+01
18–23	1Do 5–3Do 5	5–7	2157	8.64E+00	9.07E+00	3.49E−02	2.34E+00
19–23	3Do 5–3Do 5	3–7	8344	8.96E+00	9.07E+00	2.81E−04	0.00E+00
20–23	3Po 5–3Do 5	5–7	8813	8.96E+00	9.07E+00	6.43E−04	1.15E+01
22–23	3Po 5–3Do 5	3–7	72323	9.08E+00	9.07E+00	1.01E−08	0.00E+00
2–24	3Po 2–3Do 5	1–5	131.10	2.13E+00	9.08E+00	1.17E+04	0.00E+00
3–24	3Po 2–3Do 5	3–5	132.11	2.18E+00	9.08E+00	4.22E+04	6.40E+00
4–24	3Po 2–3Do 5	5–5	134.63	2.31E+00	9.08E+00	9.73E+05	3.08E+00
5–24	1Po 2–3Do 5	3–5	155.11	3.21E+00	9.08E+00	4.90E+03	7.41E+00
15–24	3Fo 5–3Do 5	5–5	1462	8.46E+00	9.08E+00	1.45E+00	4.25E+01
16–24	3Fo 5–3Do 5	7–5	1709	8.55E+00	9.08E+00	1.87E+00	1.57E+00
17–24	3Fo 5–3Do 5	9–5	2129	8.65E+00	9.08E+00	7.48E−01	0.00E+00
18–24	1Do 5–3Do 5	5–5	2078	8.64E+00	9.08E+00	2.82E−02	2.61E+01
19–24	3Do 5–3Do 5	3–5	7272	8.96E+00	9.08E+00	1.18E−03	9.23E+00
20–24	3Po 5–3Do 5	5–5	7625	8.96E+00	9.08E+00	4.90E−05	9.50E+00
21–24	3Po 5–3Do 5	1–5	136018	9.08E+00	9.08E+00	6.41E−10	0.00E+00
22–24	3Po 5–3Do 5	3–5	260363	9.08E+00	9.08E+00	2.12E−12	8.99E−04
23–24	3Do 5–3Do 5	7–5	56600	9.07E+00	9.08E+00	2.64E−08	7.73E−02
3–25	3Po 2–1Fo 5	3–7	121.53	2.18E+00	9.68E+00	5.31E+02	0.00E+00
4–25	3Po 2–1Fo 5	5–7	123.66	2.31E+00	9.68E+00	2.05E+03	1.01E+00
5–25	1Po 2–1Fo 5	3–7	140.72	3.21E+00	9.68E+00	4.75E+05	0.00E+00
15–25	3Fo 5–1Fo 5	5–7	744.74	8.46E+00	9.68E+00	4.87E+00	8.93E+01
16–25	3Fo 5–1Fo 5	7–7	803.87	8.55E+00	9.68E+00	3.25E−01	1.66E+01
17–25	3Fo 5–1Fo 5	9–7	886.02	8.65E+00	9.68E+00	3.22E−01	5.05E+01
18–25	1Do 5–1Fo 5	5–7	877.15	8.64E+00	9.68E+00	1.23E+01	1.00E+01
19–25	3Do 5–1Fo 5	3–7	1255	8.96E+00	9.68E+00	2.46E−01	0.00E+00
20–25	3Po 5–1Fo 5	5–7	1265	8.96E+00	9.68E+00	6.11E−03	1.87E+01
22–25	3Po 5–1Fo 5	3–7	1508	9.08E+00	9.68E+00	3.80E−04	0.00E+00
23–25	3Do 5–1Fo 5	7–7	1477	9.07E+00	9.68E+00	1.75E−01	6.08E+01
24–25	3Do 5–1Fo 5	5–7	1517	9.08E+00	9.68E+00	8.00E−03	1.50E+01
2–26	3Po 2–1Po 5	1–3	118.90	2.13E+00	9.80E+00	0.00E+00	1.81E+01
3–26	3Po 2–1Po 5	3–3	119.73	2.18E+00	9.80E+00	2.09E+02	9.53E+00
4–26	3Po 2–1Po 5	5–3	121.79	2.31E+00	9.80E+00	1.25E+02	1.27E+01
5–26	1Po 2–1Po 5	3–3	138.32	3.21E+00	9.80E+00	1.23E+06	4.83E−02
15–26	3Fo 5–1Po 5	5–3	681.93	8.46E+00	9.80E+00	4.86E+01	1.12E+00
16–26	3Fo 5–1Po 5	7–3	731.18	8.55E+00	9.80E+00	7.73E+00	0.00E+00
18–26	1Do 5–1Po 5	5–3	791.31	8.64E+00	9.80E+00	2.16E+02	1.37E+01
19–26	3Do 5–1Po 5	3–3	1086	8.96E+00	9.80E+00	9.34E−02	1.61E+01
20–26	3Po 5–1Po 5	5–3	1094	8.96E+00	9.80E+00	1.54E+00	2.38E+02
21–26	3Po 5–1Po 5	1–3	1265	9.08E+00	9.80E+00	0.00E+00	3.23E+01
22–26	3Po 5–1Po 5	3–3	1271	9.08E+00	9.80E+00	7.07E−03	5.93E+01
23–26	3Do 5–1Po 5	7–3	1249	9.07E+00	9.80E+00	5.37E−02	0.00E+00
24–26	3Do 5–1Po 5	5–3	1277	9.08E+00	9.80E+00	4.70E−01	2.01E+01
25–26	1Fo 5–1Po 5	7–3	8085	9.68E+00	9.80E+00	5.54E−03	0.00E+00
1–27	1Se 1–3Fe 19	1–5	72.98	0.00E+00	1.25E+01	7.51E+02	0.00E+00
6–27	3Pe 3–3Fe 19	1–5	122.58	5.05E+00	1.25E+01	1.01E+04	0.00E+00
7–27	1De 3–3Fe 19	5–5	123.35	5.10E+00	1.25E+01	1.56E+03	3.77E−02
8–27	3Pe 3–3Fe 19	3–5	124.12	5.14E+00	1.25E+01	9.65E+03	3.55E−05
9–27	3Pe 3–3Fe 19	5–5	126.83	5.30E+00	1.25E+01	3.28E+03	2.09E−03

Table 4. (*continued*)

i–j	T_iC_i–T_jC_j	g_i–g_j	λ (Å)	E_i (Ry)	E_j (Ry)	AE2	AM1
10–27	1Se 3–3Fe 19	1–5	140.71	6.01E+00	1.25E+01	4.34E+01	0.00E+00
11–27	3De 4–3Fe 19	3–5	144.61	6.19E+00	1.25E+01	9.56E+05	9.26E−01
12–27	3De 4–3Fe 19	5–5	144.82	6.19E+00	1.25E+01	6.87E+05	1.66E−01
13–27	3De 4–3Fe 19	7–5	145.16	6.21E+00	1.25E+01	6.53E+04	5.71E−02
14–27	1De 4–3Fe 19	5–5	164.42	6.94E+00	1.25E+01	2.71E+03	2.44E+00
7–28	1De 3–3Fe 19	5–7	123.09	5.10E+00	1.25E+01	5.15E+02	3.36E−01
8–28	3Pe 3–3Fe 19	3–7	123.85	5.14E+00	1.25E+01	1.41E+04	0.00E+00
9–28	3Pe 3–3Fe 19	5–7	126.54	5.30E+00	1.25E+01	6.21E+03	1.34E−01
11–28	3De 4–3Fe 19	3–7	144.24	6.19E+00	1.25E+01	3.48E+05	0.00E+00
12–28	3De 4–3Fe 19	5–7	144.46	6.19E+00	1.25E+01	8.64E+05	2.12E−01
13–28	3De 4–3Fe 19	7–7	144.79	6.21E+00	1.25E+01	5.13E+05	6.04E−01
14–28	1De 4–3Fe 19	5–7	163.95	6.94E+00	1.25E+01	2.05E+02	2.31E−01
27–28	3Fe 19–3Fe 19	5–7	56954	1.25E+01	1.25E+01	4.57E−09	1.38E−01
7–29	1De 3–3Fe 19	5–9	122.79	5.10E+00	1.25E+01	1.16E+04	0.00E+00
9–29	3Pe 3–3Fe 19	5–9	126.23	5.30E+00	1.25E+01	1.15E+04	0.00E+00
12–29	3De 4–3Fe 19	5–9	144.04	6.19E+00	1.25E+01	2.93E+05	0.00E+00
13–29	3De 4–3Fe 19	7–9	144.38	6.21E+00	1.25E+01	1.44E+06	2.88E−01
14–29	1De 4–3Fe 19	5–9	163.42	6.94E+00	1.25E+01	8.15E+02	0.00E+00
27–29	3Fe 19–3Fe 19	5–9	26802	1.25E+01	1.25E+01	5.29E−09	0.00E+00
28–29	3Fe 19–3Fe 19	7–9	50626	1.25E+01	1.25E+01	6.56E−09	1.56E−01
1–30	1Se 1–3Pe 19	1–5	71.03	0.00E+00	1.28E+01	1.11E+05	0.00E+00
6–30	3Pe 3–3Pe 19	1–5	117.19	5.05E+00	1.28E+01	5.86E+00	0.00E+00
7–30	1De 3–3Pe 19	5–5	117.89	5.10E+00	1.28E+01	4.30E+05	3.40E−02
8–30	3Pe 3–3Pe 19	3–5	118.59	5.14E+00	1.28E+01	2.39E+01	1.77E−02
9–30	3Pe 3–3Pe 19	5–5	121.06	5.30E+00	1.28E+01	8.03E+04	7.19E+00
10–30	1Se 3–3Pe 19	1–5	133.66	6.01E+00	1.28E+01	7.91E+03	0.00E+00
11–30	3De 4–3Pe 19	3–5	137.16	6.19E+00	1.28E+01	8.99E+04	1.14E+00
12–30	3De 4–3Pe 19	5–5	137.36	6.19E+00	1.28E+01	1.80E+05	2.91E−01
13–30	3De 4–3Pe 19	7–5	137.66	6.21E+00	1.28E+01	3.55E+05	1.64E−02
14–30	1De 4–3Pe 19	5–5	154.86	6.94E+00	1.28E+01	8.88E+05	4.10E−02
27–30	3Fe 19–3Pe 19	5–5	2664	1.25E+01	1.28E+01	1.15E−02	3.62E+00
28–30	3Fe 19–3Pe 19	7–5	2795	1.25E+01	1.28E+01	3.38E−02	5.84E+00
29–30	3Fe 19–3Pe 19	9–5	2958	1.25E+01	1.28E+01	1.21E−01	0.00E+00
7–31	1De 3–3Pe 19	5–1	115.72	5.10E+00	1.30E+01	8.75E+02	0.00E+00
8–31	3Pe 3–3Pe 19	3–1	116.39	5.14E+00	1.30E+01	0.00E+00	7.83E+00
9–31	3Pe 3–3Pe 19	5–1	118.77	5.30E+00	1.30E+01	2.04E+03	0.00E+00
11–31	3De 4–3Pe 19	3–1	134.22	6.19E+00	1.30E+01	0.00E+00	1.35E+00
12–31	3De 4–3Pe 19	5–1	134.41	6.19E+00	1.30E+01	2.45E+06	0.00E+00
14–31	1De 4–3Pe 19	5–1	151.13	6.94E+00	1.30E+01	7.55E+02	0.00E+00
27–31	3Fe 19–3Pe 19	5–1	1868	1.25E+01	1.30E+01	5.12E+00	0.00E+00
30–31	3Pe 19–3Pe 19	5–1	6260	1.28E+01	1.30E+01	2.97E−03	0.00E+00
1–32	1Se 1–3Pe 19	1–3	70.19	0.00E+00	1.30E+01	0.00E+00	1.77E+00
6–32	3Pe 3–3Pe 19	1–3	114.91	5.05E+00	1.30E+01	0.00E+00	2.36E+00
7–32	1De 3–3Pe 19	5–3	115.58	5.10E+00	1.30E+01	4.93E+01	3.72E−02
8–32	3Pe 3–3Pe 19	3–3	116.25	5.14E+00	1.30E+01	2.60E+02	7.86E−04
9–32	3Pe 3–3Pe 19	5–3	118.63	5.30E+00	1.30E+01	5.85E+02	9.76E+00
10–32	1Se 3–3Pe 19	1–3	130.69	6.01E+00	1.30E+01	0.00E+00	1.85E+00
11–32	3De 4–3Pe 19	3–3	134.04	6.19E+00	1.30E+01	1.12E+06	5.77E−06
12–32	3De 4–3Pe 19	5–3	134.23	6.19E+00	1.30E+01	2.06E+05	3.84E−01
13–32	3De 4–3Pe 19	7–3	134.52	6.21E+00	1.30E+01	1.14E+06	0.00E+00
14–32	1De 4–3Pe 19	5–3	150.90	6.94E+00	1.30E+01	4.14E+01	3.69E−01
27–32	3Fe 19–3Pe 19	5–3	1834	1.25E+01	1.30E+01	1.82E+00	4.78E−02
28–32	3Fe 19–3Pe 19	7–3	1895	1.25E+01	1.30E+01	3.14E+00	0.00E+00
30–32	3Pe 19–3Pe 19	5–3	5892	1.28E+01	1.30E+01	3.46E−03	3.02E+01
31–32	3Pe 19–3Pe 19	1–3	100497	1.30E+01	1.30E+01	0.00E+00	1.77E−02
1–33	1Se 1–1De 19	1–5	71.30	0.00E+00	1.28E+01	4.06E+04	0.00E+00
6–33	3Pe 3–1De 19	1–5	117.92	5.05E+00	1.28E+01	3.66E+02	0.00E+00
7–33	1De 3–1De 19	5–5	118.63	5.10E+00	1.28E+01	1.43E+05	5.99E+00
8–33	3Pe 3–1De 19	3–5	119.34	5.14E+00	1.28E+01	4.42E+02	6.66E+00
9–33	3Pe 3–1De 19	5–5	121.84	5.30E+00	1.28E+01	3.35E+04	2.77E−01
10–33	1Se 3–1De 19	1–5	134.60	6.01E+00	1.28E+01	2.61E+03	0.00E+00
11–33	3De 4–1De 19	3–5	138.16	6.19E+00	1.28E+01	1.15E+05	1.28E−01
12–33	3De 4–1De 19	5–5	138.36	6.19E+00	1.28E+01	5.64E+05	1.10E−01
13–33	3De 4–1De 19	7–5	138.67	6.21E+00	1.28E+01	8.36E+05	2.12E−01
14–33	1De 4–1De 19	5–5	156.14	6.94E+00	1.28E+01	3.39E+05	3.77E−02
27–33	3Fe 19–1De 19	5–5	3099	1.25E+01	1.28E+01	6.91E−03	4.24E−01
28–33	3Fe 19–1De 19	7–5	3277	1.25E+01	1.28E+01	4.56E−02	1.01E+00
29–33	3Fe 19–1De 19	9–5	3504	1.25E+01	1.28E+01	1.16E−01	0.00E+00
30–33	3Pe 19–1De 19	5–5	18984	1.28E+01	1.28E+01	1.26E−06	1.18E+00
31–33	3Pe 19–1De 19	1–5	4707	1.30E+01	1.28E+01	6.34E−03	0.00E+00
32–33	3Pe 19–1De 19	3–5	4497	1.30E+01	1.28E+01	1.73E−02	1.08E+02
7–34	1De 3–1Ge 19	5–9	118.00	5.10E+00	1.28E+01	1.20E+06	0.00E+00
9–34	3Pe 3–1Ge 19	5–9	121.18	5.30E+00	1.28E+01	2.21E+05	0.00E+00
12–34	3De 4–1Ge 19	5–9	137.50	6.19E+00	1.28E+01	1.10E+02	0.00E+00
13–34	3De 4–1Ge 19	7–9	137.81	6.21E+00	1.28E+01	3.75E+03	9.88E−01
14–34	1De 4–1Ge 19	5–9	155.05	6.94E+00	1.28E+01	7.65E+05	0.00E+00

(*continued on next page*)

Table 4. (*continued*)

i–j	T_iC_i–T_jC_j	g_i–g_j	λ (Å)	E_i (Ry)	E_j (Ry)	AE2	AM1
27–34	3Fe 19–1Ge 19	5–9	2720	1.25E+01	1.28E+01	9.94E−04	0.00E+00
28–34	3Fe 19–1Ge 19	7–9	2856	1.25E+01	1.28E+01	2.37E−05	1.75E+00
29–34	3Fe 19–1Ge 19	9–9	3027	1.25E+01	1.28E+01	7.57E−04	2.52E+00
30–34	3Pe 19–1Ge 19	5–9	130163	1.28E+01	1.28E+01	5.47E−10	0.00E+00
33–34	1De 19–1Ge 19	5–9	22226	1.28E+01	1.28E+01	1.83E−06	0.00E+00
7–35	1De 3–1Se 19	5–1	107.82	5.10E+00	1.36E+01	3.95E+05	0.00E+00
8–35	3Pe 3–1Se 19	3–1	108.41	5.14E+00	1.36E+01	0.00E+00	2.12E+02
9–35	3Pe 3–1Se 19	5–1	110.47	5.30E+00	1.36E+01	8.60E+04	0.00E+00
11–35	3De 4–1Se 19	3–1	123.72	6.19E+00	1.36E+01	0.00E+00	7.16E−01
12–35	3De 4–1Se 19	5–1	123.88	6.19E+00	1.36E+01	2.61E+03	0.00E+00
14–35	1De 4–1Se 19	5–1	137.94	6.94E+00	1.36E+01	2.16E+06	0.00E+00
27–35	3Fe 19–1Se 19	5–1	856.45	1.25E+01	1.36E+01	1.11E+00	0.00E+00
30–35	3Pe 19–1Se 19	5–1	1262	1.28E+01	1.36E+01	6.94E+01	0.00E+00
32–35	3Pe 19–1Se 19	3–1	1606	1.30E+01	1.36E+01	0.00E+00	2.61E+01
33–35	1De 19–1Se 19	5–1	1183	1.28E+01	1.36E+01	4.05E+01	0.00E+00
1–36	1Se 1–3Se 6	1–3	56.70	0.00E+00	1.61E+01	0.00E+00	3.27E+01
6–36	3Pe 3–3Se 6	1–3	82.70	5.05E+00	1.61E+01	0.00E+00	9.55E+00
7–36	1De 3–3Se 6	5–3	83.05	5.10E+00	1.61E+01	1.05E+00	7.76E−01
8–36	3Pe 3–3Se 6	3–3	83.40	5.14E+00	1.61E+01	8.96E+00	7.99E+00
9–36	3Pe 3–3Se 6	5–3	84.61	5.30E+00	1.61E+01	8.05E+01	6.06E+00
10–36	1Se 3–3Se 6	1–3	90.57	6.01E+00	1.61E+01	0.00E+00	2.96E−02
11–36	3De 4–3Se 6	3–3	92.17	6.19E+00	1.61E+01	3.27E+06	2.18E−02
12–36	3De 4–3Se 6	5–3	92.26	6.19E+00	1.61E+01	5.46E+06	6.47E−02
13–36	3De 4–3Se 6	7–3	92.40	6.21E+00	1.61E+01	7.67E+06	0.00E+00
14–36	1De 4–3Se 6	5–3	99.84	6.94E+00	1.61E+01	1.58E+03	8.55E−03
27–36	3Fe 19–3Se 6	5–3	254.19	1.25E+01	1.61E+01	3.88E−03	2.11E−07
28–36	3Fe 19–3Se 6	7–3	255.33	1.25E+01	1.61E+01	5.98E−03	0.00E+00
30–36	3Pe 19–3Se 6	5–3	281.00	1.28E+01	1.61E+01	7.47E−03	4.40E−03
31–36	3Pe 19–3Se 6	1–3	294.20	1.30E+01	1.61E+01	0.00E+00	1.36E−02
32–36	3Pe 19–3Se 6	3–3	295.06	1.30E+01	1.61E+01	3.17E−04	1.03E−02
33–36	1De 19–3Se 6	5–3	276.90	1.28E+01	1.61E+01	1.35E−04	1.27E−02
35–36	1Se 19–3Se 6	1–3	361.47	1.36E+01	1.61E+01	0.00E+00	5.30E−04
7–37	1De 3–1Se 6	5–1	81.48	5.10E+00	1.63E+01	8.85E+06	0.00E+00
8–37	3Pe 3–1Se 6	3–1	81.81	5.14E+00	1.63E+01	0.00E+00	3.12E+01
9–37	3Pe 3–1Se 6	5–1	82.98	5.30E+00	1.63E+01	1.61E+06	0.00E+00
11–37	3De 4–1Se 6	3–1	90.24	6.19E+00	1.63E+01	0.00E+00	9.51E−02
i–j	T_iC_i–T_jC_j	g_i–g_j	λ (Å)	E_i (Ry)	E_j (Ry)	AE3	AM2
E3 and M2, N_{tr} = 1896							
1–4	1Se 1–3Po 2	1–5	393.98	0.00E+00	2.31E+00	0.00E+00	3.38E+00
4–6	3Po 2–3Pe 3	5–1	332.55	2.31E+00	5.05E+00	0.00E+00	2.99E+00
2–7	3Po 2–1De 3	1–5	306.97	2.13E+00	5.10E+00	0.00E+00	6.54E+00
2–9	3Po 2–3Pe 3	1–5	287.38	2.13E+00	5.30E+00	0.00E+00	6.08E−02
4–10	3Po 2–1Se 3	5–1	246.42	2.31E+00	6.01E+00	0.00E+00	4.03E+01
2–12	3Po 2–3De 4	1–5	224.24	2.13E+00	6.19E+00	0.00E+00	3.19E+01
2–13	3Po 2–3De 4	1–7	223.43	2.13E+00	6.21E+00	1.63E−01	0.00E+00
3–13	3Po 2–3De 4	3–7	226.37	2.18E+00	6.21E+00	2.97E−01	2.63E+01
5–13	1Po 2–3De 4	3–7	303.48	3.21E+00	6.21E+00	2.60E−04	7.88E+00
2–14	3Po 2–1De 4	1–5	189.30	2.13E+00	6.94E+00	0.00E+00	1.32E+00
1–15	1Se 1–3Fo 5	1–5	107.73	0.00E+00	8.46E+00	0.00E+00	1.15E+00
6–15	3Pe 3–3Fo 5	1–5	267.58	5.05E+00	8.46E+00	0.00E+00	6.38E+00
10–15	1Se 3–3Fo 5	1–5	372.28	6.01E+00	8.46E+00	0.00E+00	4.06E−02
1–16	1Se 1–3Fo 5	1–7	106.60	0.00E+00	8.55E+00	1.31E−02	0.00E+00
6–16	3Pe 3–3Fo 5	1–7	260.69	5.05E+00	8.55E+00	7.10E−02	0.00E+00
8–16	3Pe 3–3Fo 5	3–7	267.72	5.14E+00	8.55E+00	1.28E−02	4.23E+00
10–16	1Se 3–3Fo 5	1–7	359.08	6.01E+00	8.55E+00	1.28E−04	0.00E+00
11–16	3De 4–3Fo 5	3–7	385.57	6.19E+00	8.55E+00	5.31E−03	1.36E+00
7–17	1De 3–3Fo 5	5–9	256.38	5.10E+00	8.65E+00	1.95E−02	4.41E+01
8–17	3Pe 3–3Fo 5	3–9	259.70	5.14E+00	8.65E+00	6.88E−02	0.00E+00
9–17	3Pe 3–3Fo 5	5–9	271.85	5.30E+00	8.65E+00	7.15E−02	1.43E−02
11–17	3De 4–3Fo 5	3–9	369.16	6.19E+00	8.65E+00	9.03E−04	0.00E+00
12–17	3De 4–3Fo 5	5–9	370.55	6.19E+00	8.65E+00	7.35E−03	1.18E+00
14–17	1De 4–3Fo 5	5–9	533.15	6.94E+00	8.65E+00	3.17E−09	1.74E−02
1–18	1Se 1–1Do 5	1–5	105.43	0.00E+00	8.64E+00	0.00E+00	9.43E+00
6–18	3Pe 3–1Do 5	1–5	253.81	5.05E+00	8.64E+00	0.00E+00	6.74E+00
10–18	1Se 3–1Do 5	1–5	346.16	6.01E+00	8.64E+00	0.00E+00	1.58E+00
13–19	3De 4–3Do 5	7–3	331.72	6.21E+00	8.96E+00	4.18E−02	8.24E−02
1–20	1Se 1–3Po 5	1–5	101.68	0.00E+00	8.96E+00	0.00E+00	5.31E−01
6–20	3Pe 3–3Po 5	1–5	233.11	5.05E+00	8.96E+00	0.00E+00	1.29E−03
10–20	1Se 3–3Po 5	1–5	308.76	6.01E+00	8.96E+00	0.00E+00	2.64E+00
7–21	1De 3–3Po 5	5–1	229.21	5.10E+00	9.08E+00	0.00E+00	9.53E−01
9–21	3Pe 3–3Po 5	5–1	241.50	5.30E+00	9.08E+00	0.00E+00	6.45E+01
12–21	3De 4–3Po 5	5–1	316.36	6.19E+00	9.08E+00	0.00E+00	7.58E+00
13–21	3De 4–3Po 5	7–1	317.99	6.21E+00	9.08E+00	7.19E−02	0.00E+00
14–21	1De 4–3Po 5	5–1	427.72	6.94E+00	9.08E+00	0.00E+00	4.49E−01
13–22	3De 4–3Po 5	7–3	317.64	6.21E+00	9.08E+00	1.26E−02	4.53E+00

Table 4. (*continued*)

i–j	T_iC_i–T_jC_j	g_i–g_j	λ (Å)	E_i (Ry)	E_j (Ry)	AE3	AM2
1–23	1Se 1–3Do 5	1–7	100.52	0.00E+00	9.07E+00	4.56E−02	0.00E+00
6–23	3Pe 3–3Do 5	1–7	227.10	5.05E+00	9.07E+00	1.92E−01	0.00E+00
8–23	3Pe 3–3Do 5	3–7	232.42	5.14E+00	9.07E+00	3.71E−01	1.85E+01
10–23	1Se 3–3Do 5	1–7	298.31	6.01E+00	9.07E+00	3.24E−04	0.00E+00
11–23	3De 4–3Do 5	3–7	316.37	6.19E+00	9.07E+00	1.22E−02	3.67E−01
1–24	1Se 1–3Do 5	1–5	100.34	0.00E+00	9.08E+00	0.00E+00	1.43E+00
6–24	3Pe 3–3Do 5	1–5	226.19	5.05E+00	9.08E+00	0.00E+00	4.17E+01
10–24	1Se 3–3Do 5	1–5	296.74	6.01E+00	9.08E+00	0.00E+00	1.41E+00
1–25	1Se 1–1Fo 5	1–7	94.12	0.00E+00	9.68E+00	1.03E+01	0.00E+00
6–25	3Pe 3–1Fo 5	1–7	196.85	5.05E+00	9.68E+00	4.02E−04	0.00E+00
8–25	3Pe 3–1Fo 5	3–7	200.83	5.14E+00	9.68E+00	7.15E−03	3.94E−01
10–25	1Se 3–1Fo 5	1–7	248.21	6.01E+00	9.68E+00	7.98E−02	0.00E+00
11–25	3De 4–1Fo 5	3–7	260.59	6.19E+00	9.68E+00	1.05E−05	6.81E+00
13–26	3De 4–1Po 5	7–3	254.15	6.21E+00	9.80E+00	3.22E−03	1.07E+01
2–27	3Po 2–3Fe 19	1–5	87.99	2.13E+00	1.25E+01	0.00E+00	2.52E+00
17–27	3Fo 5–3Fe 19	9–5	237.74	8.65E+00	1.25E+01	2.67E−02	2.35E+00
21–27	3Po 5–3Fe 19	1–5	267.09	9.08E+00	1.25E+01	0.00E+00	3.12E+00
2–28	3Po 2–3Fe 19	1–7	87.86	2.13E+00	1.25E+01	4.45E−01	0.00E+00
3–28	3Po 2–3Fe 19	3–7	88.31	2.18E+00	1.25E+01	5.65E−02	3.39E+00
5–28	1Po 2–3Fe 19	3–7	98.03	3.21E+00	1.25E+01	2.12E−04	3.24E−02
19–28	3Do 5–3Fe 19	3–7	256.96	8.96E+00	1.25E+01	1.21E−01	3.70E+00
21–28	3Po 5–3Fe 19	1–7	265.85	9.08E+00	1.25E+01	1.36E−02	0.00E+00
22–28	3Po 5–3Fe 19	3–7	266.09	9.08E+00	1.25E+01	1.94E−02	1.16E+01
26–28	1Po 5–3Fe 19	3–7	336.52	9.80E+00	1.25E+01	1.77E−04	6.96E−03
3–29	3Po 2–3Fe 19	3–9	88.16	2.18E+00	1.25E+01	5.16E−01	0.00E+00
4–29	3Po 2–3Fe 19	5–9	89.27	2.31E+00	1.25E+01	7.75E−01	5.23E+00
5–29	1Po 2–3Fe 19	3–9	97.84	3.21E+00	1.25E+01	1.17E−02	0.00E+00
15–29	3Fo 5–3Fe 19	5–9	224.33	8.46E+00	1.25E+01	1.12E−02	1.56E+01
18–29	1Do 5–3Fe 19	5–9	235.01	8.64E+00	1.25E+01	8.12E−05	2.29E+01
19–29	3Do 5–3Fe 19	3–9	255.66	8.96E+00	1.25E+01	3.40E−02	0.00E+00
20–29	3Po 5–3Fe 19	5–9	256.07	8.96E+00	1.25E+01	1.49E−01	5.95E−01
22–29	3Po 5–3Fe 19	3–9	264.70	9.08E+00	1.25E+01	2.33E−03	0.00E+00
24–29	3Do 5–3Fe 19	5–9	264.97	9.08E+00	1.25E+01	1.98E−02	1.27E+01
26–29	1Po 5–3Fe 19	3–9	334.30	9.80E+00	1.25E+01	2.47E−07	0.00E+00
2–30	3Po 2–3Pe 19	1–5	85.18	2.13E+00	1.28E+01	0.00E+00	1.52E−02
17–30	3Fo 5–3Pe 19	9–5	218.26	8.65E+00	1.28E+01	1.13E−01	7.45E+00
21–30	3Po 5–3Pe 19	1–5	242.76	9.08E+00	1.28E+01	0.00E+00	6.15E+00
4–31	3Po 2–3Pe 19	5–1	85.47	2.31E+00	1.30E+01	0.00E+00	4.50E+00
15–31	3Fo 5–3Pe 19	5–1	201.80	8.46E+00	1.30E+01	0.00E+00	8.60E+00
16–31	3Fo 5–3Pe 19	7–1	205.90	8.55E+00	1.30E+01	1.18E+00	0.00E+00
18–31	1Do 5–3Pe 19	5–1	210.40	8.64E+00	1.30E+01	0.00E+00	8.71E+00
20–31	3Po 5–3Pe 19	5–1	227.13	8.96E+00	1.30E+01	0.00E+00	1.16E+01
23–31	3Do 5–3Pe 19	7–1	233.13	9.07E+00	1.30E+01	4.99E−01	0.00E+00
24–31	3Do 5–3Pe 19	5–1	234.10	9.08E+00	1.30E+01	0.00E+00	8.27E+01
25–31	1Fo 5–3Pe 19	7–1	276.80	9.68E+00	1.30E+01	2.04E−04	0.00E+00
16–32	3Fo 5–3Pe 19	7–3	205.48	8.55E+00	1.30E+01	2.89E−02	1.51E+00
17–32	3Fo 5–3Pe 19	9–3	210.47	8.65E+00	1.30E+01	5.78E−01	0.00E+00
23–32	3Do 5–3Pe 19	7–3	232.59	9.07E+00	1.30E+01	2.89E−01	3.96E+01
25–32	1Fo 5–3Pe 19	7–3	276.04	9.68E+00	1.30E+01	3.39E−04	7.22E−02
2–33	3Po 2–1De 19	1–5	85.56	2.13E+00	1.28E+01	0.00E+00	1.05E+00
17–33	3Fo 5–1De 19	9–5	220.80	8.65E+00	1.28E+01	3.06E−01	2.17E−01
21–33	3Po 5–1De 19	1–5	245.90	9.08E+00	1.28E+01	0.00E+00	3.30E−02
3–34	3Po 2–1Ge 19	3–9	85.66	2.18E+00	1.28E+01	9.76E−02	0.00E+00
4–34	3Po 2–1Ge 19	5–9	86.71	2.31E+00	1.28E+01	3.14E−03	7.28E−03
5–34	1Po 2–1Ge 19	3–9	94.77	3.21E+00	1.28E+01	1.07E+01	0.00E+00
15–34	3Fo 5–1Ge 19	5–9	208.85	8.46E+00	1.28E+01	8.30E−02	7.09E+01
18–34	1Do 5–1Ge 19	5–9	218.08	8.64E+00	1.28E+01	4.75E−01	2.51E+00
19–34	3Do 5–1Ge 19	3–9	235.75	8.96E+00	1.28E+01	1.80E−03	0.00E+00
20–34	3Po 5–1Ge 19	5–9	236.10	8.96E+00	1.28E+01	3.64E−03	1.33E−02
22–34	3Po 5–1Ge 19	3–9	243.42	9.08E+00	1.28E+01	1.81E−06	0.00E+00
24–34	3Do 5–1Ge 19	5–9	243.65	9.08E+00	1.28E+01	1.80E−03	3.87E−01
26–34	1Po 5–1Ge 19	3–9	301.06	9.80E+00	1.28E+01	4.99E−02	0.00E+00
4–35	3Po 2–1Se 19	5–1	81.09	2.31E+00	1.36E+01	0.00E+00	6.26E−01
15–35	3Fo 5–1Se 19	5–1	178.95	8.46E+00	1.36E+01	0.00E+00	8.14E+00
16–35	3Fo 5–1Se 19	7–1	182.17	8.55E+00	1.36E+01	3.10E−02	0.00E+00
18–35	1Do 5–1Se 19	5–1	185.69	8.64E+00	1.36E+01	0.00E+00	7.13E+01
20–35	3Po 5–1Se 19	5–1	198.59	8.96E+00	1.36E+01	0.00E+00	3.64E+01
23–35	3Do 5–1Se 19	7–1	203.17	9.07E+00	1.36E+01	4.26E−03	0.00E+00
24–35	3Do 5–1Se 19	5–1	203.90	9.08E+00	1.36E+01	0.00E+00	3.93E+01
25–35	1Fo 5–1Se 19	7–1	235.55	9.68E+00	1.36E+01	1.02E+00	0.00E+00
16–36	3Fo 5–3Se 6	7–3	121.13	8.55E+00	1.61E+01	8.69E−01	1.25E−03
17–36	3Fo 5–3Se 6	9–3	122.84	8.65E+00	1.61E+01	1.03E+00	0.00E+00
23–36	3Do 5–3Se 6	7–3	130.07	9.07E+00	1.61E+01	4.01E−03	1.36E−01
25–36	1Fo 5–3Se 6	7–3	142.62	9.68E+00	1.61E+01	1.51E−04	2.97E−04
4–37	3Po 2–1Se 6	5–1	65.23	2.31E+00	1.63E+01	0.00E+00	6.30E+03
15–37	3Fo 5–1Se 6	5–1	116.45	8.46E+00	1.63E+01	0.00E+00	4.00E−02

(*continued on next page*)

Table 4. (*continued*)

i–*j*	T_iC_i–T_jC_j	g_i–g_j	λ (Å)	E_i (Ry)	E_j (Ry)	AE3	AM2
16–37	3Fo 5–1Se 6	7–1	117.81	8.55E+00	1.63E+01	5.12E−02	0.00E+00
18–37	1Do 5–1Se 6	5–1	119.27	8.64E+00	1.63E+01	0.00E+00	1.09E−01
20–37	3Po 5–1Se 6	5–1	124.46	8.96E+00	1.63E+01	0.00E+00	9.00E−01
23–37	3Do 5–1Se 6	7–1	126.25	9.07E+00	1.63E+01	6.93E−02	0.00E+00
24–37	3Do 5–1Se 6	5–1	126.53	9.08E+00	1.63E+01	0.00E+00	5.51E−01
25–37	1Fo 5–1Se 6	7–1	138.04	9.68E+00	1.63E+01	6.39E+00	0.00E+00
7–38	1De 3–3Po 7	5–1	75.30	5.10E+00	1.72E+01	0.00E+00	2.32E+02
9–38	3Pe 3–3Po 7	5–1	76.58	5.30E+00	1.72E+01	0.00E+00	8.36E+01
12–38	3De 4–3Po 7	5–1	82.79	6.19E+00	1.72E+01	0.00E+00	1.85E+03
13–38	3De 4–3Po 7	7–1	82.90	6.21E+00	1.72E+01	1.70E+03	0.00E+00
14–38	1De 4–3Po 7	5–1	88.84	6.94E+00	1.72E+01	0.00E+00	1.68E+02
27–38	3Fe 19–3Po 7	5–1	193.29	1.25E+01	1.72E+01	0.00E+00	1.70E−02
28–38	3Fe 19–3Po 7	7–1	193.94	1.25E+01	1.72E+01	3.43E−04	0.00E+00
30–38	3Pe 19–3Po 7	5–1	208.40	1.28E+01	1.72E+01	0.00E+00	2.02E−02
33–38	1De 19–3Po 7	5–1	206.14	1.28E+01	1.72E+01	0.00E+00	1.23E−02
13–39	3De 4–3Po 7	7–3	82.86	6.21E+00	1.72E+01	9.02E+02	2.15E+02
28–39	3Fe 19–3Po 7	7–3	193.69	1.25E+01	1.72E+01	4.94E−06	7.16E−03
29–39	3Fe 19–3Po 7	9–3	194.44	1.25E+01	1.72E+01	6.13E−05	0.00E+00
34–39	1Ge 19–3Po 7	9–3	207.78	1.28E+01	1.72E+01	1.38E−03	0.00E+00
1–40	1Se 1–3Po 7	1–5	52.80	0.00E+00	1.73E+01	0.00E+00	4.91E+03
6–40	3Pe 3–3Po 7	1–5	74.66	5.05E+00	1.73E+01	0.00E+00	1.24E+00
10–40	1Se 3–3Po 7	1–5	81.02	6.01E+00	1.73E+01	0.00E+00	6.22E−01
29–40	3Fe 19–3Po 7	9–5	192.34	1.25E+01	1.73E+01	1.28E−04	1.09E−02
31–40	3Pe 19–3Po 7	1–5	212.70	1.30E+01	1.73E+01	0.00E+00	4.69E−04
34–40	1Ge 19–3Po 7	9–5	205.38	1.28E+01	1.73E+01	7.56E−07	9.70E−06
35–40	1Se 19–3Po 7	1–5	245.77	1.36E+01	1.73E+01	0.00E+00	1.06E−01
37–40	1Se 6–3Po 7	1–5	934.76	1.63E+01	1.73E+01	0.00E+00	8.74E−02
13–41	3De 4–1Po 7	7–3	82.74	6.21E+00	1.72E+01	2.37E+02	1.21E+03
28–41	3Fe 19–1Po 7	7–3	193.07	1.25E+01	1.72E+01	6.21E−06	1.89E−03
29–41	3Fe 19–1Po 7	9–3	193.80	1.25E+01	1.72E+01	1.56E−04	0.00E+00
34–41	1Ge 19–1Po 7	9–3	207.06	1.28E+01	1.72E+01	6.40E−03	0.00E+00
16–42	3Fo 5–3De 8	7–3	91.47	8.55E+00	1.85E+01	2.68E+01	5.31E+01
17–42	3Fo 5–3De 8	9–3	92.45	8.65E+00	1.85E+01	3.67E+00	0.00E+00
23–42	3Do 5–3De 8	7–3	96.48	9.07E+00	1.85E+01	1.07E−01	1.36E+00
25–42	1Fo 5–3De 8	7–3	103.22	9.68E+00	1.85E+01	9.30E−02	3.70E+01
2–43	3Po 2–3De 8	1–5	55.61	2.13E+00	1.85E+01	0.00E+00	8.54E+03
17–43	3Fo 5–3De 8	9–5	92.39	8.65E+00	1.85E+01	1.59E+01	2.42E+01
21–43	3Po 5–3De 8	1–5	96.51	9.08E+00	1.85E+01	0.00E+00	1.64E+00
38–43	3Po 7–3De 8	1–5	692.77	1.72E+01	1.85E+01	0.00E+00	5.34E−01
2–44	3Po 2–3De 8	1–7	55.57	2.13E+00	1.85E+01	6.24E+03	0.00E+00
3–44	3Po 2–3De 8	3–7	55.76	2.18E+00	1.85E+01	1.23E+04	6.68E+03
5–44	1Po 2–3De 8	3–7	59.48	3.21E+00	1.85E+01	5.96E+01	3.73E+03
19–44	3Do 5–3De 8	3–7	95.21	8.96E+00	1.85E+01	2.25E−01	6.41E−01
21–44	3Po 5–3De 8	1–7	96.40	9.08E+00	1.85E+01	5.91E−02	0.00E+00
22–44	3Po 5–3De 8	3–7	96.43	9.08E+00	1.85E+01	2.41E−02	1.39E+00
26–44	1Po 5–3De 8	3–7	104.35	9.80E+00	1.85E+01	8.32E−03	2.82E+00
38–44	3Po 7–3De 8	1–7	687.03	1.72E+01	1.85E+01	4.01E−03	0.00E+00
39–44	3Po 7–3De 8	3–7	690.19	1.72E+01	1.85E+01	6.13E−03	8.44E−02
41–44	1Po 7–3De 8	3–7	698.29	1.72E+01	1.85E+01	1.52E−03	8.19E−01
2–45	3Po 2–1De 8	1–5	55.51	2.13E+00	1.85E+01	0.00E+00	8.87E+02
17–45	3Fo 5–1De 8	9–5	92.11	8.65E+00	1.85E+01	8.76E−01	4.12E+01
21–45	3Po 5–1De 8	1–5	96.21	9.08E+00	1.85E+01	0.00E+00	3.93E−03
38–45	3Po 7–1De 8	1–5	677.32	1.72E+01	1.85E+01	0.00E+00	9.43E−02
7–46	1De 3–3Po 13	5–1	66.48	5.10E+00	1.88E+01	0.00E+00	3.57E+03
9–46	3Pe 3–3Po 13	5–1	67.48	5.30E+00	1.88E+01	0.00E+00	3.97E+02
12–46	3De 4–3Po 13	5–1	72.25	6.19E+00	1.88E+01	0.00E+00	3.77E+01
13–46	3De 4–3Po 13	7–1	72.34	6.21E+00	1.88E+01	4.63E+01	0.00E+00
14–46	1De 4–3Po 13	5–1	76.82	6.94E+00	1.88E+01	0.00E+00	4.13E+02
27–46	3Fe 19–3Po 13	5–1	144.19	1.25E+01	1.88E+01	0.00E+00	5.47E−03
28–46	3Fe 19–3Po 13	7–1	144.55	1.25E+01	1.88E+01	4.32E−01	0.00E+00
30–46	3Pe 19–3Po 13	5–1	152.44	1.28E+01	1.88E+01	0.00E+00	1.79E+00
33–46	1De 19–3Po 13	5–1	151.22	1.28E+01	1.88E+01	0.00E+00	5.41E−03
43–46	3De 8–3Po 13	5–1	3141	1.85E+01	1.88E+01	0.00E+00	1.25E−06
44–46	3De 8–3Po 13	7–1	3265	1.85E+01	1.88E+01	3.17E−09	0.00E+00
45–46	1De 8–3Po 13	5–1	3504	1.85E+01	1.88E+01	0.00E+00	8.61E−07
13–47	3De 4–3Po 13	7–3	72.15	6.21E+00	1.88E+01	2.86E+01	4.37E+01
28–47	3Fe 19–3Po 13	7–3	143.80	1.25E+01	1.88E+01	1.63E−02	2.60E−04
29–47	3Fe 19–3Po 13	9–3	144.21	1.25E+01	1.88E+01	2.15E−01	0.00E+00
34–47	1Ge 19–3Po 13	9–3	151.42	1.28E+01	1.88E+01	1.93E−01	0.00E+00
44–47	3De 8–3Po 13	7–3	2920	1.85E+01	1.88E+01	4.12E−09	5.30E−07
1–48	1Se 1–3Po 13	1–5	48.01	0.00E+00	1.90E+01	0.00E+00	6.60E−06
6–48	3Pe 3–3Po 13	1–5	65.44	5.05E+00	1.90E+01	0.00E+00	2.50E+02
10–48	1Se 3–3Po 13	1–5	70.27	6.01E+00	1.90E+01	0.00E+00	5.31E+02
29–48	3Fe 19–3Po 13	9–5	141.10	1.25E+01	1.90E+01	2.44E−01	1.59E−04
31–48	3Pe 19–3Po 13	1–5	151.76	1.30E+01	1.90E+01	0.00E+00	7.79E−02
34–48	1Ge 19–3Po 13	9–5	148.00	1.28E+01	1.90E+01	3.18E−04	1.12E−05

Table 4. (*continued*)

i–j	T_iC_i–T_jC_j	g_i–g_j	λ (Å)	E_i (Ry)	E_j (Ry)	AE3	AM2
35–48	1Se 19–3Po 13	1–5	167.87	1.36E+01	1.90E+01	0.00E+00	1.35E−01
37–48	1Se 6–3Po 13	1–5	338.09	1.63E+01	1.90E+01	0.00E+00	2.96E+00
13–49	3De 4–1Po 13	7–3	70.62	6.21E+00	1.91E+01	2.00E+00	6.26E+01
28–49	3Fe 19–1Po 13	7–3	137.87	1.25E+01	1.91E+01	2.41E−03	2.13E−06
29–49	3Fe 19–1Po 13	9–3	138.25	1.25E+01	1.91E+01	5.50E−03	0.00E+00
34–49	1Ge 19–1Po 13	9–3	144.87	1.28E+01	1.91E+01	2.72E+00	0.00E+00
44–49	3De 8–1Po 13	7–3	1559	1.85E+01	1.91E+01	6.64E−08	2.61E−04
1–50	1Se 1–3Fo 9	1–5	47.43	0.00E+00	1.92E+01	0.00E+00	8.96E−04
6–50	3Pe 3–3Fo 9	1–5	64.35	5.05E+00	1.92E+01	0.00E+00	1.09E+00
10–50	1Se 3–3Fo 9	1–5	69.02	6.01E+00	1.92E+01	0.00E+00	7.30E−03
29–50	3Fe 19–3Fo 9	9–5	136.15	1.25E+01	1.92E+01	4.89E−04	9.55E−03
31–50	3Pe 19–3Fo 9	1–5	146.05	1.30E+01	1.92E+01	0.00E+00	6.08E−03
34–50	1Ge 19–3Fo 9	9–5	142.56	1.28E+01	1.92E+01	2.09E−05	6.94E−01
35–50	1Se 19–3Fo 9	1–5	160.92	1.36E+01	1.92E+01	0.00E+00	4.62E−06
37–50	1Se 6–3Fo 9	1–5	311.01	1.63E+01	1.92E+01	0.00E+00	2.17E−06
1–51	1Se 1–3Fo 9	1–7	47.42	0.00E+00	1.92E+01	1.10E+01	0.00E+00
6–51	3Pe 3–3Fo 9	1–7	64.35	5.05E+00	1.92E+01	7.90E+00	0.00E+00
8–51	3Pe 3–3Fo 9	3–7	64.77	5.14E+00	1.92E+01	1.57E+00	1.19E+00
10–51	1Se 3–3Fo 9	1–7	69.01	6.01E+00	1.92E+01	3.20E−02	0.00E+00
11–51	3De 4–3Fo 9	3–7	69.94	6.19E+00	1.92E+01	2.36E+03	1.76E+04
31–51	3Pe 19–3Fo 9	1–7	146.03	1.30E+01	1.92E+01	2.90E−03	0.00E+00
32–51	3Pe 19–3Fo 9	3–7	146.24	1.30E+01	1.92E+01	4.92E−04	8.84E−03
35–51	1Se 19–3Fo 9	1–7	160.89	1.36E+01	1.92E+01	6.12E−05	0.00E+00
36–51	3Se 6–3Fo 9	3–7	289.94	1.61E+01	1.92E+01	1.60E+00	6.35E−07
37–51	1Se 6–3Fo 9	1–7	310.91	1.63E+01	1.92E+01	1.53E−04	0.00E+00
42–51	3De 8–3Fo 9	3–7	1294	1.85E+01	1.92E+01	5.20E−05	2.48E−02
7–52	1De 3–3Fo 9	5–9	64.54	5.10E+00	1.92E+01	1.16E+00	2.01E+03
8–52	3Pe 3–3Fo 9	3–9	64.75	5.14E+00	1.92E+01	6.72E+00	0.00E+00
9–52	3Pe 3–3Fo 9	5–9	65.48	5.30E+00	1.92E+01	1.12E+01	3.54E+02
11–52	3De 4–3Fo 9	3–9	69.92	6.19E+00	1.92E+01	2.63E+02	0.00E+00
12–52	3De 4–3Fo 9	5–9	69.97	6.19E+00	1.92E+01	2.18E+03	1.42E+04
14–52	1De 4–3Fo 9	5–9	74.25	6.94E+00	1.92E+01	7.33E−01	4.97E+03
27–52	3Fe 19–3Fo 9	5–9	135.38	1.25E+01	1.92E+01	2.46E−04	1.14E−02
30–52	3Pe 19–3Fo 9	5–9	142.63	1.28E+01	1.92E+01	1.67E−03	1.85E+00
32–52	3Pe 19–3Fo 9	3–9	146.17	1.30E+01	1.92E+01	2.90E−03	0.00E+00
33–52	1De 19–3Fo 9	5–9	141.57	1.28E+01	1.92E+01	4.83E−03	9.80E−01
36–52	3Se 6–3Fo 9	3–9	289.66	1.61E+01	1.92E+01	1.61E+00	0.00E+00
42–52	3De 8–3Fo 9	3–9	1288	1.85E+01	1.92E+01	5.96E−06	0.00E+00
43–52	3De 8–3Fo 9	5–9	1299	1.85E+01	1.92E+01	4.56E−05	1.46E−02
45–52	1De 8–3Fo 9	5–9	1358	1.85E+01	1.92E+01	9.24E−07	1.54E−02
1–53	1Se 1–1Fo 9	1–7	47.10	0.00E+00	1.93E+01	7.04E+04	0.00E+00
6–53	3Pe 3–1Fo 9	1–7	63.75	5.05E+00	1.93E+01	6.60E+00	0.00E+00
8–53	3Pe 3–1Fo 9	3–7	64.16	5.14E+00	1.93E+01	1.41E−01	8.59E−02
10–53	1Se 3–1Fo 9	1–7	68.33	6.01E+00	1.93E+01	1.20E+02	0.00E+00
11–53	3De 4–1Fo 9	3–7	69.23	6.19E+00	1.93E+01	3.92E−01	4.19E+03
31–53	3Pe 19–1Fo 9	1–7	142.98	1.30E+01	1.93E+01	1.30E−03	0.00E+00
32–53	3Pe 19–1Fo 9	3–7	143.18	1.30E+01	1.93E+01	1.36E−05	8.48E−05
35–53	1Se 19–1Fo 9	1–7	157.20	1.36E+01	1.93E+01	5.19E−01	0.00E+00
36–53	3Se 6–1Fo 9	3–7	278.16	1.61E+01	1.93E+01	3.83E−04	2.17E−06
37–53	1Se 6–1Fo 9	1–7	297.41	1.63E+01	1.93E+01	1.43E+00	0.00E+00
42–53	3De 8–1Fo 9	3–7	1088	1.85E+01	1.93E+01	2.74E−08	2.00E−02
16–54	3Fo 5–1Pe 14	7–3	81.57	8.55E+00	1.97E+01	1.79E+02	1.66E+02
17–54	3Fo 5–1Pe 14	9–3	82.35	8.65E+00	1.97E+01	7.42E+01	0.00E+00
23–54	3Do 5–1Pe 14	7–3	85.53	9.07E+00	1.97E+01	1.38E+00	5.45E+02
25–54	1Fo 5–1Pe 14	7–3	90.78	9.68E+00	1.97E+01	2.31E+02	2.06E+02
51–54	3Fo 9–1Pe 14	7–3	1804	1.92E+01	1.97E+01	4.30E−08	6.80E−05
52–54	3Fo 9–1Pe 14	9–3	1815	1.92E+01	1.97E+01	1.92E−08	0.00E+00
53–54	1Fo 9–1Pe 14	7–3	2449	1.93E+01	1.97E+01	9.81E−09	5.92E−07
16–55	3Fo 5–3De 14	7–3	80.71	8.55E+00	1.98E+01	9.65E+02	6.41E+02
17–55	3Fo 5–3De 14	9–3	81.47	8.65E+00	1.98E+01	1.03E+02	0.00E+00
23–55	3Do 5–3De 14	7–3	84.58	9.07E+00	1.98E+01	1.94E+02	1.03E+02
25–55	1Fo 5–3De 14	7–3	89.72	9.68E+00	1.98E+01	7.11E+01	5.09E+01
51–55	3Fo 9–3De 14	7–3	1458	1.92E+01	1.98E+01	2.59E−07	1.33E−04
52–55	3Fo 9–3De 14	9–3	1465	1.92E+01	1.98E+01	8.11E−09	0.00E+00
53–55	1Fo 9–3De 14	7–3	1853	1.93E+01	1.98E+01	3.66E−08	4.72E−05
2–56	3Po 2–3De 14	1–5	51.39	2.13E+00	1.99E+01	0.00E+00	1.57E+02
17–56	3Fo 5–3De 14	9–5	81.29	8.65E+00	1.99E+01	8.00E+02	7.15E+02
21–56	3Po 5–3De 14	1–5	84.46	9.08E+00	1.99E+01	0.00E+00	5.31E+00
38–56	3Po 7–3De 14	1–5	342.28	1.72E+01	1.99E+01	0.00E+00	3.48E+00
46–56	3Po 13–3De 14	1–5	862.21	1.88E+01	1.99E+01	0.00E+00	3.10E−02
52–56	3Fo 9–3De 14	9–5	1410	1.92E+01	1.99E+01	2.35E−07	3.07E−04
4–57	3Po 2–3Pe 14	5–1	51.82	2.31E+00	1.99E+01	0.00E+00	9.97E+02
15–57	3Fo 5–3Pe 14	5–1	79.66	8.46E+00	1.99E+01	0.00E+00	4.79E+02