# *Energies, electric dipole (E1), quadrupole (E2), octupole (E3) and magnetic dipole (M1), quadrupole (M2) transition rates for Ca XII, Ti XIV, Cr XVI, Fe XVIII and Ni XX*

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ORIGINAL PAPER

# Energies, electric dipole (E1), quadrupole (E2), octupole (E3) and magnetic dipole (M1), quadrupole (M2) transition rates for Ca XII, Ti XIV, Cr XVI, Fe XVIII and Ni XX

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**Abstract:** Energies, weighted oscillator strengths (*gf*), line strengths (*S*) and radiative rates (*A*) for allowed and forbidden transitions are presented for $2s2p^6\ ^2S_{1/2} - 2s^22p^5\ ^2P_{1/2}$, $^2P_{3/2}$ and $2s^22p^5\ ^2P_{1/2} - 2s^22p^5\ ^2P_{3/2}$ transitions in fluorine-like Ca XII ($Z = 20$), Ti XIV ($Z = 22$), Cr XVI ($Z = 24$), Fe XVIII ($Z = 26$) and Ni XX ($Z = 28$) ions. Moreover, the allowed electric dipole (E1) and the forbidden electric quadrupole (E2), octupole (E3), magnetic dipole (M1) and quadrupole (M2) transition rates for some transitions are obtained. The $2s^22p^5$–$2s\ 2p^6$-type transitions of F-like ions are prominent in high-temperature plasmas and are useful for diagnostics. The present results are obtained from configuration interaction atomic structure calculations using the code *SUPERSTRUCTURE* (*SS*) which includes relativistic effects in Breit–Pauli approximation. The comparison of the present energies with the available observed energies displayed very good agreement (< 1%). The presented excitation energy results have been compared with other detailed relativistic approaches such as Dirac–Fock, coupled cluster and configuration interaction for a few ionic states.

**Keywords:** Atomic processes; Atomic data; Allowed and forbidden transitions; F-like ions

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## 1. Introduction

Observations from the several space missions such as Hubble, Chandra and Spitzer provide the lines of highly charged ions. The highly stripped F-like ions are very important for astrophysical applications, high-temperature plasma diagnostics and in laboratory sources [1–3]. The detection of the forbidden transition lines in stellar spectra is very useful to search high-temperature corona for transitions between $2s^22p^5$ and $2s2p^6$ levels. In quasar spectra, such lines are also used to demonstrate the presence of high-temperature plasma associated with these objects. Many forbidden transitions within $np^k$ configurations in F-like ions have identified in tokamak discharges, in the solar corona and flares [4, 5].

By now, numerous experimental and theoretical studies have been done for fluorine-like ions such as transition energies measured using laser-irradiated solid targets by Reader et al. [6, 7], the energy levels, oscillator strengths and transition probabilities calculated using the multiconfigurational Dirac–Fock (MCDF) method by Cheng et al. [8], transition energies determined using semiempirical method by Edlen [9] and oscillator strengths calculated using CIV3 code by Mohan and Hibbert [10] and Blackford and Hibbert [11]. Moreover, the energy levels and transition rates were calculated using multiconfigurational Breit–Pauli wave functions by Froese Fischer and Tachiev [12]. Jonauskas et al. [13] calculated the energy levels and transition probabilities using the MCDF GRASP code. The relativistic configuration interaction calculations were done for energies, E1, M1, E2 transition rates by Jönsson et al. [14], and the spectral properties such as oscillator strengths, transition probabilities, lifetimes and hyperfine shifts were computed using relativistic coupled cluster method by Nandy and Sahoo [15].

**Electronic supplementary material** The online version of this article (https://doi.org/10.1007/s12648-019-01501-y) contains supplementary material, which is available to authorized users.

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The present paper reports the atomic data for several fluorine-like ions such as Ca XII, Ti XIV, Cr XVI, Fe XVIII and Ni XX having $2p$ open-shell configurations. Energy levels, weighted oscillator strengths, line strengths and transition rates for allowed and forbidden lines have been presented using the *SS* code [16, 17].

## 2. Method and formulation

The energies and $\psi = \psi(\gamma \mathrm{SLM}_S M_L | r_1, \ldots, r_N)$ wave functions can be obtained by solving time-independent Schrödinger equation for an N-electron system which is given as

$$\left[\sum_{i=1}^{N}\left\{-\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N}\frac{2}{r_{ij}}\right\}\right]\psi = E\psi; \quad H_{\mathrm{NR}}\psi = E\psi \tag{1}$$

where $H_{\mathrm{NR}}$ is the nonrelativistic Hamiltonian. While approximate solutions in the nonrelativistic bound-state problems are obtained from Eq. (1), for the ones in the relativistic bound-state problems require the additional Hamiltonian terms.

The computer program *SUPERSTRUCTURE* and the code's properties which yield bound-state energies in *LS* coupling and intermediate coupling had been described by Eissner [16, 17]. In this approach, the configuration expansion (CI) wave functions are given by

$$\psi = \sum_i \phi_i c_i \tag{2}$$

where $\phi_i$ is the configuration basis functions and $c_i$ is the mixing coefficients. In *SS*, these functions are constructed from one-electron orbitals generated in two-type potential such as both spectroscopic orbitals $P(nl)$ calculated in Thomas–Fermi–Dirac statistical model potential and correlation orbitals $P(\bar{n}l)$ obtained in a Coulomb potential [17–19]

The statistical Thomas–Fermi–Dirac–Amaldi model potential is

$$V^{\mathrm{SM}}(r) = \frac{Zeff(\lambda_{nl}, r)}{r} \tag{3}$$

where $Zeff(\lambda_{nl}, r) = Z\left[e^{-Zr/2} + \lambda_{nl}(1 - e^{-Zr/2})\right]\lambda_{nl}$ is the Thomas–Fermi scaling parameters for the orbitals [20].

Since the relativistic effects taken into account through Breit–Pauli (BP) approximation in *SS* calculations, the relativistic N-electron Breit–Pauli Hamiltonian is given in the form

$$H_{\mathrm{BP}} = H_{\mathrm{NR}} + H_{rc} \tag{4}$$

where $H_{rc}$ is a sum of relativistic correction operators consisting of one- and two-body parts and may be written as

$$H_{rc} = H_{\mathrm{Mass}} + H_{\mathrm{Dar}} + H_{SO} + \frac{1}{2}\left[g_{ij}(so + so') + g_{ij}(ss') + g_{ij}(css') + g_{ij}(d) + g_{ij}(oo')\right] \tag{5}$$

The first three terms in Eq. (5) are the one-body relativistic correction terms: $H_{\mathrm{Mass}}$ is the relativistic correction due to the variation of mass with velocity, Darwin term $H_{\mathrm{Dar}}$ is the correction term due to the retardation of the electromagnetic field produced by an electron, and $H_{\mathrm{SO}}$ is spin–orbit interaction term which is the operator representing spin–orbit interaction of the *i*th electron in the field of the nucleus [21], and they are given in Eq. (6), respectively [20]

$$H_{\mathrm{Mass}} = -\frac{\alpha^2}{4}\sum_i p_i^4, \quad H_{\mathrm{Dar}} = -\frac{\alpha^2}{4}\sum_i \nabla^2\left(\frac{Z}{r_i}\right), \quad H_{\mathrm{SO}} = \alpha^2\sum_i \frac{Z}{r_i^3} l(i)\cdot s(i) \tag{6}$$

The remaining terms consist of the two-body fine structure terms and the two-body non-fine structure terms. $g_{ij}(so + so')$; spin-other-orbit term and $g_{ij}(ss')$ spin–spin interaction term are the two-body fine structure terms. $g_{ij}(css')$; spin–spin contact interaction term, $g_{ij}(d)$; the two-body Darwin term and $g_{ij}(oo')$; the orbit–orbit interaction term are the two-body non-fine structure terms [16].

The principal physical quantities are determined depending on the line strength. The generalized *S* line strength for a transition between *i* and *j* levels is

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

where $O^{X\lambda}$ is the appropriate multipole operator. *X* represents the electric and magnetic type of *O* operator, and λ refers to a multipolarity [22, 23].

In electric dipole case, transition rate is

$$A_{ji}^{E1} = 2.6773 \times 10^9 (E_j - E_i)^3 \frac{1}{g_j} S^{E1}(i,j) \quad \mathrm{s}^{-1} \tag{8}$$

where $E_{ji} = E_j - E_i$ is the excitation energy. The absorption oscillator strength is

$$f_{ij} = \frac{E_{ji}}{3g_i} S_{ij}, \quad g_i f_{ij} = g_j f_{ji} \tag{9}$$

where energies are expressed in Rydberg and $g_i$ and $g_j$ are the statistical weights of the initial and final states, respectively. Also, the relation between transition rate and oscillator strength is given by the expression

$$A_{ji}.\tau_o = \alpha^3 \frac{g_i}{g_j} E_{ji}^2 f_{ij} \tag{10}$$

where the time unit is $\tau_o = \hbar / Ry = 4.838 \times 10^{-17}$ s [23, 24].

The electric quadrupole (E2), magnetic dipole (M1), electric octupole (E3) and magnetic quadrupole (M2) radiative transition rates depending on line strengths are

$$A_{ji}^{E2} = 2.6773 \times 10^3 (E_j - E_i)^5 \frac{1}{g_j} S^{E2}(i,j) \quad \mathrm{s}^{-1} \tag{11}$$

$$A_{ji}^{M1} = 3.5644 \times 10^4 (E_j - E_i)^3 \frac{1}{g_j} S^{M1}(i,j) \quad \mathrm{s}^{-1} \tag{12}$$

$$A_{ji}^{E3} = 1.2050 \times 10^{-3} (E_j - E_i)^7 \frac{1}{g_j} S^{E3}(i,j) \quad \mathrm{s}^{-1} \tag{13}$$

$$A_{ji}^{M2} = 2.3727 \times 10^{-2} (E_j - E_i)^5 \frac{1}{g_j} S^{M2}(i,j) \quad \mathrm{s}^{-1} \tag{14}$$

## 3. Results and discussion

In this work, allowed and forbidden fine structure transitions are studied in fluorine-like Ca XII, Ti XIV, Cr XVI, Fe XVIII and Ni XX ions using the code *SS*. All calculated energy values for these ions are given by electronic form in Table 1 as supplemental materials. In Table 1, the obtained energies are compared with some experimental data compiled by NIST [25]. These comparisons in Table 1 show that most of the calculated levels are well within < 1% of the observed energies for Ca XII, within 1.3% for Ti XIV, within < 1% for Cr XVI, within < 1% for Fe XVIII and within < 1% for Ni XX. Moreover, the largest discrepancies are 1.2% for the $2p^4 3d\ ^2D_{3/2,5/2}$ levels in Ca XII, 1.8% for the $2p^4 3p\ ^2P_{1/2,3/2}$ levels in Ti XIV, 1.4% for the $2p^4 3d\ ^4P_{5/2}$ levels in Cr XVI, 2.8% for the $2p^4 3d\ ^4P_{3/2,5/2}$ levels in Fe XVIII and 1.3% for the $2p^4 3d\ ^2F_{5/2}$ levels in Ni XX. Therefore, we can say that the overall computed energies are well agreed with the experimental values.

Table 2 presents excitation energies for $2s^2 2p^5\ ^2P_{1/2}$ and $2s2p^6\ ^2S_{1/2}$ levels obtained with the *SS* code. These energies are given in Rydberg. The obtained results are compared to some results given in the literature. They agreed very well with those by NIST [25], Jönsson et al. [14] and other results reported using the Dirac–Hartree–Fock (DHF) method and obtained from the CCSD with perturbative treatment of triple excitations CCSD(T) (CCSD; coupled cluster method with single and double excitations) method considering the Dirac–Coulomb (DC), Dirac–Coulomb–Breit (DCB), DCBV (the lower-order vacuum polarization effects incorporating the Uehling and Wichmann-Kroll potentials along with DCB) and DCBVS (the lowest-order self-energy correction to the DCBV) Hamiltonians given by Nandy and Sahoo [15]. Most of the NIST data include the results of

**Table 1** Energy levels (Ry) for (a) Ca XII, (b) Ti XIV, (c) Cr XVI, (d) Fe XVIII and (e) Ni XX

| Config. number | Configuration | Term | $J$ | $E^{SS}$ | $E^{NIST}$ |
|---|---|---|---|---|---|
| (a) | | | | | |
| 1 | $2s^2 2p^5$ | $^2P^o$ | 3/2 | 0 | 0 |
| 1 | | | 1/2 | 0.2737 | 0.2737 |
| 2 | $2s2p^6$ | $^2S$ | 1/2 | 6.461 | 6.461 |
| 3 | $2s^2 2p^4(^3P)3s$ | $^4P$ | 5/2 | 28.045 | 27.906 |
| 3 | | | 3/2 | 28.167 | 28.041 |
| 3 | $2s^2 2p^4(^3P)3s$ | $^2P$ | 1/2 | 28.270 | 28.152 |
| 3 | | | 3/2 | 28.340 | 28.229 |
| 3 | $2s^2 2p^4(^1D)3s$ | $^2D$ | 1/2 | 28.480 | 28.384 |
| 3 | | | 5/2 | 28.905 | 28.782 |
| 3 | $2s^2 2p^4(^1S)3s$ | $^2S$ | 3/2 | 28.911 | 28.79 |
| 6 | $2s^2 2p^4(^3P)3d$ | $^4P$ | 1/2 | 29.619 | 29.613 |
| 6 | | | 1/2 | 31.883 | 31.674 |
| 6 | | | 3/2 | 31.940 | 31.708 |
| 6 | $2s^2 2p^4(^3P)3d$ | $^4F$ | 5/2 | 32.019 | 31.798 |
| 6 | $2s^2 2p^4(^3P)3d$ | $^2P$ | 5/2 | 31.917 | 31.712 |
| 6 | | | 1/2 | 31.987 | 31.773 |
| 6 | $2s^2 2p^4(^3P)3d$ | $^2D$ | 3/2 | 32.189 | 31.969 |
| 6 | | | 3/2 | 32.081 | 31.845 |
| 6 | $2s^2 2p^4(^3P)3d$ | $^2F$ | 5/2 | 32.243 | 31.999 |
| 6 | $2s^2 2p^4(^1D)3d$ | $^2S$ | 5/2 | 32.089 | 31.848 |
| 6 | $2s^2 2p^4(^1D)3d$ | $^2F$ | 1/2 | 32.692 | 32.435 |
| 6 | $2s^2 2p^4(^1D)3d$ | $^2D$ | 5/2 | 32.694 | 32.467 |
| 6 | | | 5/2 | 32.243 | 32.577 |
| 6 | $2s^2 2p^4(^1D)3d$ | $^2P$ | 3/2 | 32.081 | 32.668 |
| 6 | $2s^2 2p^4(^1S)3d$ | $^2D$ | 3/2 | 32.189 | 32.577 |
| 6 | | | 5/2 | 33.650 | 33.242 |
| 16 | $2s2p^5(^3P^o)3s$ | $^2P^o$ | 3/2 | 32.974 | 33.282 |
| 16 | | | 3/2 | 34.133 | 34.063 |
| | $2s^2 2p^5$ | $^2P^o$ | 1/2 | 34.286 | 34.226 |
| (b) | | | | | |
| 1 | $2s^2 2p^5$ | $^2P^o$ | 3/2 | 0 | 0.00000 |
| 1 | | | 1/2 | 0.430307 | 0.43029 |
| 2 | $2s2p^6$ | $^2S$ | 1/2 | 7.56258 | 7.47031 |
| 3 | $2s^2 2p^4(^3P)3s$ | $^4P$ | 5/2 | 36.7471 | 36.40662 |
| 3 | | | 3/2 | 36.9201 | 36.58687 |
| 3 | | | 1/2 | 36.99811 | 36.7798 |
| 3 | $2s^2 2p^4(^3P)3s$ | $^2P$ | 3/2 | 37.18655 | 36.8464 |
| 3 | | | 1/2 | 37.63268 | 37.0498 |
| 3 | $2s^2 2p^4(^1D)3s$ | $^2D$ | 5/2 | 37.64474 | 37.478 |
| 3 | | | 3/2 | 38.29952 | 37.49021 |
| 5 | $2s^2 2p^4(^3P)3p$ | $^4P^o$ | 5/2 | 38.31211 | 38.11543 |
| 5 | | | 3/2 | 38.44815 | 38.1259 |
| 5 | | | 1/2 | 38.50655 | 38.2740 |
| 5 | $2s^2 2p^4(^3P)3p$ | $^4D^o$ | 7/2 | 38.56637 | 38.3269 |
| 5 | | | 5/2 | 38.7278 | 38.36803 |
| 5 | | | 3/2 | 38.79661 | 38.5663 |

**Table 1** continued

| Config. number | Configuration | Term | $J$ | $E^{SS}$ | $E^{NIST}$ |
|---|---|---|---|---|---|
| 5 | | | 1/2 | 38.85878 | 38.6137 |
| 3 | $2s^22p^4(^1S)3s$ | $^2S$ | 1/2 | 38.5197 | 38.466 |
| 5 | $2s^22p^4(^3P)3p$ | $^2P^\circ$ | 1/2 | 38.7526 | 38.5423 |
| 5 | | | 3/2 | 38.97527 | 38.6743 |
| 5 | $2s^22p^4(^3P)3p$ | $^2D^\circ$ | 5/2 | 38.86455 | 38.68251 |
| 5 | | | 3/2 | 39.03456 | 38.8643 |
| 5 | $2s^22p^4(^3P)3p$ | $^4S^\circ$ | 3/2 | 39.40343 | 38.7940 |
| 5 | $2s^22p^4(^3P)3p$ | $^2S^\circ$ | 1/2 | 39.04287 | 38.8571 |
| 5 | $2s^22p^4(^1D)3p$ | $^2F^\circ$ | 5/2 | 39.47704 | 39.2131 |
| 5 | | | 7/2 | 39.63661 | 39.2957 |
| 5 | $2s^22p^4(^1D)3p$ | $^2D^\circ$ | 3/2 | 39.68574 | 39.4507 |
| 5 | | | 5/2 | 40.15311 | 39.5027 |
| 5 | $2s^22p^4(^1D)3p$ | $^2P^\circ$ | 3/2 | 40.25205 | 39.90106 |
| 5 | $2s^22p^4(^1S)3p$ | $^2P^\circ$ | 3/2 | 40.75559 | 40.3985 |
| 5 | | | 1/2 | 40.86491 | 40.4881 |
| 6 | $2s^22p^4(^3P)3d$ | $^4D$ | 7/2 | 40.6686 | 40.4610 |
| 6 | | | 5/2 | 40.70292 | 40.470 |
| 6 | | | 3/2 | 40.75519 | 40.50933 |
| 6 | | | 1/2 | 40.83401 | 40.5670 |
| 6 | $2s^22p^4(^3P)3d$ | $^4F$ | 9/2 | 40.94615 | 40.6503 |
| 6 | | | 7/2 | 41.01778 | 40.73241 |
| 6 | | | 5/2 | 41.15384 | 40.90673 |
| 6 | | | 3/2 | 41.19113 | 40.99222 |
| 6 | $2s^22p^4(^3P)3d$ | $^4P$ | 1/2 | 41.10139 | 40.81896 |
| 6 | | | 3/2 | 41.10417 | 40.902 |
| 6 | | | 5/2 | 41.26551 | 41.021 |
| 6 | $2s^22p^4(^3P)3d$ | $^2P$ | 1/2 | 41.18808 | 40.960 |
| 6 | | | 3/2 | 41.49438 | 41.236 |
| 6 | $2s^22p^4(^3P)3d$ | $^2F$ | 7/2 | 42.14633 | 40.9902 |
| 6 | | | 5/2 | 42.02777 | 41.11705 |
| 6 | $2s^22p^4(^3P)3d$ | $^2D$ | 3/2 | 41.31567 | 41.066 |
| 6 | | | 5/2 | 41.75617 | 41.298 |
| 6 | $2s^22p^4(^1D)3d$ | $^2G$ | 7/2 | 41.77071 | 41.5587 |
| | | | 9/2 | 41.95383 | 41.56786 |
| 6 | $2s^22p^4(^1D)3d$ | $^2S$ | 1/2 | 41.98146 | 41.76 |
| 6 | $2s^22p^4(^1D)3d$ | $^2F$ | 5/2 | 42.02777 | 41.7731 |
| | | | 7/2 | 42.14633 | 41.8260 |
| 6 | $2s^22p^4(^1D)3d$ | $^2P$ | 3/2 | 42.16627 | 41.92205 |
| 6 | $2s^22p^4(^1D)3d$ | $^2D$ | 5/2 | 42.29234 | 41.94802 |
| | | | 3/2 | 42.2928 | 42.077 |
| 6 | $2s^22p^4(^1S)3d$ | $^2D$ | 5/2 | 43.15206 | 42.700 |
| | | | 3/2 | 43.23661 | 42.77 |
| 16 | $2s2p^5(^3P^\circ)3s$ | $^2P^\circ$ | 3/2 | 44.01267 | 43.546 |
| | | | 1/2 | 44.85627 | 43.796 |
| (c) | | | | | |
| 1 | $2s^22p^5$ | $^2P^\circ$ | 3/2 | 0 | 0.00000 |
| 1 | | | 1/2 | 0.64604 | 0.64602 |

**Table 1** continued

| Config. number | Configuration | Term | $J$ | $E^{SS}$ | $E^{NIST}$ |
|---|---|---|---|---|---|
| 2 | $2s2p^6$ | $^2S$ | 1/2 | 8.54576 | 8.5458 |
| 3 | $2s^22p^4(^3P)3s$ | $^4P$ | 5/2 | 46.537 | 46.007 |
| 3 | | | 3/2 | 46.7707 | 46.222 |
| 3 | | | 1/2 | 47.0336 | 46.559 |
| 3 | $2s^22p^4(^3P)3s$ | $^2P$ | 3/2 | 47.148 | 46.640 |
| 3 | | | 1/2 | 47.3884 | 46.870 |
| 3 | $2s^22p^4(^1D)3s$ | $^2D$ | 5/2 | 47.846 | 47.327 |
| 3 | | | 3/2 | 47.8705 | 47.350 |
| 3 | $2s^22p^4(^1S)3s$ | $^2S$ | 1/2 | 48.9196 | 48.511 |
| 6 | $2s^22p^4(^3P)3d$ | $^4P$ | 1/2 | 51.6667 | 51.100 |
| 6 | | | 3/2 | 51.7832 | 51.219 |
| 6 | | | 5/2 | 52.1206 | 51.397 |
| 6 | $2s^22p^4(^3P)3d$ | $^4F$ | 5/2 | 51.8168 | 51.238 |
| 6 | $2s^22p^4(^3P)3d$ | $^2P$ | 1/2 | 51.8612 | 51.291 |
| 6 | | | 3/2 | 52.2388 | 51.680 |
| 6 | $2s^22p^4(^3P)3d$ | $^2D$ | 3/2 | 52.0146 | 51.469 |
| 6 | | | 5/2 | 52.3344 | 51.767 |
| 6 | $2s^22p^4(^3P)3d$ | $^2F$ | 5/2 | 51.9653 | 51.57 |
| 6 | $2s^22p^4(^1D)3d$ | $^2S$ | 1/2 | 52.8226 | 52.258 |
| 6 | $2s^22p^4(^1D)3d$ | $^2P$ | 3/2 | 53.0769 | 52.454 |
| 6 | $2s^22p^4(^1D)3d$ | $^2D$ | 5/2 | 53.1018 | 52.463 |
| 6 | | | 3/2 | 53.2738 | 52.676 |
| 6 | $2s^22p^4(^1S)3d$ | $^2D$ | 5/2 | 54.1376 | 53.375 |
| 6 | | | 3/2 | 54.2467 | 53.497 |
| 16 | $2s2p^5(^3P^\circ)3s$ | $^2P^\circ$ | 3/2 | 54.5008 | 54.222 |
| 16 | | | 1/2 | 54.8431 | 54.554 |
| (d) | | | | | |
| 1 | $2s^22p^5$ | $^2P^\circ$ | 3/2 | 0.0 | 0.0 |
| 1 | | | 1/2 | 0.9347 | 0.9348 |
| 2 | $2s2p^6$ | $^2S$ | 1/2 | 9.70 | 9.70 |
| 3 | $2s^22p^4(^3P)3s$ | $^4P$ | 5/2 | 57.21 | 56.70 |
| 3 | | | 1/2 | 57.50 | 57.50 |
| 3 | | | 3/2 | 57.88 | 57.57 |
| 3 | $2s^22p^4(^3P)3s$ | $^2P$ | 3/2 | 57.50 | 56.94 |
| 3 | | | 1/2 | 58.35 | 57.80 |
| 3 | $2s^22p^4(^1D)3s$ | $^2D$ | 5/2 | 58.83 | 58.32 |
| 3 | | | 3/2 | 58.87 | 58.36 |
| 3 | $2s^22p^4(^1S)3s$ | $^2S$ | 1/2 | 60.16 | 59.92 |
| 6 | $2s^22p^4(^3P)3d$ | $^4P$ | 1/2 | 63.94 | 62.50 |
| 6 | | | 3/2 | 64.46 | 62.63 |
| 6 | | | 5/2 | 64.62 | 62.91 |
| 6 | $2s^22p^4(^3P)3d$ | $^2F$ | 5/2 | 64.17 | 62.70 |
| 6 | $2s^22p^4(^3P)3d$ | $^4D$ | 1/2 | 63.58 | 62.91 |
| 6 | | | 3/2 | 63.49 | 63.05 |
| 6 | $2s^22p^4(^3P)3d$ | $^2P$ | 3/2 | 64.74 | 63.31 |
| 6 | $2s^22p^4(^3P)3d$ | $^2D$ | 5/2 | 64.09 | 63.40 |
| 6 | $2s^22p^4(^1D)3d$ | $^2S$ | 1/2 | 65.97 | 63.92 |

**Table 1** continued

| Config. number | Configuration | Term | $J$ | $E^{SS}$ | $E^{NIST}$ |
|---|---|---|---|---|---|
| 6 | $2s^22p^4(^1D)3d$ | $^2P$ | 3/2 | 66.38 | 64.14 |
| 6 | | | 1/2 | 66.86 | 64.46 |
| 6 | $2s^22p^4(^1D)3d$ | $^2D$ | 5/2 | 65.37 | 64.16 |
| 6 | | | 3/2 | 64.09 | 64.39 |
| 6 | $2s^22p^4(^1S)3d$ | $^2D$ | 5/2 | 65.64 | 65.31 |
| 6 | | | 3/2 | 65.69 | 65.47 |
| 16 | $2s2p^5(^3P°)3s$ | $^4P°$ | 5/2 | 65.56 | 65.48 |
| 16 | | | 3/2 | 65.88 | 65.59 |
| | | | 1/2 | 66.28 | 65.84 |
| 16 | $2s2p^5(^3P°)3s$ | $^2P°$ | 3/2 | 66.38 | 66.08 |
| 17 | $2s2p^5(^3P°)3p$ | $^4D$ | 3/2 | 68.21 | 68.02 |
| 17 | $2s2p^5(^3P°)3p$ | $^2D$ | 5/2 | 68.33 | 68.14 |
| 17 | | | 3/2 | 69.16 | 68.96 |
| 16 | $2s2p^5(^3P°)3p$ | $^2P$ | 3/2 | 68.91 | 68.23 |
| 16 | | | 1/2 | 68.96 | 68.42 |
| 17 | $2s2p^5(^3P°)3p$ | $^4P$ | 5/2 | 68.74 | 68.42 |
| 17 | | | 3/2 | 68.77 | 68.62 |
| | $2s2p^5(^3P°)3p$ | $^2S$ | 1/2 | 69.38 | 69.25 |
| 17 | $2s2p^5(^1P°)3p$ | $^2D$ | 3/2 | 71.17 | 70.75 |
| 17 | | | 5/2 | 71.37 | 70.93 |
| 17 | $2s2p^5(^1P°)3p$ | $^2P$ | 1/2 | 71.41 | 70.95 |
| 17 | | | 3/2 | 71.51 | 71.03 |
| (e) | | | | | |
| 1 | $2s^22p^5$ | $^2P°$ | 3/2 | 0 | 0.00000 |
| 1 | | | 1/2 | 1.31185 | 1.31185 |
| 2 | $2s2p^6$ | $^2S$ | 1/2 | 10.955 | 10.955 |
| 3 | $2s^22p^4(^3P)3s$ | $^4P$ | 5/2 | 68.971 | 68.470 |
| 3 | | | 1/2 | 69.830 | 69.377 |
| 3 | | | 3/2 | 69.288 | 69.696 |
| 3 | $2s^22p^4(^3P)3s$ | $^2P$ | 3/2 | 69.288 | 68.744 |
| 3 | | | 1/2 | 70.426 | 69.923 |
| 3 | $2s^22p^4(^1D)3s$ | $^2D$ | 5/2 | 70.976 | 70.493 |
| 3 | | | 3/2 | 71.031 | 70.552 |
| 5 | $2s^22p^4(^3P)3p$ | $^4D°$ | 7/2 | 71.956 | 71.384 |
| 5 | | | 3/2 | 72.571 | 71.982 |
| 5 | | | 5/2 | 73.021 | 72.325 |
| 5 | $2s^22p^4(^3P)3p$ | $^2D°$ | 5/2 | 71.940 | 71.568 |
| 5 | $2s^22p^4(^3P)3p$ | $^4P°$ | 5/2 | 71.547 | |
| | | | 1/2 | 71.870 | 72.271 |
| 3 | $2s^22p^4(^1S)3s$ | $^2S$ | 1/2 | 72.639 | 72.44 |
| 5 | $2s^22p^4(^1D)3p$ | $^2F°$ | 5/2 | 73.505 | 73.044 |
| 5 | | | 7/2 | 73.825 | 73.289 |
| 5 | $2s^22p^4(^1D)3p$ | $^2D°$ | 5/2 | 73.287 | 73.558 |
| 6 | $2s^22p^4(^3P)3d$ | $^4F$ | 9/2 | 75.335 | 74.691 |
| 6 | | | 5/2 | 75.906 | 75.34 |
| 6 | | | 7/2 | 76.3766 | 75.749 |
| 6 | $2s^22p^4(^3P)3d$ | $^2F$ | 7/2 | 75.428 | 74.853 |
| 6 | | | 5/2 | 76.213 | 75.23 |

**Table 1** continued

| Config. number | Configuration | Term | $J$ | $E^{SS}$ | $E^{NIST}$ |
|---|---|---|---|---|---|
| 6 | $2s^22p^4(^3P)3d$ | $^4P$ | 1/2 | 75.608 | 74.96 |
| 6 | | | 3/2 | 75.788 | 75.12 |
| 6 | $2s^22p^4(^3P)3d$ | $^4D$ | 7/2 | 76.376 | |
| 6 | | | 3/2 | 76.169 | 75.90 |
| 6 | $2s^22p^4(^3P)3d$ | $^2P$ | 3/2 | 76.7136 | 76.12 |
| 6 | $2s^22p^4(^3P)3d$ | $^2D$ | 5/2 | 76.81 | 76.2 |
| 6 | $2s^22p^4(^1D)3d$ | $^2G$ | 7/2 | 77.084 | 76.542 |
| 6 | $2s^22p^4(^1D)3d$ | $^2S$ | 1/2 | 77.37 | 76.76 |
| 6 | $2s^22p^4(^1D)3d$ | $^2F$ | 7/2 | 77.504 | 76.895 |
| 6 | $2s^22p^4(^1D)3d$ | $^2P$ | 3/2 | 77.646 | 76.96 |
| | | | 1/2 | 78.084 | 77.41 |
| 6 | $2s^22p^4(^1D)3d$ | $^2D$ | 5/2 | 77.712 | 77.02 |
| 6 | | | 3/2 | 77.998 | 77.31 |
| 6 | $2s^22p^4(^1S)3d$ | $^2D$ | 3/2 | 79.462 | 78.68 |
| 17 | $2s2p^5(^3P°)3p$ | $^2D$ | 5/2 | 82.138 | 81.18 |
| 17 | | | 3/2 | 82.755 | 82.49 |
| 17 | $2s2p^5(^3P°)3p$ | $^4D$ | 3/2 | 81.402 | 81.18 |
| 17 | $2s2p^5(^3P°)3p$ | $^2P$ | 3/2 | 81.839 | 81.67 |
| 17 | | | 1/2 | 82.021 | 81.81 |
| 17 | $2s2p^5(^3P°)3p$ | $^4P$ | 3/2 | 82.184 | 82.09 |
| 17 | $2s2p^5(^3P°)3p$ | $^2S$ | 1/2 | 82.916 | 82.85 |
| 17 | $2s2p^5(^1P°)3p$ | $^2D$ | 3/2 | 84.685 | 84.3 |
| 17 | | | 5/2 | 85.035 | 84.59 |
| 17 | $2s2p^5(^1P°)3p$ | $^2P$ | 1/2 | 85.031 | 84.64 |
| 17 | | | 3/2 | 85.190 | 84.78 |
| 7 | $2s^22p^4(^3P)4s$ | $^2P$ | 3/2 | 93.531 | 92.79 |
| 7 | $2s^22p^4(^3P)4s$ | $^4P$ | 3/2 | 94.549 | 94.02 |
| | $2s^22p^4(^3P)4d$ | $^2D$ | 5/2 | 94.595 | 95.34 |
| 9 | $2s^22p^4(^3P)4d$ | $^4F$ | 5/2 | 96.089 | 96.0 |
| 9 | | | 3/2 | 96.686 | 96.0 |
| 9 | $2s^22p^4(^3P)4d$ | $^4P$ | 5/2 | 95.756 | 96.38 |
| 9 | $2s^22p^4(^3P)4d$ | $^2P$ | 3/2 | 96.924 | 96.42 |
| 9 | $2s^22p^4(^1D)4d$ | $^2D$ | 5/2 | 97.049 | 97.10 |
| 9 | | | 3/2 | 97.101 | 97.27 |
| 9 | $2s^22p^4(^1D)4d$ | $^2S$ | 1/2 | 97.769 | 97.10 |
| 9 | $2s^22p^4(^1D)4d$ | $^2F$ | 5/2 | 97.761 | 97.30 |
| 9 | $2s^22p^4(^1S)4d$ | $^2D$ | 3/2 | 99.719 | 98.90 |

Sugar and Corlis [26], Sugar and Musgrove [27–29], and Shirai et al. [30] obtained either from the tokamak plasma experiments or from the Dirac–Fock calculations.

We presented the line strengths, oscillator strengths and transition rates of the first two excited states for some F-like ions in Table 3. The line strengths ($S$) were given for both the allowed E1 and forbidden M1 and E2 transitions. Also, in same table, we evaluated the transition rates and given the weighted oscillator strengths. We compared our

**Table 2** Excitation energies (in Ry) for some F-like ions obtained with the SUPERSTRUCTURE code

| Ions | This Work SS | Kramida et al. [25] | Jönsson et al. [14] | Nandy and Sahoo [15] | | | |
|---|---|---|---|---|---|---|---|
| | | | | DC | DCB | DCBV | DCBVS |
| Ca XII | | | | | | | |
| $2s^22p^5\ ^2P_{3/2}$ | 0.0 | 0.0 | 0.0 | | | | |
| $2s^22p^5\ ^2P_{1/2}$ | 0.274124 | 0.274097 | 0.274191 | | | | |
| $2s2p^6\ ^2S_{1/2}$ | 6.469717 | 6.469252 | 6.472679 | | | | |
| Ti XIV | | | | | | | |
| $2s^22p^5\ ^2P_{3/2}$ | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| $2s^22p^5\ ^2P_{1/2}$ | 0.430812 | 0.43083 | 0.430777 | 0.443125 | 0.430086 | 0.430083 | 0.431062 |
| $2s2p^6\ ^2S_{1/2}$ | 7.485995 | 7.476934 | 7.486043 | 7.494727 | 7.494569 | 7.494889 | 7.494881 |
| Cr XVI | | | | | | | |
| $2s^22p^5\ ^2P_{3/2}$ | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| $2s^22p^5\ ^2P_{1/2}$ | 0.646843 | 0.646825 | 0.646766 | 0.663504 | 0.645647 | 0.645644 | 0.647875 |
| $2s2p^6\ ^2S_{1/2}$ | 8.556469 | 8.553741 | 8.562196 | 8.571693 | 8.571873 | 8.580975 | 8.5811 |
| Fe XVIII | | | | | | | |
| $2s^22p^5\ ^2P_{3/2}$ | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| $2s^22p^5\ ^2P_{1/2}$ | 0.935931 | 0.935027 | 0.934951 | 0.953402 | 0.935093 | 0.935089 | 0.935005 |
| $2s2p^6\ ^2S_{1/2}$ | 9.714425 | 9.714434 | 9.715859 | 9.738228 | 9.742777 | 9.745331 | 9.752225 |
| Ni XX | | | | | | | |
| $2s^22p^5\ ^2P_{3/2}$ | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| $2s^22p^5\ ^2P_{1/2}$ | 1.313495 | 1.313495 | 1.308806 | 1.345581 | 1.309149 | 1.309143 | 1.318372 |
| $2s2p^6\ ^2S_{1/2}$ | 10.96901 | 10.96898 | 10.97065 | 11.00286 | 11.00946 | 11.01298 | 11.02631 |

transition rate results with the other calculations: Jönsson et al. [14], Tachiev and Fischer [12], Kaufman and Sugar [31] and Nandy and Sahoo [15]. It was seen that our transition probability results differ from those by Jönsson et al. [14] with 4–6% for E1 transitions, with 0.2–4% for M1 transitions and with 0.8–3% for E2 transitions, from those by Tachiev and Fischer [12] with 4–5% for E1 transitions, with 3% for E2 transitions, with 2–5% for M1 transitions, from those by Kaufman and Sugar [31] with 2–4% for M1 transitions and from those by Nandy and Sahoo [15], with 5–7% for E1 transitions, with 2–3% for E2 transitions and with 2–8% for M1 transitions. Moreover, some radiative E3 and M2 decay rates for the forbidden transitions of relevant F-like ions are given in Table 4 as new data for these ions. In Table 4, $(i, j)$ is the level numbers, $(C_i, C_j)$ is configuration indices: $2s^22p^5(1)$, $2s2p^6(2)$, $2s^22p^43s(3)$, $2s^22p^43p(5)$, $2s^22p^43d(6)$, $2s^22p^4$4s(7), $2s^22p^4$4p(8), $2s^22p^4$4d(9), $2s^22p^4$4f(10) and $2s2p^53s(11)$, and $T$ denotes the LS term. Moreover, $g_i$ and $g_j$ are the statistical weights of the lower and upper levels, and $E_i$ and $E_j$ are the energies in Rydberg unit of the lower and upper levels, respectively. It is seen from all comparisons that the present results have good agreement with other results for the same spin-dipole transitions.

## 4. Conclusions

We determined energy levels, excitation energies, weighted oscillator strengths and transition rates using *SS* code for some considered F-like highly charged ions. The determined quantities were compared with available results from the literature. For energies, very good agreements were obtained with those of the measured levels. The average agreement of energies is within $< 1\%$. Also, E1, E2 and M1 transition rates are in very good agreement with the earlier data given in the literature.

We expect that the obtained atomic properties such as radiative decay rates and weighted oscillator strengths are enough accurate data and very useful for the astrophysical plasma analysis.

**Table 3** Line strengths ($S_{ik}$ in au), weighted oscillator strengths (*gf*) and transition rates ($A$ in $s^{-1}$), for the considered ions

| | | | $S_{ik}$ | $g_i f_{ik}$ | $A_{ki}$ | Jönsson et al. [14] | Tachiev and Fischer [12] | Kaufman and Sugar [31] | Nandy and Sahoo [15] |
|---|---|---|---|---|---|---|---|---|---|
| Ca XII | | | | | | | | | |
| $2s\,2p^6$ $^2S_{1/2}$ | $2s^22p^5$ $^2P_{1/2}$ | E1 | 0.120412 | 2.594e−01 | 4.349e+10 | 4.146e+10 | 4.167e+10 | | |
| $2s\,2p^6$ $^2S_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | E1 | 0.059892 | 1.235e−01 | 1.900e+10 | 1.803e+10 | 1.810e+10 | | |
| $2s^22p^5$ $^2P_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | M1 | 1.33 | | 1.619e−02 | 1.547e−02 | 1.6285e−02 | | |
| $2s^22p^5$ $^2P_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | E2 | 7.876e−03 | | 4.875e+02 | 4.871e+02 | 5.0376e+02 | | |
| Ti XIV | | | | | | | | | |
| $2s\,2p^6$ $^2S_{1/2}$ | $2s^22p^5$ $^2P_{1/2}$ | E1 | 0.048847 | 1.147e−01 | 2.285e+10 | 2.136e+10 | 2.151e+10 | | 2.141e+10 |
| $2s\,2p^6$ $^2S_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | E1 | 0.098218 | 2.447e−01 | 5.49e+10 | 5.163e+10 | 5.212e+10 | | 5.097e+10 |
| $2s^22p^5$ $^2P_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | M1 | 1.333 | | 1.839e+03 | 1.888e+03 | 1.976e+03 | 1.890 e+03 | 1.881e+03 |
| $2s^22p^5$ $^2P_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | E2 | 4.768e−03 | | 9.467e−02 | 9.124e−02 | 9.793e−02 | | 9.110e−02 |
| Cr XVI | | | | | | | | | |
| $2s\,2p^6$ $^2S_{1/2}$ | $2s^22p^5$ $^2P_{1/2}$ | E1 | 0.40309 | 1.061e−01 | 2.660e+10 | 2.476e+10 | | | 2.481e+10 |
| $2s\,2p^6$ $^2S_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | E1 | 0.081178 | 2.312e−01 | 6.782e+10 | 6.358e+10 | | | 6.29e+10 |
| $2s^22p^5$ $^2P_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | M1 | 1.333 | | 6.403e+03 | 6.386e+03 | | 6.390e+03 | 6.341e+03 |
| $2s^22p^5$ $^2P_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | E2 | 3.084e−03 | | 4.639e−01 | 4.518e−01 | | | 4.512e−01 |
| Fe XVIII | | | | | | | | | |
| $2s\,2p^6$ $^2S_{1/2}$ | $2s^22p^5$ $^2P_{1/2}$ | E1 | 0.033822 | 9.884e−02 | 3.051e+10 | 2.824e+10 | | | 2.826e+10 |
| $2s\,2p^6$ $^2S_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | E1 | 0.068209 | 2.206e−01 | 8.340e+10 | 7.784e+10 | | | 7.715e+10 |
| $2s^22p^5$ $^2P_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | M1 | 1.332 | | 1.939e+04 | 1.933e+04 | | 1.930e+04 | 1.923e+04 |
| $2s^22p^5$ $^2P_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | E2 | 2.080e−03 | | 1.984e+00 | 1.939e+00 | | | 1.937e+00 |
| Ni XX | | | | | | | | | |
| $2s\,2p^6$ $^2S_{1/2}$ | $2s^22p^5$ $^2P_{1/2}$ | E1 | 0.028079 | 9.031e−02 | 3.373e+10 | 3.181e+10 | | | 3.180e+10 |
| $2s\,2p^6$ $^2S_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | E1 | 0.056779 | 2.075e−01 | 1.00e+11 | 9.512e+10 | | | 9.441e+10 |
| $2s^22p^5$ $^2P_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | M1 | 1.332 | | 5.359e+04 | 5.340e+04 | | 5.342e+04 | 5.315e+04 |
| $2s^22p^5$ $^2P_{1/2}$ | $2s^22p^5$ $^2P_{3/2}$ | E2 | 1.455e−03 | | 7.55e+00 | 7.386e+00 | | | 7.387e+00 |

**Table 4** Transition probabilities $A_{ji}$ ($s^{-1}$) for the forbidden electric octupole (E3) and magnetic quadrupole (M2) transitions in relevant F-like ions such as (a) Ca XII, (b) Ti XIV, (c) Cr XVI, (d) Fe XVIII and (e) Ni XX

| *i–j* | $T_iC_i$–$T_jC_j$ | $g_i$–$g_j$ | $\lambda$ (Å) | $E_i$ (Ry) | $E_j$ (Ry) | $A_{ji}$ | |
|---|---|---|---|---|---|---|---|
| | | | | | | E3 | M2 |
| (a) | | | | | | | |
| 2–4 | $2P_0$ 1–$4P_e$ 3 | 2–6 | 25.21513 | 2.7377E−01 | 28.045E+00 | 2.349E+02 | 3.470E+03 |
| 2–9 | $2P_0$ 1–$2D_e$ 3 | 2–6 | 24.49662 | 2.7377E−01 | 28.905E+00 | 1.463E+04 | 1.555E+04 |
| 3–11 | $2S_e$ 2–$4P_O$ 5 | 2–6 | 29.65592 | 6.4616E+00 | 29.572E+00 | 2.178E−02 | 9.551E+00 |
| 6–11 | $4P_e$ 3–$4P_0$ 5 | 2–6 | 665.1585 | 28.270E+00 | 29.572E+00 | 8.050E−06 | 2.69E−02 |
| 8–11 | $2P_e$ 3–$4P_0$ 5 | 2–6 | 820.9614 | 28.480E+00 | 29.572E+00 | 8.770E−09 | 2.661E−02 |
| 4–14 | $4P_e$ 3–$4P_0$ 5 | 6–2 | 472.1591 | 28.045E+00 | 29.675E+00 | 1.316E−04 | 1.108E−01 |
| 9–14 | $2D_e$ 3–$4P_0$ 5 | 6–2 | 23.93681 | 28.905E+00 | 29.675E+00 | 9.150E−07 | 1.89E−03 |
| 3–15 | $2S_e$ 2–$4D_0$ 5 | 2–8 | 29.4451 | 6.4616E+00 | 29.765E+00 | 1.219E+00 | 0.00E+00 |
| 5–15 | $4P_e$ 3–$4D_0$ 5 | 4–8 | 514.8402 | 28.167E+00 | 29.765E+00 | 1.686E−03 | 3.158E−03 |
| 6–15 | $4P_e$ 3–$4D_0$ 5 | 2–8 | 573.124 | 28.270E+00 | 29.765E+00 | 1.114E−03 | 0.00E+00 |
| 7–15 | $2P_e$ 3–$4D_0$ 5 | 4–8 | 599.5178 | 28.340E+00 | 29.765E+00 | 2.397E−04 | 3.174E−01 |
| 8–15 | $2P_e$ 3–$4D_0$ 5 | 2–8 | 685.1632 | 28.480E+00 | 29.765E+00 | 1.926E−06 | 0.00E+00 |
| 10–15 | $2D_e$ 3–$4D_0$ 5 | 4–8 | 1047.433 | 28.911E+00 | 29.765E+00 | 1.484E−07 | 2.719E−03 |
| 13–15 | $4P_e$ 5–$4D_0$ 5 | 2–6 | 13018.1 | 29.619E+00 | 29.765E+00 | 2.204E−12 | 0.00E+00 |
| 6–16 | $4P_e$ 3–$4D_0$ 5 | 2–8 | 555.6507 | 28.270E+00 | 29.812E+00 | 9.807E−05 | 5.144E−02 |
| 8–16 | $2P_e$ 3–$4D_0$ 5 | 2–6 | 660.3385 | 28.480E+00 | 29.812E+00 | 3.621E−04 | 7.369E−02 |
| (b) | | | | | | | |
| 2–4 | $2P_0$ 1–$4P_e$ 3 | 2–6 | 36570 | 4.303E−01 | 3.657E+04 | 1.137E+03 | 7.652E+03 |
| 2–9 | $2P_0$ 1–$2D_e$ 3 | 2–6 | 37.63 | 4.303E−01 | 3.763E+01 | 4.254E+04 | 4.346E+04 |
| 3–11 | $2S_e$ 2–$4P_O$ 5 | 2–6 | 30.728 | 7.562E+00 | 3.829E+01 | 1.73E−01 | 1.441E+01 |
| 6–11 | $4P_e$ 3–$4P_0$ 5 | 2–6 | 1.37 | 3.692E+01 | 3.829E+01 | 8.048E−06 | 3.351E−02 |
| 8–11 | $2P_e$ 3–$4P_0$ 5 | 2–6 | 1.11 | 3.718E+01 | 3.829E+01 | 2.143E−08 | 2.363E−02 |
| 4–13 | $4P_e$ 3–$4P_0$ 3 | 6–2 | 36531.5 | 3.657E+04 | 3.844E+01 | 2.349E−04 | 1.138E−01 |
| 9–13 | $2D_e$ 3–$4P_0$ 3 | 6–2 | 0.87 | 3.763E+01 | 3.844E+01 | 1.402E−06 | 3.714E−03 |
| 11–14 | $4P_0$ 5–2 $S_e$ 3 | 6–2 | 0.21 | 3.829E+01 | 3.850E+01 | 2.115E−12 | 1.392E−06 |
| 3–15 | $2S_e$ 2–$4D_0$ 5 | 2–8 | 30.948 | 7.562E+00 | 3.851E+01 | 4.112E+00 | 0 |
| 5–15 | $4P_e$ 3–$4D_0$ 5 | 4–8 | 1.77 | 3.674E+01 | 3.851E+01 | 1.335E−03 | 2.504E−02 |
| 6–15 | $4P_e$ 3–$4D_0$ 5 | 2–8 | 1.59 | 3.692E+01 | 3.851E+01 | 7.942E−04 | 0 |
| 7–15 | $2P_e$ 3–$4D_0$ 5 | 4–8 | 1.52 | 3.699E +01 | 3.851E+01 | 2.571E−04 | 3.037E−01 |
| 8–15 | $2P_e$ 3–$4D_0$ 5 | 2–8 | 1.33 | 3.718E+01 | 3.851E+01 | 9.352E−08 | 0 |
| 10–15 | $2D_e$ 3–$4D_0$ 5 | 4–8 | 0.87 | 3.764E+01 | 3.851E+01 | 1.401E−07 | 3.853E−03 |
| 14–15 | 2 $S_e$ 3–$4D_0$ 5 | 2–6 | 0.07 | 3.8506E+01 | 3.851E+01 | 8.808E−20 | 0 |
| 3–16 | $2S_e$ 2–$4D_0$ 5 | 2–6 | 30.998 | 7.562E+00 | 3.856E+01 | 5.141E+00 | 8.868E+01 |
| 6–16 | $4P_e$ 3–$4D_0$ 5 | 2–8 | 1.64 | 3.692E+01 | 3.856E+01 | 5.350E−05 | 4.717E−02 |
| 8–16 | $2P_e$ 3–$4D_0$ 5 | 2–6 | 1.38 | 3.718E+01 | 3.856E+01 | 2.531E−04 | 4.965E−02 |
| 14–16 | 2 $S_e$ 3–$4D_0$ 5 | 2–6 | 0.12 | 3.8506E+01 | 3.856E+01 | 4.247E−15 | 9.457E−10 |
| (c) | | | | | | | |
| 2–4 | $2P_0$ 1–$4P_e$ 3 | 2–6 | 2.52E+01 | 6.4603E−01 | 46.536E+00 | 4.589E+03 | 1.465E+04 |
| 2–9 | $2P_0$ 1–$2D_e$ 3 | 2–6 | 2.45E+01 | 6.4603E−01 | 47.845E+00 | 1.145E+05 | 1.069E+05 |
| 3–12 | $2S_e$ 2–$4P_O$ 5 | 2–6 | 2.96E+01 | 8.545E+00 | 48.545E+00 | 1.373E+00 | 5.267E−02 |
| 6–12 | $4P_e$ 3–$4P_0$ 5 | 2–6 | 6.56E+02 | 47.033E+00 | 48.545E+00 | 1.003E−05 | 5.267E−02 |
| 8–12 | $2P_e$ 3–$4P_0$ 5 | 2–6 | 8.06E+02 | 47.388E+00 | 48.545E+00 | 1.341E−07 | 2.150E−02 |
| 4–13 | $4P_e$ 3–$4P_0$ 3 | 6–2 | 4.87E+02 | 46.536E+00 | 48.741E+00 | 4.275E−04 | 1.064E−01 |
| 9–13 | $2D_e$ 3–$4P_0$ 3 | 6–2 | 1.13E+03 | 47.84E+00 | 48.741E+00 | 2.248E−06 | 7.273E−03 |
| 3–14 | $4P_o$ 5–$4D_0$ 3 | 6–2 | 2.95E+01 | 8.545E+00 | 48.806E+00 | 1.592E+01 | 0.00E+00 |

**Table 4** continued

| *i–j* | $T_iC_i$–$T_jC_j$ | $g_i$–$g_j$ | λ (Å) | $E_i$ (Ry) | $E_j$ (Ry) | $A_{ji}$ | |
|---|---|---|---|---|---|---|---|
| | | | | | | E3 | M2 |
| 5–14 | $2S_e$ 2–$4D_0$ 5 | 2–8 | 5.18E+02 | 46.770E+00 | 48.806E+00 | 1.489E−03 | 6.172E−02 |
| 6–14 | $4P_e$ 3–$4D_0$ 5 | 4–8 | 5.77E+02 | 47.033E+00 | 48.806E+00 | 7.528E−04 | 0.00E+00 |
| 7–14 | $4P_e$ 3–$4D_0$ 5 | 2–8 | 6.03E+02 | 47.148E+00 | 48.806E+00 | 2.754E−04 | 3.192E−01 |
| 8–14 | $2P_e$ 3–$4D_0$ 5 | 4–8 | 6.90E+02 | 47.388E+00 | 48.806E+00 | 7.337E−07 | 0.00E+00 |
| 10–14 | $2P_e$ 3–$4D_0$ 5 | 2–8 | 1.06E+03 | 47.870E+00 | 48.806E+00 | 1.756E−07 | 6.212E−03 |
| 3–15 | $2D_e$ 3–$4D_0$ 5 | 4–8 | 2.94E+01 | 8.545E+00 | 48.841E+00 | 2.041E+01 | 3.051E+02 |
| 6–15 | 2 $S_e$ 3–$4D_0$ 5 | 2–6 | 5.70E+02 | 47.033E+00 | 48.841E+00 | 5.33E−05 | 5.005E−02 |
| 8–15 | $2S_e$ 2–$4D_0$ 5 | 2–6 | 6.80E+02 | 47.388E+00 | 48.841E+00 | 1.826E−04 | 3.216E−02 |
| 12–16 | $4P_e$ 3–$4D_0$ 5 | 2–8 | 3.65E+03 | 48.545E+00 | 48.919E+00 | 2.233E−10 | 4.275E−05 |
| 14–16 | $2P_e$ 3–$4D_0$ 5 | 2–6 | 1.52E+04 | 48.806E+00 | 48.919E+00 | 9.955E−13 | 0.00E+00 |
| 15–16 | 2 $S_e$ 3–$4D_0$ 5 | 2–6 | 2.28E+04 | 48.841E+00 | 48.919E+00 | 6.578E−14 | 1.039E−08 |
| (d) | | | | | | | |
| 2–4 | $2P_0$ 1–$4P_e$ 3 | 2–6 | 16.19308 | 9.349E−01 | 5.721E+01 | 1.577E+04 | 2.665E+04 |
| 2–9 | $2P_0$ 1–$2D_e$ 3 | 2–6 | 15.86879 | 9.349E−01 | 5.836E+01 | 2.605E+05 | 2.556E+05 |
| 3–12 | $2S_e$ 2–$4P_O$ 5 | 2–6 | 18.26699 | 9.702E+00 | 5.959E+01 | 6.232E+00 | 2.96E+02 |
| 6–12 | $4P_e$ 3–$4P_0$ 5 | 2–6 | 532.9047 | 5.788E+01 | 5.959E+01 | 1.772E−05 | 1.055E−01 |
| 8–12 | $2P_e$ 3–$4P_0$ 5 | 2–6 | 729.0137 | 5.834E+01 | 5.959E+01 | 3.848E−07 | 2.364E−02 |
| 4–13 | $4P_e$ 3–$4P_0$ 5 | 6–2 | 346.4894 | 5.721E+01 | 5.984E+01 | 8.672E−04 | 9.197E−02 |
| 9–13 | $2D_e$ 3–$4P_0$ 5 | 6–2 | 615.721 | 5.836E+01 | 5.984E+01 | 4.131E−06 | 1.475E−02 |
| 3–14 | $2S_e$ 2–$4D_0$ 5 | 2–8 | 18.15418 | 9.704E+00 | 5.990E+01 | 3.615E+01 | 0.00E +00 |
| 5–14 | $2P_e$ 3–$4D_0$ 5 | 4–8 | 379.6946 | 5.750E+01 | 5.990E+01 | 2.218E−03 | 1.612E−01 |
| 6–14 | $4P_e$ 3–$4D_0$ 5 | 2–8 | 451.1223 | 5.788E+01 | 5.990E+01 | 9.44E−04 | 0.00E+00 |
| 7–14 | $4P_e$ 3–$4D_0$ 5 | 4–8 | 497.9602 | 5.807E+01 | 5.990E+01 | 3.629E−04 | 3.861E−01 |
| 8–14 | $2P_e$ 3–$4D_0$ 5 | 2–8 | 584.1456 | 5.834E+01 | 5.990E+01 | 5.964E−06 | 0.00E+00 |
| 10–14 | $2D_e$ 3–$4D_0$ 5 | 4–8 | 884.7253 | 5.887E+01 | 5.990E+01 | 2.938E−07 | 1.185E−02 |
| 3–15 | $2S_e$ 2–$2D_0$ 5 | 2–6 | 18.14695 | 9.704E+00 | 5.992E+01 | 4.853E+01 | 6.867E+02 |
| 6–15 | $4P_e$ 3–$2D_0$ 5 | 2–6 | 446.6996 | 5.788E+01 | 5.992E+01 | 8.779E−05 | 5.929E−02 |
| 8–15 | $2P_e$ 3–$2D_0$ 5 | 2–6 | 576.7513 | 5.834E+01 | 5.992E+01 | 1.722E−04 | 2.218E−02 |
| (e) | | | | | | | |
| 2–4 | $2P_0$ 1–$4P_e$ 3 | 2–6 | 16.35733 | 1.311E+01 | 6.882E+01 | 4.276E+04 | 4.07E+04 |
| 2–9 | $2P_0$ 1–$2D_e$ 3 | 2–6 | 15.79319 | 1.311E+01 | 7.081E+01 | 5.498E+05 | 5.626E+05 |
| 3–12 | $2S_e$ 2–$4P_O$ 5 | 2–6 | 15.11222 | 1.103E+01 | 7.133E+01 | 2.677E+01 | 1.022 +00 |
| 6–12 | $4P_e$ 3–$4P_0$ 5 | 2–6 | 548.9561 | 6.967E+01 | 7.133E+01 | 1.502E−05 | 1.067E−01 |
| 8–12 | $2P_e$ 3–$4P_0$ 5 | 2–6 | 836.0249 | 7.024E+01 | 7.133E+01 | 3.584E−07 | 8.359E−03 |
| 4–13 | $4P_e$ 3–$4P_0$ 5 | 6–2 | 320.8687 | 6.882E+01 | 7.166E+01 | 8.946E−04 | 3.191E−02 |
| 9–13 | $2D_e$ 3–$4P_0$ 5 | 6–2 | 1072.079 | 7.081E+01 | 7.166E+01 | 1.090E−06 | 6.906E−03 |
| 3–14 | $2S_e$ 2–$4D_0$ 5 | 6–2 | 15.01511 | 1.103E+01 | 7.172E+01 | 8.21E+01 | 1.788E+03 |
| 6–14 | $4P_e$ 3–$4D_0$ 5 | 4–8 | 444.5205 | 6.967E+01 | 7.172E+01 | 7.713E−05 | 2.398E−02 |
| 8–14 | $2P_e$ 3–$4D_0$ 5 | 4–8 | 615.721 | 7.024E+01 | 7.172E+01 | 5.856E−05 | 4.279E−03 |
| 3–15 | $2S_e$ 2–$4D_0$ 5 | 2–8 | 15.01016 | 1.103E+01 | 7.174E+01 | 7.196E+01 | 0.00E+00 |
| 5–15 | $2D_e$ 3–$4D_0$ 5 | 4–8 | 346.4894 | 6.911E+01 | 7.174E+01 | 2.038E−03 | 2.709E−01 |
| 6–15 | 2 $S_e$ 3–$4D_0$ 5 | 2–6 | 440.2257 | 6.967E+01 | 7.174E+01 | 6.082E−04 | 0.00 |
| 7–15 | $2S_e$ 2–$4D_0$ 5 | 2–6 | 517.7654 | 6.998E+01 | 7.174E+01 | 1.953E−04 | 2.386E−01 |
| 8–15 | $4P_e$ 3–$4D_0$ 5 | 2–8 | 312.0778 | 6.882E+01 | 7.174E+01 | 8.046E−06 | 0.00 |
| 10–15 | $2P_e$ 3–$4D_0$ 5 | 2–6 | 1035.531 | 7.086E+01 | 7.174E+01 | 8.748E−08 | 6.163E−03 |
| 4–16 | 2 $S_e$ 3–$4D_0$ 5 | 2–6 | 262.613 | 6.882E+01 | 7.229E+01 | 5.461E−03 | 7.741E−01 |
| 9–16 | $2D_e$ 3–$4D_0$ 5 | 6–2 | 615.721 | 7.081E+01 | 7.229E+01 | 2.982E−05 | 2.414E−04 |

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