

Relativistic distorted-wave excitation cross sections of F-like selenium by electron collision

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Abstract. RDWB procedures were applied to study the excitation cross sections induced by electron collision for F-like selenium. GRASP² code was used for atomic structure calculations. By approaching from the 'post' form approximation, it was possible to overcome the complexity involved in using non-orthogonal orbits. From the multipole expansion of the inter-electron potential used, it was found justifiable to add a correction term to the exchange Slater integrals due to the non-orthogonal orbitals. Comparisons are made of the resulting cross sections for excitation from the three low-lying levels as calculated using 113-level and 279-level MCDF configuration expansion both between themselves as well as with existing data. More than 10% in difference has been found in these comparisons.

1. Introduction

It is of interest to accurately calculate electron impact excitation (EIE) for F-like ions because of the absence of F-like lasers in Ne-like x-ray laser plasmas in contrast to Co-like analogue lasers observed in Ni-like ones [1, 2]. Although extensive investigations of F-like selenium have been made by Hagelstein recently [1], some of the cross sections he obtained are greatly in disagreement with ours. As our calculations may be accurate, our results may be useful for the analysis and diagnosis of F-like selenium plasma. Comprehensive relativistic distorted-wave Born (RDWB) calculations of collision strengths for different F-like ions have also been published by Sampson *et al* [3]. They extended Cowan's atomic structure code [4] to the relativistic case and used Dirac–Fock–Slater (DFS) potential, which is energy-independent, to evaluate continuum orbitals. Comparison of their results with ours indicates that the agreement is generally good for relatively large excitation processes, but some differences still exist under certain circumstances.

Rapid RDWB method [5] was also used in the present EIE calculation of F-like selenium. Approximations made in this method are elaborated in the next section. The multiconfiguration Dirac–Fock (MCDF) method [6] was used to treat the necessary atomic structure input of EIE. Because different potentials were used in the calculations of the bound and free orbitals, the orbitals of the free electrons are not orthogonal to those of the bound electrons. As a result of these non-orthogonal orbitals, there will be various overlapping integrals appearing in the transition matrix elements. Several approximations which will be discussed in detail in the subsequent section were also used in computing these transition matrix elements. This work was preliminarily performed on the SUN workstation in the Beijing Institute of Applied Physics

and Computational Mathematics and subsequently on the SGI PowerChallenge and/or the Cray supercomputer in the National University of Singapore.

To compare the results with others, we have used almost identical approximations. Continuum orbitals were calculated with or without exchange potential, and it was found that inclusion of the energy-dependent local semi-classical exchange (SCE) [7–9] potential has a bit of influence on the cross sections. Comparisons of the EIE results for excitations to singly excited M shell states calculated by including configurations from single excitation to only the M shell involving 113-level MCDF configuration expansion and from single excitation to both M and N shells involving 279-level MCDF configuration expansion have also been made. The difference obtained is sometimes greater than 10%. This difference indicates that the more elaborate latter procedure is necessary to achieve sufficient accuracy.

In this paper more elaborate calculation procedures than before are given. Also, the results are extensively compared and discussed. In section 2 the calculation procedures of the relativistic atomic structure and the RDWB are reviewed briefly. Detailed discussions of the distorted potentials used in the calculations of free-electron orbitals and the approximations made in the calculations of the transition matrix elements are also given in this section. In section 3, the $n = 2-3$ collisional excitation cross sections are presented and compared in detail with some literature data.

2. Theory

2.1. Relativistic atomic structure

The relativistic atomic structure code GRASP² which is based on MCDF theory and intermediate coupling is applied to calculate the present relativistic atomic structure. Atomic orbitals are taken to be four-component spinors. Multiconfiguration self-consistent-field (SCF) calculations are based on the Dirac–Coulomb Hamiltonian. Nuclear potential is modelled as a spherically symmetric distribution of nuclear charge. The one-body operator is based upon the Dirac kinetic energy operator. The transverse photon interaction is added to the two-body operator. It is calculated perturbatively in the atomic structure section. The Dirac Hamiltonian H_D adequately describes the relativistic interaction [10, 11],

$$H_D = c\vec{\alpha} \cdot \vec{p} + (\beta - 1)c^2 + V(r), \quad (2.1)$$

where $c \sim 137.036$ is the light speed in au. $\vec{\alpha}, \beta$ are the usual Dirac matrices.

Generalized Breit interaction in Coulomb gauge for photon propagator was used to account for the transverse photon interaction.

$$H_B(1, 2) = -(\vec{\alpha}_1 \cdot \vec{\alpha}_2) \frac{\exp(i\omega r_{12})}{r_{12}} + (\vec{\alpha}_1 \cdot \vec{\nabla}_1)(\vec{\alpha}_2 \cdot \vec{\nabla}_2) \frac{\exp(i\omega r_{12}) - 1}{\omega^2 r_{12}}, \quad (2.2)$$

where ω is the wavenumber of the virtual photon exchanged between the two electrons. Coulomb interaction $1/r_{12}$ is not included in $H_B(1, 2)$. Nuclear potential assumes the Fermi charge distribution [12], for which nuclear volume effect is considered. The vacuum polarization potential of Fullerton and Rinker [13, 14] is calculated via perturbation-theory (i.e. added to the matrix elements of Dirac–Coulomb Hamiltonian prior to diagonalizing the resulting matrix). Self-energy is estimated by interpolation of the screened hydrogenic self-energy [15]. With the addition of transverse photon interaction, the mixing coefficients may be somewhat changed. However, in the collision section, we exclude transverse photon scattering because the incident energy was found to be not high enough to make the transverse interaction scattering between the incident electron and bound electrons significant.

All the present atomic structure data were obtained from the GRASP² code including bound-state orbitals, angular coefficients, and other required radial functions. All these functions were transformed to the new hybrid grid using a well-tested cubic spline interpolation [5].

2.2. Relativistic distorted-wave Born

To outline the theoretical method of this paper we will sometimes refer to equations given in [5]. In doing so equation (X) of that paper will be called equation (I.X). It is convenient to express relativistic cross section $\sigma_{if}(\epsilon)$ for a transition $i \rightarrow f$ in term of collision strength $\Omega_{if}(\epsilon)$ by the relation

$$\sigma_{if}(\epsilon) = \frac{\pi a_0^2}{k_i^2 g_i} \Omega_{if}(\epsilon), \quad (2.3)$$

where the subscripts i and f refer to the initial and final states, a_0 is the Bohr radius, k_i is the relativistic wavenumber of the impact electron, $g_i = [J_i] = 2J_i + 1$ is the statistical weight of the initial state of the N -electron target ion. The total collision strength is computed by summing over the partial collision strength in equation (I.28), which is computed from the transition matrix T . Matrix T can be expressed in terms of reactance matrix K in equation (I.30). F-like selenium is a highly charged ion, and in some tested cases it has been found that the elements of matrix K are small, so that the weak-coupling approximation used here should give a good treatment. After applying the factorization method proposed by Bar-Shalom *et al* [16] to the RDWB model by Sampson *et al* [17], the final expression for the collision strength is given in equation (I.32).

2.3. Distorted potentials

In the RDWB method, the distorted potential $V(r)$,

$$V(r) = V'(r) + V^{ex}(r), \quad (2.4)$$

$$V'(r) = -\frac{Z(r)}{r} + V_c(r), \quad (2.5)$$

$$V_c(r) = \sum_{n\kappa} \omega_{n\kappa} \int_0^\infty \frac{1}{r_{>}} [P_{n\kappa}^2(r') + Q_{n\kappa}^2(r')] dr', \quad (2.6)$$

is used to distort the wavefunctions. $V^{ex}(r)$ and $V_c(r)$ are the spherical average of the electron–electron interaction including free electron. $V^{ex}(r)$ will be explained below. $V_c(r)$ is the spherically averaged classical potential. Hence the residual potential $U(r)$ is

$$\begin{aligned} U(r) &= -\frac{Z(r)}{r} + \sum_{i=1}^N \frac{1}{|\vec{r} - \vec{r}_i|} - V(r) \\ &= \sum_{i=1}^N \frac{1}{|\vec{r} - \vec{r}_i|} - (V_c(r) + V^{ex}(r)) \end{aligned} \quad (2.7)$$

which is used as a perturbation potential for the subsequent RDWB approximation. \vec{r}_i ($i = 1, \dots, N$) are the radii of the N bound electrons. The meanings of the finite nuclear charge $Z(r)$, occupation number $\omega_{n\kappa}$, large and small orbital components $P_{n\kappa}$ and $Q_{n\kappa}$ of the bound electrons were explained in detail in [5]. The exchange potential $V^{ex}(r)$ used in determining the continuum wavefunction is chosen to be the semi-classical exchange (SCE) approximation

proposed by Riley and Truhlar [7], which is the local energy-dependent exchange potential. It is the second choice of exchange potential appearing in [5].

$$V^{ex}(r) = \frac{1}{2}[V'(r) - \epsilon][(1 + \beta^2)^{1/2} - 1], \quad (2.8)$$

where

$$\beta^2 = \frac{4\pi\rho(r)}{[V'(r) - \epsilon]^2}. \quad (2.9)$$

Here, ϵ is the free-electron kinetic energy in atomic units. The direct potential $V'(r)$ is the spherically averaged potential given in equation (2.5). As stated in [7], the SCE exchange-distorted potentials would be more appropriate for determining the free-electron orbitals in collision calculation. The potential used in calculating the orbitals of the impact and scattered electrons for a transition differed only by different free-electron energies. Finite nuclear charge $Z(r)$, which differs from ordinary Z only for small r , is chosen to be the Fermi charge distribution [12] and can be obtained from GRASP² code [6]. A set of fictitious occupation numbers in equation (2.10), which is sometimes called a mean configuration, is used in the present calculation if no special mention is given.

$$1s_{1/2}^{2.0} 2s_{1/2}^{1.9} 2p_{1/2}^{1.9} 2p_{3/2}^{2.7} 3s_{1/2}^{0.04} 3p_{1/2}^{0.04} 3p_{3/2}^{0.04} 3d_{3/2}^{0.04} 3d_{5/2}^{0.04} 4s_{1/2}^{0.04} 4p_{1/2}^{0.04} 4p_{3/2}^{0.04} 4d_{3/2}^{0.04} 4d_{5/2}^{0.04} 4f_{5/2}^{0.05} 4f_{7/2}^{0.05}. \quad (2.10)$$

In equation (2.10) half an electron is excited. The original reason to use a fictitious occupation number was to make all bound and free orbitals orthogonal. However, from tests mentioned in [1] as well as made by us, it may be concluded that there is little influence on the F-like selenium system when different fictitious occupation numbers are used. The fictitious occupation number here is used solely to determine the spherically averaged Dirac–Fock central field potential for free orbitals. In the above-mentioned choice of potential, since two different potentials (MCDF and SCE) were used in the calculations of the bound and free orbitals, the orbitals of the free electron are not orthogonal to those of the bound electrons. As a result of these non-orthogonal orbitals, there will be various overlapping integrals appearing in the transition matrix elements, which are very difficult to calculate. It will be explained in the next section that, after making some approximations, the calculations can be simplified merely by replacing the factor $[r_{<}^\lambda / r_{>}^{\lambda+1}]$ with $[r_{<}^\lambda / r_{>}^{\lambda+1} - \delta_{\lambda 0} \frac{V_c(r)}{N}]$ in the exchange Slater integrals E^λ [17].

2.4. Approximations in calculating matrix elements

According to the first-order perturbation theory, the differential cross section for a transition from initial state i to final state f is the ratio of the transition probability per unit time to the incident electron flux. In the uncoupled representation, relativistic scattering amplitude B_{if} can be given by equation (20) of [18] for a transition from initial channel γ_i to final channel γ_f (free electron from spin m_{si} , wavenumber k_i and its direction \hat{k}_i to spin m_{sf} , wavenumber k_f and its direction \hat{k}_f),

$$B_{if} = \frac{2\pi}{k_i} \sum_{\substack{l_i, j_i, m_i \\ l_f, j_f, m_f}} i^{l_i - l_f + 1} e^{i(\delta_{\kappa_i} + \delta_{\kappa_f})} C(l_i \frac{1}{2} j_i; m_i - m_{si}, m_i) Y_{l_i}^{m_i - m_{si}*}(\hat{k}_i) \\ \times C(l_f \frac{1}{2} j_f; m_f - m_{sf}, m_f) Y_{l_f}^{m_f - m_{sf}}(\hat{k}_f) T(\gamma_i, \gamma_f). \quad (2.11)$$

Here Y and C are spherical harmonics and Clebsch–Gordan coefficients, respectively. δ are phases shifted by pure Coulomb potentials and other short-range distorted potentials. The relation between relativistic quantum number κ_i and total angular momentum j_i of the initial

free electron is: $j_i = |\kappa_i| - \frac{1}{2}$. If the weak-coupling approximation equation (I.30) is used, the relativistic T matrix can be expressed by equation (22) of [18],

$$T(\gamma_i, \gamma_f) = -4i\langle\gamma_i|U|\gamma_f\rangle, \quad (2.12)$$

where U is the residual perturbation potential as given in equation (2.7). T matrix elements in equation (2.12) are given in terms of the uncoupled representation. In our present calculation, both the target and the incident and scattering free-electron beams are unpolarized, and it is more convenient for us to transform the expression of cross sections in terms of the coupled representation T matrix. According to the definition of equation (2.11), the differential cross section $(d\sigma/d\Omega)_{if}$ for a transition $i \rightarrow f$ is,

$$(d\sigma/d\Omega)_{if} = |B_{if}|^2. \quad (2.13)$$

After involving derivation and summing over the final spins m_{sf} and averaging over the initial spins m_{si} , we get the following well known expression for cross sections σ_{if} (see equation (34) of [18] or equation (16) of [19]),

$$\sigma_{if} = \frac{\pi}{2g_i k_i^2} \sum_J [J] \sum_{\kappa_i, \kappa_f} |T(\Gamma_i, \Gamma_f)|^2, \quad (2.14)$$

where J is the total angular momentum of the $(N+1)$ -electron system. Γ are coupled angular momentum representation. Like equation (2.12), if weak-coupling approximation is applied, we have,

$$T(\Gamma_i, \Gamma_f) = -2iK(\Gamma_i, \Gamma_f) = -4i\langle\Gamma_i|U|\Gamma_f\rangle. \quad (2.15)$$

According to the definition of equation (2.3), the collision strength Ω_{if} can be expressed by

$$\Omega_{if} = 8 \sum_J [J] \sum_{\kappa_i, \kappa_f} |\langle\Gamma_i|U|\Gamma_f\rangle|^2. \quad (2.16)$$

If all the bound and continuum orbitals are orthogonal to one another, the one-electron operators in U have no contribution to the T (or K) matrix and henceforth can be eliminated. This is because there exists one integral between a pair of active orbitals in the initial and final states which is zero because of their orthogonality. Because the initial and final free-electron orbitals are orthogonal, each matrix element in equation (I.31) vanishes except when one index of r_{qk} is for the free electron, i.e. $k = N+1$. Then we find that equation (2.16) is equivalent to equation (I.31) or equation (3) of [17]. Both equation (2.16) and equation (I.31) hold for the calculation of excitation cross sections when unitarization is not necessary for the T matrix such as for the case of the highly charged F-like selenium of interest here. If appropriate approximations (see the next paragraph) are made, equation (2.16), like equation (I.31), can be factorized into the form of equation (I.32), namely, the angular part and the radial part of the matrix elements can be separated. As the angular part is independent of the free-electron orbitals and can be determined by only the properties of the target, the computing time can be saved by a few orders of magnitude. This possibility of factorization of the cross section expression is an extremely important advantage for very large-scale and time-consuming calculations and should be duly capitalized. Indeed, all our calculations including the previous calculations within the framework of RDWB procedures are based on equation (I.32), which makes the large-scale electron impact excitation calculation feasible.

In this paper, although all the bound orbitals are orthogonal (bound orbitals were calculated in a MCDF potential and Lagrange multipliers were used to ensure their orthogonalities), the continuum orbitals are not orthogonal to the bound orbitals because different potentials were used in their calculation. Hence, those one-electron operators in U cannot be eliminated automatically. Also, the calculations of T (K) matrix elements become extremely complex

Table 1. Level definitions and energies E (in eV) for the lowest 113 states of F-like selenium in increasing energy order. $2J$ is twice the total angular momentum quantum number. The occupied subshell is omitted for brevity. p means $p_{3/2}$ and p^* means $p_{1/2}$, etc.

| Level | Designation | $2J$ | E (eV) | Level | Designation | $2J$ | E (eV) |
|-------|----------------------|------|----------|-------|----------------------|------|----------|
| 1 | $[2p^3]_{3/2}$ | 3 | 0.0 | 58 | $[2p^*2p^3]_{23d^*}$ | 1 | 1684.54 |
| 2 | $[2p^*]_{1/2}$ | 1 | 42.87 | 59 | $[2s2p^3]_{23s}$ | 5 | 1688.23 |
| 3 | $[2s]_{1/2}$ | 1 | 213.20 | 60 | $[2s2p^3]_{23s}$ | 3 | 1696.45 |
| 4 | $[2p^2]_{23s}$ | 5 | 1499.34 | 61 | $[2s2p^3]_{13s}$ | 3 | 1712.74 |
| 5 | $[2p^2]_{23s}$ | 3 | 1504.02 | 62 | $[2s2p^3]_{13s}$ | 1 | 1713.21 |
| 6 | $[2p^2]_{03s}$ | 1 | 1518.61 | 63 | $[2s^22p^4]_{03d}$ | 5 | 1717.59 |
| 7 | $[2p^*2p^3]_{13s}$ | 3 | 1539.99 | 64 | $[2s^22p^4]_{03d^*}$ | 3 | 1721.63 |
| 8 | $[2p^*2p^3]_{13s}$ | 1 | 1543.69 | 65 | $[2s2p^3]_{23p^*}$ | 3 | 1732.56 |
| 9 | $[2p^2]_{23p^*}$ | 3 | 1544.27 | 66 | $[2s2p^3]_{23p^*}$ | 5 | 1736.01 |
| 10 | $[2p^2]_{03p^*}$ | 5 | 1546.10 | 67 | $[2s2p^*]_{03s}$ | 1 | 1736.45 |
| 11 | $[2p^*2p^3]_{23s}$ | 5 | 1552.87 | 68 | $[2s2p^3]_{23p}$ | 7 | 1743.82 |
| 12 | $[2p^*2p^3]_{23s}$ | 3 | 1554.23 | 69 | $[2s2p^3]_{23p}$ | 3 | 1746.41 |
| 13 | $[2p^2]_{23p}$ | 1 | 1554.91 | 70 | $[2s2p^3]_{23p}$ | 5 | 1749.06 |
| 14 | $[2p^2]_{23p}$ | 5 | 1555.77 | 71 | $[2s2p^3]_{23p}$ | 1 | 1753.93 |
| 15 | $[2p^2]_{23p}$ | 7 | 1556.57 | 72 | $[2s2p^3]_{13p^*}$ | 3 | 1756.37 |
| 16 | $[2p^2]_{03p^*}$ | 1 | 1565.14 | 73 | $[2s2p^3]_{13p^*}$ | 1 | 1757.42 |
| 17 | $[2p^2]_{23p}$ | 3 | 1570.85 | 74 | $[2s2p^*]_{13s}$ | 3 | 1766.12 |
| 18 | $[2p^2]_{03p}$ | 3 | 1576.43 | 75 | $[2s2p^3]_{13p}$ | 5 | 1766.29 |
| 19 | $[2p^*2p^3]_{13p^*}$ | 1 | 1583.60 | 76 | $[2s2p^3]_{13p}$ | 3 | 1767.18 |
| 20 | $[2p^*2p^3]_{13p^*}$ | 3 | 1588.56 | 77 | $[2s2p^*]_{13s}$ | 1 | 1769.58 |
| 21 | $[2p^*2p^3]_{13p}$ | 5 | 1595.69 | 78 | $[2s2p^3]_{13p}$ | 1 | 1773.03 |
| 22 | $[2p^*2p^3]_{23p^*}$ | 5 | 1598.07 | 79 | $[2s2p^*]_{03p^*}$ | 1 | 1784.88 |
| 23 | $[2p^*2p^3]_{13p}$ | 1 | 1598.74 | 80 | $[2s2p^*]_{03p}$ | 3 | 1790.62 |
| 24 | $[2p^*2p^3]_{13p}$ | 3 | 1599.38 | 81 | $[2s2p^3]_{23d^*}$ | 1 | 1795.57 |
| 25 | $[2s^22p^4]_{03s}$ | 1 | 1601.39 | 82 | $[2s2p^3]_{23d^*}$ | 3 | 1797.83 |
| 26 | $[2p^*2p^3]_{23p}$ | 7 | 1608.37 | 83 | $[2s2p^3]_{23d}$ | 9 | 1799.87 |
| 27 | $[2p^*2p^3]_{23p}$ | 3 | 1609.16 | 84 | $[2s2p^3]_{23d^*}$ | 5 | 1801.15 |
| 28 | $[2p^2]_{23d^*}$ | 5 | 1611.39 | 85 | $[2s2p^3]_{23d^*}$ | 7 | 1801.34 |
| 29 | $[2p^2]_{23d^*}$ | 3 | 1611.81 | 86 | $[2s2p^3]_{23d}$ | 5 | 1807.16 |
| 30 | $[2p^2]_{23d}$ | 7 | 1612.46 | 87 | $[2s2p^3]_{23d}$ | 7 | 1808.48 |
| 31 | $[2p^*2p^3]_{23p}$ | 5 | 1612.74 | 88 | $[2s2p^*]_{13p^*}$ | 3 | 1810.81 |
| 32 | $[2p^2]_{23d^*}$ | 1 | 1613.47 | 89 | $[2s2p^3]_{23d}$ | 3 | 1811.73 |
| 33 | $[2p^*2p^3]_{23p^*}$ | 3 | 1614.34 | 90 | $[2s2p^3]_{23d}$ | 1 | 1819.56 |
| 34 | $[2p^2]_{23d}$ | 9 | 1615.82 | 91 | $[2s2p^*]_{13p}$ | 1 | 1820.35 |
| 35 | $[2p^2]_{23d^*}$ | 7 | 1616.76 | 92 | $[2s2p^*]_{13p}$ | 5 | 1821.57 |
| 36 | $[2p^2]_{23d}$ | 1 | 1621.48 | 93 | $[2s2p^3]_{13d^*}$ | 5 | 1823.80 |
| 37 | $[2p^2]_{23d}$ | 3 | 1625.10 | 94 | $[2s2p^*]_{13p}$ | 3 | 1824.29 |
| 38 | $[2p^*2p^3]_{23p}$ | 1 | 1627.13 | 95 | $[2s2p^3]_{13d^*}$ | 3 | 1824.77 |
| 39 | $[2p^2]_{23d}$ | 5 | 1628.33 | 96 | $[2s2p^3]_{13d^*}$ | 1 | 1825.19 |
| 40 | $[2p^2]_{03d^*}$ | 3 | 1634.35 | 97 | $[2s2p^3]_{13d}$ | 7 | 1825.38 |
| 41 | $[2p^2]_{03d}$ | 5 | 1636.95 | 98 | $[2s2p^3]_{13d}$ | 5 | 1825.46 |
| 42 | $[2p^*2p^3]_{13d^*}$ | 1 | 1649.82 | 99 | $[2s2p^*]_{13p^*}$ | 1 | 1827.16 |
| 43 | $[2p^*2p^3]_{13d^*}$ | 3 | 1653.87 | 100 | $[2s2p^3]_{13d}$ | 3 | 1832.11 |
| 44 | $[2p^*2p^3]_{13d}$ | 7 | 1654.64 | 101 | $[2s2p^*]_{03d}$ | 5 | 1849.25 |
| 45 | $[2s^22p^4]_{03p^*}$ | 1 | 1655.74 | 102 | $[2s2p^*]_{03d^*}$ | 3 | 1852.38 |
| 46 | $[2s^22p^4]_{03p}$ | 3 | 1657.76 | 103 | $[2s2p^*]_{13d^*}$ | 5 | 1877.99 |
| 47 | $[2p^*2p^3]_{13d}$ | 5 | 1658.48 | 104 | $[2s2p^*]_{13d}$ | 7 | 1879.09 |
| 48 | $[2p^*2p^3]_{13d^*}$ | 5 | 1660.07 | 105 | $[2s2p^*]_{13d}$ | 3 | 1880.94 |
| 49 | $[2p^*2p^3]_{13d}$ | 3 | 1660.70 | 106 | $[2s2p^*]_{13d^*}$ | 1 | 1884.15 |

Table 1. (Continued)

| Level | Designation | 2J | E (eV) | Level | Designation | 2J | E (eV) |
|-------|--|----|---------|-------|--|----|---------|
| 50 | [2p*2p ³] ₂ 3d* | 7 | 1665.19 | 107 | [2s2p*] ₁ 3d | 5 | 1884.16 |
| 51 | [2p*2p ³] ₂ 3d | 9 | 1666.90 | 108 | [2s2p*] ₁ 3d* | 3 | 1884.70 |
| 52 | [2p*2p ³] ₂ 3d | 5 | 1670.19 | 109 | [2p* ² 2p ⁴] ₀ 3s | 1 | 1935.60 |
| 53 | [2p*2p ³] ₂ 3d* | 1 | 1670.27 | 110 | [2p* ² 2p ⁴] ₀ 3p* | 1 | 1978.05 |
| 54 | [2p*2p ³] ₂ 3d | 7 | 1673.03 | 111 | [2p* ² 2p ⁴] ₀ 3p | 3 | 1988.75 |
| 55 | [2p*2p ³] ₂ 3d* | 3 | 1673.31 | 112 | [2p* ² 2p ⁴] ₀ 3d* | 3 | 2043.42 |
| 56 | [2p*2p ³] ₂ 3d* | 5 | 1674.78 | 113 | [2p* ² 2p ⁴] ₀ 3d | 5 | 2045.68 |
| 57 | [2p*2p ³] ₂ 3d | 3 | 1682.07 | | | | |

due to the overlapping integrals between free and bound orbitals. Therefore, a couple of approximations must be made to simplify our calculations. First, we make an approximation that exchange matrix elements from the overlapping of core (inactive shell) electrons and the free orbitals may be eliminated. These exchange matrix elements are the so-called three-electron exchange terms in equation (4.7) of [20]. Next, we make a minor approximation to omit the small energy-dependence exchange potential $V^{ex}(r)$ in U when performing the perturbation calculation so that $\langle i|V_c(r)/N|f\rangle$ can cancel out the zeroth order term of the multipole expansion of $\frac{1}{|\vec{r}_N - \vec{r}|} = \sum_{\lambda} \frac{r_{<}^{\lambda}}{r_{>}^{\lambda+1}} P_{\lambda}$ (P_{λ} are Legendre polynomials), i.e. $\langle i|\frac{1}{r_{>}}|f\rangle$. Hence, overlapping integrals over r do not need to be performed and thus the factorization form of cross sections like equation (I.32) can still be employed in the present calculation except for a minor modification in the expression of the exchange Slater integrals as mentioned above. The error introduced can be seen to be small from a direct comparison of the results (Present1 and Present2) in the next section. The \mathbf{K} matrix elements thus become [8],

$$K(\Gamma_i, \Gamma_f) = 2N \langle \Psi_i(\vec{r}^{-1}) F_i(\vec{r}) | \frac{1}{|\vec{r}_N - \vec{r}|} - \delta_{\Gamma_i \Gamma_f} \frac{V_c(r)}{N} | \Psi_f(\vec{r}^{-1}) F_f(\vec{r}) \rangle - 2N \langle \Psi_i(\vec{r}^{-1}) F_i(\vec{r}) | \frac{1}{|\vec{r}_N - \vec{r}|} - \frac{V_c(r)}{N} | \Psi_f(\vec{r}_N^{-1}) F_f(\vec{r}_N) \rangle, \quad (2.17)$$

where Ψ and F are N -electron bound wavefunctions and free-electron wavefunctions, respectively. $\vec{r} = \vec{r}_{N+1}$ is the coordinate of the free electron. The notation \vec{r}_N^{-1} indicates all the coordinates except the N th. The first and second integrals are the direct and exchange matrix elements, respectively. Normal Racah algebra is applicable for the angular coupling coefficients with the presence of the one-electron operator term $V_c(r)/N$. We further omit the $V_c(r)/N$ term from the direct matrix elements because of the orthogonality of the bound orbitals between the initial and final N -electron ions. This approximation may have a bit of influence on the results as in the one special case of $\Gamma_i = \Gamma_f$ in which the same J and parity term is a component of both the initial and final states in the MCDF configuration-expansion. After this approximation, the direct Slater integrals D^{λ} are the same as those used in equations (I.31) and (I.32) or equation (9) of [17]. From the multipole expansion of the perturbation potential used, however, the factor $[r_{<}^{\lambda}/r_{>}^{\lambda+1} - \delta_{\lambda 0} \frac{V_c(r)}{N}]$ should replace the factor $[r_{<}^{\lambda}/r_{>}^{\lambda+1}]$ in the exchange Slater integrals E^{λ} in equation (10) of [17].

It should be mentioned that $V_c(r)$ used and discussed above for the incident free electron are different from those for the scattering free electron. The choice of using the former $V_c(r)$ is called the ‘prior’ form approximation whereas using the latter ones is called the ‘post’ form approximation [21]. In this work, the so-called ‘post’ form was used. The ‘prior’ form will cause slightly different results [21].

Table 2. Electron collisional cross sections (cm^2) for all 2–3 transitions from the $2s^22p^5\ ^2P_{3/2}$ state in F-like selenium. Three different calculation models employed in this paper are tabulated and compared with those of Hagelstein [1] and Sampson *et al* [3] at energy 1000 eV above threshold. The level indices for transition are given under the heading levels: I, F, where I stands for the initial level and F the final level. $[n]$ means $\times 10^n$.

| I | F | Present1 | Present2 | Present3 | Hagel ^a | Samp ^b |
|---|----|------------|------------|------------|--------------------|-------------------|
| 1 | 2 | 4.792[–21] | 4.761[–21] | 4.806[–21] | | 4.73[–21] |
| 1 | 3 | 4.655[–20] | 4.645[–20] | 4.725[–20] | | 4.98[–20] |
| 1 | 4 | 2.027[–22] | 2.017[–22] | 2.040[–22] | 1.922[–22] | 1.95[–22] |
| 1 | 5 | 4.126[–22] | 4.127[–22] | 4.216[–22] | 4.521[–22] | 3.93[–22] |
| 1 | 6 | 1.071[–22] | 1.069[–22] | 1.083[–22] | 1.096[–22] | 1.07[–22] |
| 1 | 7 | 1.257[–22] | 1.256[–22] | 1.277[–22] | 1.323[–22] | 1.21[–22] |
| 1 | 8 | 8.286[–23] | 8.284[–23] | 8.423[–23] | 8.799[–23] | 8.00[–23] |
| 1 | 9 | 2.889[–22] | 2.854[–22] | 2.877[–22] | 2.795[–22] | 2.72[–22] |
| 1 | 10 | 4.574[–22] | 4.528[–22] | 4.545[–22] | 4.598[–22] | 4.34[–22] |
| 1 | 11 | 2.970[–22] | 2.970[–22] | 3.038[–22] | 3.344[–22] | 2.83[–22] |
| 1 | 12 | 6.878[–23] | 6.840[–23] | 6.882[–23] | 8.016[–23] | 6.64[–23] |
| 1 | 13 | 1.929[–22] | 1.910[–22] | 1.937[–22] | 1.953[–22] | 1.85[–22] |
| 1 | 14 | 4.694[–22] | 4.648[–22] | 4.680[–22] | 4.542[–22] | 4.45[–22] |
| 1 | 15 | 4.009[–22] | 3.945[–22] | 3.962[–22] | 3.758[–22] | 3.77[–22] |
| 1 | 16 | 9.283[–23] | 9.159[–23] | 9.170[–23] | 9.306[–23] | 8.79[–23] |
| 1 | 17 | 1.883[–21] | 1.892[–21] | 1.863[–21] | 1.125[–21] | 1.80[–21] |
| 1 | 18 | 6.983[–22] | 6.991[–22] | 6.815[–22] | 3.592[–22] | 6.86[–22] |
| 1 | 19 | 4.664[–23] | 4.583[–23] | 4.610[–23] | 3.058[–22] | 4.37[–23] |
| 1 | 20 | 4.902[–22] | 4.913[–22] | 4.769[–22] | 1.054[–21] | 4.52[–22] |
| 1 | 21 | 2.052[–22] | 2.029[–22] | 2.042[–22] | 2.290[–22] | 1.93[–22] |
| 1 | 22 | 1.447[–22] | 1.420[–22] | 1.424[–22] | 4.362[–22] | 1.34[–22] |
| 1 | 23 | 7.215[–23] | 7.140[–23] | 7.190[–23] | 1.373[–22] | 6.78[–23] |
| 1 | 24 | 2.693[–22] | 2.689[–22] | 2.711[–22] | 5.319[–22] | 2.60[–22] |
| 1 | 25 | 7.955[–24] | 7.951[–24] | 8.081[–24] | 7.432[–24] | 8.38[–24] |
| 1 | 26 | 3.479[–22] | 3.453[–22] | 3.490[–22] | 3.791[–22] | 3.33[–22] |
| 1 | 27 | 5.697[–22] | 5.711[–22] | 6.222[–22] | 7.768[–22] | 5.45[–22] |
| 1 | 28 | 4.900[–22] | 4.855[–22] | 4.909[–22] | 4.833[–22] | 4.64[–22] |
| 1 | 29 | 3.455[–22] | 3.425[–22] | 3.457[–22] | 3.385[–22] | 3.27[–22] |
| 1 | 30 | 5.692[–22] | 5.634[–22] | 5.706[–22] | 5.637[–22] | 5.35[–22] |
| 1 | 31 | 1.898[–22] | 1.879[–22] | 1.879[–22] | 2.073[–22] | 1.81[–22] |
| 1 | 32 | 1.859[–22] | 1.844[–22] | 1.850[–22] | 1.783[–22] | 1.76[–22] |
| 1 | 33 | 7.314[–21] | 7.362[–21] | 6.923[–21] | 1.267[–20] | 7.08[–21] |
| 1 | 34 | 4.737[–22] | 4.686[–22] | 4.733[–22] | 4.702[–22] | 4.49[–22] |
| 1 | 35 | 4.978[–22] | 4.953[–22] | 4.991[–22] | 4.923[–22] | 4.78[–22] |
| 1 | 36 | 1.275[–21] | 1.277[–21] | 1.274[–21] | 1.309[–21] | 1.25[–21] |
| 1 | 37 | 2.686[–21] | 2.690[–21] | 2.682[–21] | 2.578[–21] | 2.62[–21] |
| 1 | 38 | 6.507[–23] | 6.446[–23] | 6.317[–23] | 7.004[–23] | 6.27[–23] |
| 1 | 39 | 5.148[–21] | 5.157[–21] | 5.169[–21] | 5.237[–21] | 5.13[–21] |
| 1 | 40 | 1.854[–21] | 1.857[–21] | 1.820[–21] | 1.822[–21] | 1.86[–21] |
| 1 | 41 | 3.232[–21] | 3.236[–21] | 3.148[–21] | 3.410[–21] | 3.34[–21] |
| 1 | 42 | 5.191[–23] | 5.137[–23] | 5.178[–23] | 5.466[–23] | 4.91[–23] |
| 1 | 43 | 2.438[–22] | 2.432[–22] | 2.408[–22] | 2.397[–22] | 2.36[–22] |
| 1 | 44 | 2.719[–22] | 2.696[–22] | 2.728[–22] | 2.700[–22] | 2.58[–22] |
| 1 | 45 | 1.180[–23] | 1.162[–23] | 1.070[–23] | 1.451[–23] | 1.12[–23] |
| 1 | 46 | 8.756[–24] | 8.626[–24] | 8.907[–24] | 1.187[–23] | 8.79[–24] |
| 1 | 47 | 1.447[–21] | 1.449[–21] | 1.520[–21] | 1.382[–21] | 1.41[–21] |
| 1 | 48 | 2.562[–21] | 2.566[–21] | 2.477[–21] | 2.592[–21] | 2.57[–21] |
| 1 | 49 | 1.925[–22] | 1.913[–22] | 1.945[–22] | 1.975[–22] | 1.84[–22] |

Table 2. (Continued)

| I | F | Present1 | Present2 | Present3 | Hagel ^a | Samp ^b |
|---|-----|------------|------------|------------|--------------------|-------------------|
| 1 | 50 | 1.919[−22] | 1.895[−22] | 1.911[−22] | 1.842[−22] | 1.80[−22] |
| 1 | 51 | 3.202[−22] | 3.188[−22] | 3.230[−22] | 3.410[−22] | 3.11[−22] |
| 1 | 52 | 5.683[−22] | 5.674[−22] | 5.833[−22] | 6.329[−22] | 5.84[−22] |
| 1 | 53 | 2.722[−21] | 2.728[−21] | 2.732[−21] | 2.916[−21] | 2.55[−21] |
| 1 | 54 | 2.166[−22] | 2.152[−22] | 2.162[−22] | 2.355[−22] | 2.08[−22] |
| 1 | 55 | 6.050[−21] | 6.063[−21] | 5.935[−21] | 5.940[−21] | 5.96[−21] |
| 1 | 56 | 9.162[−21] | 9.183[−21] | 8.779[−21] | 9.628[−21] | 9.42[−21] |
| 1 | 57 | 1.619[−21] | 1.623[−21] | 1.555[−21] | 1.689[−21] | 1.64[−21] |
| 1 | 58 | 6.895[−22] | 6.904[−22] | 6.567[−22] | 6.289[−22] | 7.25[−22] |
| 1 | 59 | 7.692[−23] | 7.566[−23] | 7.650[−23] | 6.275[−23] | 7.16[−23] |
| 1 | 60 | 1.964[−21] | 1.977[−21] | 1.885[−21] | 1.839[−21] | 1.88[−21] |
| 1 | 61 | 2.662[−21] | 2.680[−21] | 2.518[−21] | 4.242[−21] | 2.63[−21] |
| 1 | 62 | 1.648[−23] | 1.621[−23] | 1.661[−23] | 8.015[−23] | 1.58[−23] |
| 1 | 63 | 6.796[−23] | 6.796[−23] | 6.893[−23] | 7.049[−23] | 7.28[−23] |
| 1 | 64 | 1.365[−23] | 1.351[−23] | 1.294[−23] | 1.509[−23] | 1.40[−23] |
| 1 | 65 | 5.643[−23] | 5.623[−23] | 5.680[−23] | 5.733[−23] | 5.59[−23] |
| 1 | 66 | 2.173[−22] | 2.174[−22] | 2.215[−22] | 2.195[−22] | 2.29[−22] |
| 1 | 67 | 1.509[−24] | 1.490[−24] | 1.514[−24] | 1.321[−23] | 1.76[−24] |
| 1 | 68 | 8.364[−23] | 8.313[−23] | 8.324[−23] | 8.447[−23] | 8.06[−23] |
| 1 | 69 | 2.308[−22] | 2.311[−22] | 2.344[−22] | 2.828[−22] | 2.33[−22] |
| 1 | 70 | 2.954[−22] | 2.957[−22] | 3.002[−22] | 3.722[−22] | 3.14[−22] |
| 1 | 71 | 4.005[−23] | 4.001[−23] | 4.187[−23] | 5.400[−23] | 4.17[−23] |
| 1 | 72 | 2.546[−22] | 2.551[−22] | 2.564[−22] | 2.779[−22] | 2.71[−22] |
| 1 | 73 | 2.503[−22] | 2.508[−22] | 2.516[−22] | 2.601[−22] | 2.74[−22] |
| 1 | 74 | 3.257[−22] | 3.277[−22] | 3.229[−22] | 6.174[−22] | 3.38[−22] |
| 1 | 75 | 2.581[−22] | 2.585[−22] | 2.633[−22] | 2.776[−22] | 2.75[−22] |
| 1 | 76 | 9.087[−23] | 9.087[−23] | 9.184[−23] | 1.117[−22] | 1.01[−22] |
| 1 | 77 | 5.394[−24] | 5.308[−24] | 5.431[−24] | 1.861[−23] | 5.15[−24] |
| 1 | 78 | 1.644[−23] | 1.640[−23] | 1.605[−23] | 1.374[−23] | 1.96[−23] |
| 1 | 79 | 1.678[−23] | 1.679[−23] | 1.565[−23] | 1.171[−23] | 2.14[−23] |
| 1 | 80 | 1.643[−24] | 1.640[−24] | 1.594[−24] | 1.163[−24] | 1.47[−24] |
| 1 | 81 | 4.336[−23] | 4.302[−23] | 4.335[−23] | 5.789[−23] | 4.13[−23] |
| 1 | 82 | 8.569[−23] | 8.503[−23] | 8.582[−23] | 1.670[−22] | 8.17[−23] |
| 1 | 83 | 2.182[−22] | 2.166[−22] | 2.218[−22] | 3.489[−22] | 2.05[−22] |
| 1 | 84 | 1.297[−22] | 1.287[−22] | 1.305[−22] | 2.382[−22] | 1.24[−22] |
| 1 | 85 | 3.302[−22] | 3.291[−22] | 3.317[−22] | 3.959[−22] | 3.18[−22] |
| 1 | 86 | 5.715[−22] | 5.711[−22] | 5.750[−22] | 7.235[−22] | 5.57[−22] |
| 1 | 87 | 1.018[−21] | 1.017[−21] | 1.025[−21] | 1.063[−21] | 1.00[−21] |
| 1 | 88 | 2.483[−23] | 2.481[−23] | 2.510[−23] | 2.174[−23] | 2.88[−23] |
| 1 | 89 | 3.275[−22] | 3.272[−22] | 3.286[−22] | 4.338[−22] | 3.21[−22] |
| 1 | 90 | 1.142[−22] | 1.140[−22] | 1.156[−22] | 1.762[−22] | 1.12[−22] |
| 1 | 91 | 5.298[−24] | 5.269[−24] | 5.280[−24] | 5.529[−24] | 5.83[−24] |
| 1 | 92 | 7.671[−23] | 7.679[−23] | 7.820[−23] | 7.191[−23] | 7.95[−23] |
| 1 | 93 | 6.222[−22] | 6.220[−22] | 6.174[−22] | 6.812[−22] | 6.09[−22] |
| 1 | 94 | 2.323[−23] | 2.319[−23] | 2.277[−23] | 2.655[−23] | 2.98[−23] |
| 1 | 95 | 6.370[−22] | 6.371[−22] | 6.463[−22] | 6.911[−22] | 6.34[−22] |
| 1 | 96 | 4.404[−22] | 4.406[−22] | 4.386[−22] | 5.229[−22] | 4.46[−22] |
| 1 | 97 | 9.330[−22] | 9.329[−22] | 9.510[−22] | 1.001[−21] | 9.40[−22] |
| 1 | 98 | 4.102[−22] | 4.098[−22] | 4.282[−22] | 4.261[−22] | 4.23[−22] |
| 1 | 99 | 8.398[−24] | 8.357[−24] | 7.601[−24] | 7.401[−24] | 1.18[−23] |
| 1 | 100 | 1.164[−22] | 1.161[−22] | 1.129[−22] | 1.593[−22] | 1.22[−22] |
| 1 | 101 | 3.920[−24] | 3.890[−24] | 3.960[−24] | 5.994[−23] | 3.82[−24] |

Table 2. (Continued)

| I | F | Present1 | Present2 | Present3 | Hagel ^a | Samp ^b |
|---|-----|------------|------------|------------|--------------------|-------------------|
| 1 | 102 | 5.070[−23] | 5.063[−23] | 4.725[−23] | 2.021[−22] | 5.44[−23] |
| 1 | 103 | 1.232[−22] | 1.230[−22] | 1.265[−22] | 1.263[−22] | 1.28[−22] |
| 1 | 104 | 2.233[−22] | 2.231[−22] | 2.305[−22] | 2.487[−22] | 2.31[−22] |
| 1 | 105 | 2.830[−23] | 2.813[−23] | 3.201[−23] | 8.358[−23] | 2.71[−23] |
| 1 | 106 | 1.797[−23] | 1.791[−23] | 2.125[−23] | 2.411[−23] | 1.56[−23] |
| 1 | 107 | 1.141[−22] | 1.139[−22] | 1.162[−22] | 1.166[−22] | 1.18[−22] |
| 1 | 108 | 6.670[−23] | 6.662[−23] | 6.983[−23] | 8.161[−23] | 6.60[−23] |
| 1 | 109 | 1.459[−24] | 1.458[−24] | 1.050[−24] | 1.337[−24] | 2.32[−24] |
| 1 | 110 | 1.301[−24] | 1.292[−24] | 1.382[−24] | 1.315[−24] | 1.11[−24] |
| 1 | 111 | 2.755[−24] | 2.741[−24] | 3.363[−24] | 2.946[−24] | 3.05[−24] |
| 1 | 112 | 2.680[−24] | 2.670[−24] | 2.961[−24] | 4.581[−24] | 3.60[−24] |
| 1 | 113 | 1.082[−23] | 1.083[−23] | 1.021[−23] | 2.879[−23] | 1.91[−23] |

^a These entries were obtained by Hagelstein [1].

^b These entries were obtained by Sampson *et al* [3]. Note that the energy above threshold was 1016.8 eV, which is slightly larger than 1000 eV chosen for the present calculations.

3. Result

The level designations and energies are given in table 1. The energy levels relative to the ground level are obtained with the 279-level MCDF configuration expansion, which is the total number of energy levels of the ground and singly excited M and N shell states.

We tabulate the cross sections in units of cm² for 2–3 excitation transitions from the 2s²2p⁵ 2P_{3/2} state in table 2. Results for excitation cross sections from the 2s²2p⁵ 2P_{1/2} state are presented in table 3, and those from the 2s¹2p⁶ 2S_{1/2} state are given in table 4. In tables 2–4, the five calculational models are tabulated at energy 1000 eV above threshold. The entry ‘Present1’ is obtained by 113-level MCDF configuration expansion. In this case, the continuum orbitals were computed without exchange potential, whereas the distorted-wave potential used was the spherically averaged potential of the nucleus plus the potential due to the bound electrons of the bound state; the fictitious mean configuration given in equation (3.1) was used in determining the potential in the calculation of free-electron orbitals. Equation (3.1)

$$1s_{1/2}^{2.0} 2s_{1/2}^{1.27} 2p_{1/2}^{1.27} 2p_{3/2}^{3.82} 3s_{1/2}^{0.128} 3p_{1/2}^{0.128} 3p_{3/2}^{0.128} 3d_{3/2}^{0.128} 3d_{5/2}^{0.128} \quad (3.1)$$

is just the same as equation (2.1) of [1], except that occupation numbers 0.127 in that equation were all replaced by 0.128. The above choice of occupation numbers gives 6.36 electrons in the L shell and 0.64 electrons in the M shell, which is not far from a 50–50% split. The approximations made here are almost the same as in [1]. The purpose of this choice is to make the comparison between the two sets of results as meaningful as possible. The entries ‘Present2’ were obtained with the same approximations as the entries ‘Present1’, except that SCE exchange potential was added in ‘Present2’. By direct comparison of ‘Present1’ and ‘Present2’ we can gauge the influence of this exchange potential on the final values of the cross sections. The entries ‘Present3’ were obtained with the 279-level MCDF configuration expansion which includes the ground and all singly excited MCDF states in both the M and N shells. SCE exchange potential was also added. The fictitious mean configuration given in equation (2.10), in which exactly half an electron is excited, was used in determining the potential required in the calculation of the free-electron orbitals. The entries ‘Hagel’ are the results calculated by Hagelstein [1] using his RDWB code. The entries ‘Samp’ are the results calculated by Sampson *et al* [3]. Detailed comparisons among the above-mentioned five groups of entries will be given in the following three paragraphs.

Table 3. Electron collisional cross sections (cm^2) for all 2–3 transitions from the $2s^2 2p^5 \ ^2P_{1/2}$ state in F-like selenium. Three different calculation models employed in this paper are tabulated and compared with those of Hagelstein [1] and Sampson *et al* [3] at energy 1000 eV above threshold. The level indices for transition are given under the heading levels: I, F, where I stands for the initial level and F the final level. $[n]$ means $\times 10^n$.

| I | F | Present1 | Present2 | Present3 | Hagel ^a | Samp ^b |
|---|----|------------|------------|------------|--------------------|-------------------|
| 2 | 3 | 4.972[–20] | 4.962[–20] | 5.070[–20] | | 5.26[–20] |
| 2 | 4 | 5.076[–24] | 5.038[–24] | 5.107[–24] | 4.953[–24] | 4.93[–24] |
| 2 | 5 | 6.392[–24] | 6.383[–24] | 6.471[–24] | 7.825[–24] | 5.85[–24] |
| 2 | 6 | 7.937[–24] | 7.890[–24] | 8.085[–24] | 8.739[–24] | 6.85[–24] |
| 2 | 7 | 1.162[–22] | 1.154[–22] | 1.163[–22] | 1.129[–22] | 1.11[–22] |
| 2 | 8 | 2.538[–22] | 2.540[–22] | 2.598[–22] | 2.880[–22] | 2.44[–22] |
| 2 | 9 | 9.848[–24] | 9.738[–24] | 9.995[–24] | 1.429[–23] | 9.07[–24] |
| 2 | 10 | 1.096[–23] | 1.082[–23] | 1.088[–23] | 1.836[–23] | 1.04[–23] |
| 2 | 11 | 1.515[–22] | 1.504[–22] | 1.510[–22] | 1.427[–22] | 1.45[–22] |
| 2 | 12 | 5.241[–22] | 5.246[–22] | 5.372[–22] | 5.073[–22] | 4.99[–22] |
| 2 | 13 | 3.513[–23] | 3.528[–23] | 3.251[–23] | 2.590[–23] | 2.80[–23] |
| 2 | 14 | 1.366[–23] | 1.353[–23] | 1.364[–23] | 2.311[–23] | 1.27[–23] |
| 2 | 15 | 9.812[–24] | 9.621[–24] | 9.663[–24] | 3.323[–23] | 9.17[–24] |
| 2 | 16 | 8.868[–24] | 8.722[–24] | 8.836[–24] | 2.823[–23] | 8.64[–24] |
| 2 | 17 | 3.952[–23] | 3.910[–23] | 3.974[–23] | 1.261[–22] | 3.73[–23] |
| 2 | 18 | 4.963[–23] | 4.880[–23] | 4.890[–23] | 5.200[–23] | 4.71[–23] |
| 2 | 19 | 1.664[–22] | 1.644[–22] | 1.656[–22] | 1.552[–22] | 1.56[–22] |
| 2 | 20 | 3.556[–22] | 3.521[–22] | 3.556[–22] | 5.501[–22] | 3.35[–22] |
| 2 | 21 | 3.025[–22] | 2.971[–22] | 2.985[–22] | 8.861[–22] | 2.83[–22] |
| 2 | 22 | 5.562[–22] | 5.524[–22] | 5.568[–22] | 5.251[–22] | 5.35[–22] |
| 2 | 23 | 2.575[–22] | 2.568[–22] | 2.524[–22] | 1.940[–22] | 2.38[–22] |
| 2 | 24 | 3.063[–22] | 3.041[–22] | 3.058[–22] | 2.059[–21] | 2.92[–22] |
| 2 | 25 | 2.600[–22] | 2.598[–22] | 2.639[–22] | 2.720[–22] | 2.59[–22] |
| 2 | 26 | 3.792[–22] | 3.718[–22] | 3.733[–22] | 1.200[–21] | 3.51[–22] |
| 2 | 27 | 2.374[–22] | 2.346[–22] | 2.368[–22] | 1.123[–21] | 2.25[–22] |
| 2 | 28 | 2.353[–23] | 2.332[–23] | 2.419[–23] | 2.194[–23] | 2.17[–23] |
| 2 | 29 | 5.760[–23] | 5.754[–23] | 5.756[–23] | 4.501[–23] | 4.97[–23] |
| 2 | 30 | 1.757[–23] | 1.736[–23] | 1.802[–23] | 1.726[–23] | 1.64[–23] |
| 2 | 31 | 3.844[–22] | 3.819[–22] | 3.831[–22] | 1.483[–21] | 3.72[–22] |
| 2 | 32 | 1.675[–23] | 1.671[–23] | 1.660[–23] | 2.055[–23] | 1.69[–23] |
| 2 | 33 | 2.400[–22] | 2.375[–22] | 2.316[–22] | 2.652[–22] | 2.29[–22] |
| 2 | 34 | 1.167[–23] | 1.153[–23] | 1.162[–23] | 1.175[–23] | 1.08[–23] |
| 2 | 35 | 9.963[–24] | 9.916[–24] | 9.940[–24] | 9.302[–24] | 9.19[–24] |
| 2 | 36 | 1.156[–23] | 1.147[–23] | 1.207[–23] | 1.371[–23] | 9.45[–24] |
| 2 | 37 | 1.503[–22] | 1.504[–22] | 1.483[–22] | 1.548[–22] | 1.44[–22] |
| 2 | 38 | 4.929[–21] | 4.961[–21] | 4.841[–21] | 1.466[–21] | 4.74[–21] |
| 2 | 39 | 1.904[–23] | 1.884[–23] | 1.938[–23] | 1.984[–23] | 1.80[–23] |
| 2 | 40 | 4.522[–23] | 4.490[–23] | 4.577[–23] | 4.936[–23] | 4.82[–23] |
| 2 | 41 | 5.916[–23] | 5.850[–23] | 5.902[–23] | 5.862[–23] | 5.59[–23] |
| 2 | 42 | 2.907[–22] | 2.884[–22] | 2.909[–22] | 2.870[–22] | 2.75[–22] |
| 2 | 43 | 6.289[–22] | 6.256[–22] | 6.296[–22] | 6.144[–22] | 5.99[–22] |
| 2 | 44 | 4.100[–22] | 4.052[–22] | 4.100[–22] | 4.029[–22] | 3.86[–22] |
| 2 | 45 | 5.439[–21] | 5.473[–21] | 5.165[–21] | 3.197[–21] | 5.30[–21] |
| 2 | 46 | 5.092[–22] | 5.042[–22] | 5.080[–22] | 5.040[–22] | 4.89[–22] |
| 2 | 47 | 3.747[–22] | 3.709[–22] | 3.728[–22] | 3.733[–22] | 3.54[–22] |
| 2 | 48 | 3.619[–22] | 3.610[–22] | 3.634[–22] | 3.741[–22] | 3.49[–22] |
| 2 | 49 | 1.256[–21] | 1.256[–21] | 1.265[–21] | 1.278[–21] | 1.22[–21] |
| 2 | 50 | 5.720[–22] | 5.699[–22] | 5.766[–22] | 5.449[–22] | 5.56[–22] |

Table 3. (Continued)

| I | F | Present1 | Present2 | Present3 | Hagel ^a | Samp ^b |
|---|-----|------------|------------|------------|--------------------|-------------------|
| 2 | 51 | 5.120[−22] | 5.057[−22] | 5.114[−22] | 5.228[−22] | 4.82[−22] |
| 2 | 52 | 3.675[−22] | 3.646[−22] | 3.699[−22] | 3.733[−22] | 3.50[−22] |
| 2 | 53 | 8.554[−22] | 8.545[−22] | 8.460[−22] | 9.285[−22] | 8.79[−22] |
| 2 | 54 | 3.349[−22] | 3.329[−22] | 3.335[−22] | 3.241[−22] | 3.22[−22] |
| 2 | 55 | 2.627[−21] | 2.630[−21] | 2.561[−21] | 2.416[−21] | 2.54[−21] |
| 2 | 56 | 3.085[−22] | 3.060[−22] | 3.031[−22] | 2.953[−22] | 2.93[−22] |
| 2 | 57 | 1.215[−20] | 1.217[−20] | 1.200[−20] | 1.249[−20] | 1.24[−20] |
| 2 | 58 | 9.788[−21] | 9.810[−21] | 9.668[−21] | 9.382[−21] | 9.51[−21] |
| 2 | 59 | 2.790[−24] | 2.736[−24] | 2.526[−24] | 4.248[−23] | 2.41[−24] |
| 2 | 60 | 7.428[−24] | 7.328[−24] | 7.125[−24] | 5.678[−23] | 7.38[−24] |
| 2 | 61 | 2.373[−23] | 2.333[−23] | 2.394[−23] | 4.603[−23] | 2.17[−23] |
| 2 | 62 | 7.776[−22] | 7.825[−22] | 7.371[−22] | 5.968[−22] | 7.29[−22] |
| 2 | 63 | 6.844[−22] | 6.795[−22] | 6.855[−22] | 6.838[−22] | 6.56[−22] |
| 2 | 64 | 1.167[−20] | 1.170[−20] | 1.133[−20] | 1.183[−20] | 1.19[−20] |
| 2 | 65 | 2.579[−24] | 2.570[−24] | 2.449[−24] | 4.276[−24] | 2.62[−24] |
| 2 | 66 | 2.445[−24] | 2.429[−24] | 2.421[−24] | 2.852[−24] | 2.62[−24] |
| 2 | 67 | 1.446[−21] | 1.455[−21] | 1.370[−21] | 2.202[−21] | 1.39[−21] |
| 2 | 68 | 1.710[−24] | 1.689[−24] | 1.752[−24] | 2.458[−24] | 1.67[−24] |
| 2 | 69 | 1.234[−23] | 1.233[−23] | 1.126[−23] | 9.986[−24] | 1.05[−23] |
| 2 | 70 | 1.069[−24] | 1.065[−24] | 1.099[−24] | 1.075[−24] | 1.25[−24] |
| 2 | 71 | 3.915[−23] | 3.919[−23] | 3.918[−23] | 3.932[−23] | 3.26[−23] |
| 2 | 72 | 6.516[−23] | 6.514[−23] | 6.663[−23] | 7.489[−23] | 6.80[−23] |
| 2 | 73 | 4.998[−24] | 4.977[−24] | 4.866[−24] | 6.327[−24] | 4.42[−24] |
| 2 | 74 | 6.032[−23] | 6.917[−23] | 7.043[−23] | 8.738[−23] | 6.80[−23] |
| 2 | 75 | 3.400[−23] | 3.379[−23] | 3.390[−23] | 3.247[−23] | 3.22[−23] |
| 2 | 76 | 1.110[−22] | 1.111[−22] | 1.140[−22] | 1.251[−22] | 1.13[−22] |
| 2 | 77 | 2.774[−21] | 2.793[−21] | 2.659[−21] | 3.348[−21] | 2.78[−21] |
| 2 | 78 | 2.764[−23] | 2.751[−23] | 2.810[−23] | 3.114[−23] | 2.80[−23] |
| 2 | 79 | 3.706[−22] | 3.713[−22] | 3.727[−22] | 3.664[−22] | 3.90[−22] |
| 2 | 80 | 3.356[−22] | 3.358[−22] | 3.406[−22] | 3.478[−22] | 3.50[−22] |
| 2 | 81 | 3.686[−25] | 3.659[−25] | 3.562[−25] | 1.571[−22] | 4.06[−25] |
| 2 | 82 | 2.203[−24] | 2.187[−24] | 2.131[−24] | 1.027[−22] | 2.12[−24] |
| 2 | 83 | 7.639[−27] | 7.605[−27] | 3.209[−26] | 4.397[−25] | |
| 2 | 84 | 4.113[−24] | 4.088[−24] | 4.027[−24] | 7.450[−23] | 3.94[−24] |
| 2 | 85 | 3.599[−24] | 3.572[−24] | 3.809[−24] | 3.790[−23] | 3.16[−24] |
| 2 | 86 | 1.359[−23] | 1.351[−23] | 1.374[−23] | 3.760[−23] | 1.30[−23] |
| 2 | 87 | 6.723[−25] | 6.664[−25] | 6.887[−25] | 1.183[−23] | 6.19[−25] |
| 2 | 88 | 3.822[−22] | 3.828[−22] | 3.888[−22] | 4.264[−22] | 3.97[−22] |
| 2 | 89 | 3.573[−23] | 3.566[−23] | 3.642[−23] | 1.202[−22] | 3.23[−22] |
| 2 | 90 | 1.345[−23] | 1.335[−23] | 1.328[−23] | 4.280[−23] | 1.21[−23] |
| 2 | 91 | 2.760[−22] | 2.765[−22] | 2.752[−22] | 3.062[−22] | 3.22[−22] |
| 2 | 92 | 8.713[−23] | 8.661[−23] | 8.757[−23] | 8.589[−23] | 8.42[−23] |
| 2 | 93 | 1.994[−22] | 1.990[−22] | 2.046[−22] | 1.965[−22] | 1.93[−22] |
| 2 | 94 | 2.865[−22] | 2.868[−22] | 2.895[−22] | 3.525[−22] | 3.24[−22] |
| 2 | 95 | 3.817[−23] | 3.788[−23] | 3.769[−23] | 6.566[−23] | 3.58[−23] |
| 2 | 96 | 7.429[−24] | 7.373[−24] | 7.363[−24] | 7.672[−24] | 6.91[−24] |
| 2 | 97 | 9.156[−23] | 9.087[−23] | 9.210[−23] | 1.213[−22] | 8.60[−23] |
| 2 | 98 | 3.455[−22] | 3.452[−22] | 3.411[−22] | 4.551[−22] | 3.28[−22] |
| 2 | 99 | 2.674[−23] | 2.658[−23] | 2.680[−23] | 2.871[−23] | 2.68[−23] |
| 2 | 100 | 1.298[−22] | 1.293[−22] | 1.289[−22] | 1.367[−22] | 1.26[−22] |
| 2 | 101 | 9.598[−22] | 9.586[−22] | 9.661[−22] | 9.344[−22] | 9.38[−22] |
| 2 | 102 | 8.349[−22] | 8.345[−22] | 8.254[−22] | 1.072[−21] | 8.24[−22] |

Table 3. (Continued)

| I | F | Present1 | Present2 | Present3 | Hagel ^a | Samp ^b |
|---|-----|------------|------------|------------|--------------------|-------------------|
| 2 | 103 | 9.343[−22] | 9.337[−22] | 9.525[−22] | 9.741[−22] | 9.33[−22] |
| 2 | 104 | 2.441[−22] | 2.422[−22] | 2.480[−22] | 2.959[−22] | 2.34[−22] |
| 2 | 105 | 7.287[−22] | 7.285[−22] | 7.202[−22] | 7.755[−22] | 6.94[−22] |
| 2 | 106 | 6.369[−23] | 6.320[−23] | 6.406[−23] | 6.674[−23] | 6.28[−23] |
| 2 | 107 | 1.282[−21] | 1.282[−21] | 1.307[−21] | 1.304[−21] | 1.32[−21] |
| 2 | 108 | 6.897[−22] | 6.894[−22] | 7.314[−22] | 7.294[−22] | 7.37[−22] |
| 2 | 109 | 3.071[−24] | 3.071[−24] | 2.431[−24] | 2.977[−24] | 4.48[−24] |
| 2 | 110 | 3.268[−24] | 3.259[−24] | 3.813[−24] | 2.694[−24] | 3.78[−24] |
| 2 | 111 | 3.947[−24] | 3.918[−24] | 4.133[−24] | 4.875[−24] | 3.50[−24] |
| 2 | 112 | 1.974[−23] | 1.979[−23] | 1.841[−23] | 4.610[−23] | 3.16[−23] |
| 2 | 113 | 4.184[−24] | 4.153[−24] | 4.810[−24] | 4.519[−24] | 4.19[−24] |

^a These entries were obtained by Hagelstein [1].^b These entries were obtained by Sampson *et al* [3]. Note that the energy above threshold was 1016.8 eV, which is slightly larger than 1000 eV chosen for the present calculations.

From table 2, we can obtain the following comparisons: (1) comparisons of ‘Present1’ and ‘Present2’, which are referred to as ‘Comparison A’, reveal generally good agreement with each other. This indicates that exchange potential has only a little influence on the calculation. Most of the discrepancies are less than 1%. The largest discrepancy is nearly 2% for transition 1–77. The discrepancies are greater than 1% for the transitions from ground state to levels 9, 10, 13, 15, 16, 19, 21–23, 30, 31, 34, 38, 46, 50, 59, and 67. (2) ‘Comparison B’ which refers to comparisons of ‘Present2’ and ‘Present3’ does show some differences. The largest discrepancies (>5%) are 9% for transition 1–27, 6% for 1–33, 7% for 1–79, 5% for 1–98, 10% for 1–99, 14% for 1–105, 19% for 1–106, 39% for 1–109, 7% for 1–110, 23% for 1–111, 11% for 1–112, and 6% for 1–113. There are about one-fourth of the total transitions whose discrepancies are more than a few per cent. This indicates the necessity of the calculation with 279-level MCDF configuration expansion. (3) ‘Comparison C’ represents comparisons between ‘Present2’ and ‘Samp’. There is generally very good agreement. However, some differences exist especially for transitions 1–67, 1–76, 1–78, 1–79, 1–80, 1–88, 1–91, 1–94, 1–99, 1–107, 1–109, 1–110, 1–111, 1–112, and 1–113. The collision strengths for these transitions are very small ($<10^{-3}$ or even $<10^{-4}$). The largest three discrepancies are 41% for transition 1–99, 59% for 1–109, and 76% for 1–113. (4) ‘Comparison D’ refers to the comparisons of ‘Present1’ and ‘Hagel’. Here, the agreement is often very poor. This conclusion was also drawn by Sampson *et al* [3]. About half of all the transitions have more than 10% in discrepancy. About one-third of all the transitions have discrepancies greater than 30%. For transitions from level 1 to levels 18, 22–24, 61, 62, 74, 77, 82–84, 102, 105, 112, and 113, respectively, the discrepancies are about 100% or even higher. For transition 1–62, the difference is about a factor of five. This is the largest discrepancy in this comparison mode. Paradoxically, however, some of the transitions which have large differences in ‘Comparison C’, are in good agreement or have fewer discrepancies in ‘Comparison D’. This is a consequence of the fact that the atomic structure used in the three calculational codes are more or less different from one another.

We can do the same four comparison modes for table 3. (1) When ‘Comparison A’ is made in table 3, the conclusion is the same as in table 2. The discrepancies are greater than 1% for transitions from level 2 to levels 9, 10, 15, 16, 18, 19, 21, 26, 30, 34, 39, 51, 60, and 75 respectively. (2) In ‘Comparison B’, some large discrepancies are found for transitions from level 2 to levels 3, 13, 45, 59, 62, 64, 67, 69, 76, 81, 83, 85, 108–110, and 113 respectively. The

Table 4. Electron collisional cross sections (cm^2) for all 2–3 transitions from the $2s2p^6\ ^2S_{1/2}$ state in F-like selenium. Three different calculation models employed in this paper are tabulated and compared with those of Hagelstein [1] and Sampson *et al* [3] at energy 1000 eV above threshold. The level indices for transition are given under the heading levels: I, F, where I stands for the initial level and F the final level. $[n]$ means $\times 10^n$.

| I | F | Present1 | Present2 | Present3 | Hagel ^a | Samp ^b |
|---|----|------------|------------|------------|--------------------|-------------------|
| 3 | 4 | 1.408[–24] | 1.402[–24] | 1.372[–24] | 3.967[–24] | 6.97[–25] |
| 3 | 5 | 1.123[–24] | 1.118[–24] | 1.070[–24] | 4.494[–24] | 4.04[–25] |
| 3 | 6 | 5.003[–24] | 5.018[–24] | 4.016[–24] | 6.319[–24] | 1.73[–24] |
| 3 | 7 | 3.974[–25] | 3.924[–25] | 4.321[–25] | 1.314[–24] | 4.49[–25] |
| 3 | 8 | 4.908[–25] | 4.899[–25] | 4.404[–25] | 3.787[–25] | 3.61[–25] |
| 3 | 9 | 1.957[–24] | 1.951[–24] | 2.037[–24] | 2.210[–24] | 1.08[–24] |
| 3 | 10 | 9.665[–25] | 9.584[–25] | 9.889[–25] | 9.785[–25] | 8.09[–25] |
| 3 | 11 | 4.801[–24] | 4.789[–24] | 4.515[–24] | 3.847[–24] | 1.22[–24] |
| 3 | 12 | 3.692[–24] | 3.683[–24] | 3.490[–24] | 3.190[–24] | 1.04[–24] |
| 3 | 13 | 1.095[–24] | 1.091[–24] | 1.115[–24] | 1.041[–24] | 1.13[–24] |
| 3 | 14 | 1.146[–24] | 1.136[–24] | 1.177[–24] | 1.252[–24] | 9.94[–25] |
| 3 | 15 | 6.736[–25] | 6.694[–25] | 6.191[–25] | 6.465[–25] | 3.47[–25] |
| 3 | 16 | 4.834[–24] | 4.835[–24] | 4.832[–24] | 4.033[–24] | 1.80[–24] |
| 3 | 17 | 7.453[–24] | 7.461[–24] | 7.084[–24] | 1.047[–23] | 6.33[–24] |
| 3 | 18 | 3.404[–24] | 3.397[–24] | 3.546[–24] | 2.231[–24] | 6.59[–25] |
| 3 | 19 | 5.937[–25] | 5.886[–25] | 6.234[–25] | 9.709[–25] | 5.52[–25] |
| 3 | 20 | 2.650[–24] | 2.646[–24] | 2.770[–24] | 2.550[–24] | 2.00[–24] |
| 3 | 21 | 1.089[–24] | 1.079[–24] | 1.132[–24] | 4.044[–24] | 1.05[–24] |
| 3 | 22 | 1.285[–24] | 1.281[–24] | 1.189[–24] | 1.310[–24] | 5.03[–25] |
| 3 | 23 | 9.193[–25] | 9.166[–25] | 9.236[–25] | 2.201[–24] | 1.13[–24] |
| 3 | 24 | 4.632[–25] | 4.583[–25] | 4.792[–25] | 2.867[–24] | 4.85[–25] |
| 3 | 25 | 6.803[–24] | 6.820[–24] | 5.769[–24] | 4.277[–24] | 3.20[–24] |
| 3 | 26 | 1.764[–24] | 1.758[–24] | 1.600[–24] | 1.718[–24] | 6.26[–25] |
| 3 | 27 | 8.312[–24] | 8.322[–24] | 8.859[–24] | 1.128[–23] | 3.34[–24] |
| 3 | 28 | 1.958[–24] | 1.926[–24] | 1.996[–24] | 2.405[–24] | 9.96[–25] |
| 3 | 29 | 1.314[–24] | 1.295[–24] | 1.327[–24] | 4.271[–23] | 6.57[–25] |
| 3 | 30 | 1.948[–24] | 1.909[–24] | 2.030[–24] | 2.863[–24] | 9.61[–25] |
| 3 | 31 | 7.056[–25] | 7.008[–25] | 7.072[–25] | 7.868[–25] | 5.08[–25] |
| 3 | 32 | 1.082[–24] | 1.076[–24] | 9.962[–25] | 3.561[–23] | 4.23[–25] |
| 3 | 33 | 2.027[–23] | 2.030[–23] | 1.864[–23] | 3.181[–23] | 1.76[–23] |
| 3 | 34 | 5.454[–26] | 5.440[–26] | 7.171[–26] | 5.442[–26] | |
| 3 | 35 | 1.894[–25] | 1.864[–25] | 2.075[–25] | 3.886[–24] | 7.15[–26] |
| 3 | 36 | 1.428[–23] | 1.435[–23] | 1.189[–23] | 1.748[–23] | 4.14[–24] |
| 3 | 37 | 1.347[–24] | 1.341[–24] | 1.292[–24] | 3.149[–23] | 8.10[–25] |
| 3 | 38 | 2.467[–23] | 2.471[–23] | 2.425[–23] | 3.794[–23] | 1.61[–23] |
| 3 | 39 | 9.729[–25] | 9.663[–25] | 1.009[–24] | 3.986[–23] | 5.69[–25] |
| 3 | 40 | 1.053[–23] | 1.052[–23] | 1.008[–23] | 1.600[–23] | 7.05[–24] |
| 3 | 41 | 1.764[–23] | 1.763[–23] | 1.661[–23] | 9.818[–23] | 1.24[–23] |
| 3 | 42 | 7.432[–25] | 7.287[–25] | 7.694[–25] | 2.550[–21] | 3.82[–25] |
| 3 | 43 | 1.211[–24] | 1.194[–24] | 1.208[–24] | 4.845[–21] | 6.21[–25] |
| 3 | 44 | 1.710[–24] | 1.676[–24] | 1.750[–24] | 1.330[–21] | 1.03[–24] |
| 3 | 45 | 1.831[–24] | 1.825[–24] | 1.628[–24] | 5.153[–24] | 3.40[–24] |
| 3 | 46 | 1.434[–23] | 1.433[–23] | 1.432[–23] | 1.234[–23] | 7.35[–24] |
| 3 | 47 | 2.052[–24] | 2.042[–24] | 2.021[–24] | 3.025[–21] | 1.39[–24] |
| 3 | 48 | 4.413[–24] | 4.406[–24] | 3.984[–24] | 1.302[–23] | 3.42[–24] |
| 3 | 49 | 8.900[–25] | 8.781[–25] | 8.833[–25] | 5.190[–22] | 5.07[–25] |
| 3 | 50 | 1.928[–25] | 1.913[–25] | 2.355[–25] | 8.572[–25] | 3.48[–26] |
| 3 | 51 | 1.875[–25] | 1.870[–25] | 2.393[–25] | 1.860[–25] | |

Table 4. (Continued)

| I | F | Present1 | Present2 | Present3 | Hagel ^a | Samp ^b |
|---|-----|------------|------------|------------|--------------------|-------------------|
| 3 | 52 | 2.449[−24] | 2.440[−24] | 2.464[−24] | 4.560[−23] | 1.19[−24] |
| 3 | 53 | 4.707[−23] | 4.731[−23] | 3.899[−23] | 5.797[−23] | 1.53[−23] |
| 3 | 54 | 4.680[−25] | 4.592[−25] | 4.917[−25] | 3.394[−23] | 2.82[−25] |
| 3 | 55 | 1.196[−24] | 1.183[−24] | 1.194[−24] | 3.061[−23] | 9.10[−25] |
| 3 | 56 | 4.341[−24] | 4.319[−24] | 3.717[−24] | 1.788[−22] | 4.49[−24] |
| 3 | 57 | 1.530[−24] | 1.520[−24] | 1.768[−24] | 5.855[−22] | 8.92[−25] |
| 3 | 58 | 1.257[−23] | 1.264[−23] | 1.118[−23] | 1.486[−22] | 5.92[−24] |
| 3 | 59 | 1.532[−22] | 1.520[−22] | 1.519[−22] | 1.474[−22] | 1.46[−22] |
| 3 | 60 | 4.371[−22] | 4.373[−22] | 4.476[−22] | 4.371[−22] | 4.06[−22] |
| 3 | 61 | 1.794[−22] | 1.788[−22] | 1.776[−22] | 1.820[−22] | 1.66[−22] |
| 3 | 62 | 2.456[−22] | 2.458[−22] | 2.523[−22] | 2.539[−22] | 2.30[−22] |
| 3 | 63 | 2.914[−23] | 2.911[−23] | 2.848[−23] | 2.563[−23] | 2.10[−23] |
| 3 | 64 | 3.193[−23] | 3.189[−23] | 3.008[−23] | 6.826[−23] | 2.50[−23] |
| 3 | 65 | 3.361[−22] | 3.316[−22] | 3.323[−22] | 4.266[−22] | 3.13[−22] |
| 3 | 66 | 4.759[−22] | 4.717[−22] | 4.720[−22] | 4.491[−22] | 4.47[−22] |
| 3 | 67 | 2.086[−22] | 2.087[−22] | 2.109[−22] | 2.280[−22] | 1.94[−22] |
| 3 | 68 | 3.940[−22] | 3.863[−22] | 3.864[−22] | 8.506[−22] | 3.66[−22] |
| 3 | 69 | 2.822[−22] | 2.790[−22] | 2.796[−22] | 8.443[−22] | 2.64[−22] |
| 3 | 70 | 4.489[−22] | 4.461[−22] | 4.467[−22] | 8.322[−22] | 4.26[−22] |
| 3 | 71 | 4.634[−22] | 4.648[−22] | 4.697[−22] | 3.358[−22] | 4.44[−22] |
| 3 | 72 | 2.144[−22] | 2.118[−22] | 2.119[−22] | 3.275[−22] | 2.01[−22] |
| 3 | 73 | 1.080[−21] | 1.084[−21] | 1.042[−21] | 1.112[−21] | 1.01[−21] |
| 3 | 74 | 4.603[−22] | 4.606[−22] | 4.692[−22] | 3.907[−22] | 4.42[−22] |
| 3 | 75 | 2.725[−22] | 2.676[−22] | 2.672[−22] | 8.065[−22] | 2.53[−22] |
| 3 | 76 | 3.829[−22] | 3.807[−22] | 3.822[−22] | 1.158[−21] | 3.65[−22] |
| 3 | 77 | 6.052[−23] | 6.011[−23] | 6.031[−23] | 5.630[−23] | 6.07[−23] |
| 3 | 78 | 1.236[−21] | 1.243[−21] | 1.219[−21] | 8.982[−22] | 1.19[−21] |
| 3 | 79 | 2.277[−21] | 2.290[−21] | 2.175[−21] | 6.095[−22] | 2.11[−21] |
| 3 | 80 | 2.852[−22] | 2.826[−22] | 2.835[−22] | 3.050[−22] | 2.69[−22] |
| 3 | 81 | 2.962[−22] | 2.935[−22] | 2.959[−22] | 2.790[−22] | 2.75[−22] |
| 3 | 82 | 5.169[−22] | 5.123[−22] | 5.154[−22] | 4.782[−22] | 4.83[−22] |
| 3 | 83 | 5.355[−22] | 5.289[−22] | 5.322[−22] | 5.506[−22] | 5.03[−22] |
| 3 | 84 | 4.741[−22] | 4.694[−22] | 4.698[−22] | 4.515[−22] | 4.41[−22] |
| 3 | 85 | 4.270[−22] | 4.230[−22] | 4.236[−22] | 4.166[−22] | 4.04[−22] |
| 3 | 86 | 3.980[−22] | 3.947[−22] | 3.981[−22] | 3.890[−22] | 3.75[−22] |
| 3 | 87 | 5.234[−22] | 5.224[−22] | 5.203[−22] | 4.910[−22] | 5.04[−22] |
| 3 | 88 | 2.366[−22] | 2.333[−22] | 2.332[−22] | 3.410[−22] | 2.22[−22] |
| 3 | 89 | 2.276[−21] | 2.279[−21] | 2.254[−21] | 2.110[−21] | 2.22[−21] |
| 3 | 90 | 4.386[−21] | 4.395[−21] | 4.390[−21] | 4.382[−21] | 4.28[−21] |
| 3 | 91 | 3.764[−22] | 3.771[−22] | 4.035[−22] | 4.196[−22] | 3.66[−22] |
| 3 | 92 | 5.375[−22] | 5.335[−22] | 5.361[−22] | 6.492[−22] | 5.13[−22] |
| 3 | 93 | 2.669[−22] | 2.642[−22] | 2.649[−22] | 2.841[−22] | 2.52[−22] |
| 3 | 94 | 1.440[−22] | 1.416[−22] | 1.409[−22] | 4.312[−22] | 1.33[−22] |
| 3 | 95 | 9.363[−22] | 9.351[−22] | 9.199[−22] | 8.353[−22] | 8.48[−22] |
| 3 | 96 | 2.869[−21] | 2.873[−21] | 2.707[−21] | 2.726[−21] | 2.81[−21] |
| 3 | 97 | 3.754[−22] | 3.714[−22] | 3.710[−22] | 3.626[−22] | 3.54[−22] |
| 3 | 98 | 5.058[−22] | 5.037[−22] | 5.052[−22] | 4.992[−22] | 4.80[−22] |
| 3 | 99 | 9.150[−21] | 9.210[−21] | 8.565[−21] | 4.319[−21] | 8.68[−21] |
| 3 | 100 | 7.296[−21] | 7.311[−21] | 7.234[−21] | 7.008[−21] | 7.32[−21] |
| 3 | 101 | 3.966[−22] | 3.944[−22] | 3.959[−22] | 4.013[−22] | 3.76[−22] |
| 3 | 102 | 8.594[−21] | 8.612[−21] | 8.333[−21] | 8.180[−21] | 8.44[−21] |
| 3 | 103 | 3.012[−22] | 2.980[−22] | 3.002[−22] | 3.057[−22] | 2.84[−22] |

Table 4. (Continued)

| I | F | Present1 | Present2 | Present3 | Hagel ^a | Samp ^b |
|---|-----|------------|------------|------------|--------------------|-------------------|
| 3 | 104 | 5.115[−22] | 5.089[−22] | 5.160[−22] | 4.871[−22] | 4.93[−22] |
| 3 | 105 | 6.620[−21] | 6.632[−21] | 6.821[−21] | 6.648[−21] | 6.94[−21] |
| 3 | 106 | 8.217[−21] | 8.236[−21] | 7.958[−21] | 8.091[−21] | 8.29[−21] |
| 3 | 107 | 2.053[−22] | 2.028[−22] | 2.023[−22] | 1.945[−22] | 1.92[−22] |
| 3 | 108 | 5.491[−21] | 5.503[−21] | 4.823[−21] | 5.131[−21] | 5.27[−21] |
| 3 | 109 | 1.964[−21] | 1.975[−21] | 1.861[−21] | 1.892[−21] | 1.94[−21] |
| 3 | 110 | 2.493[−22] | 2.493[−22] | 2.538[−22] | 2.806[−22] | 2.72[−22] |
| 3 | 111 | 4.980[−22] | 4.980[−22] | 5.060[−22] | 5.604[−22] | 5.40[−22] |
| 3 | 112 | 1.285[−21] | 1.283[−21] | 1.305[−21] | 1.285[−21] | 1.29[−21] |
| 3 | 113 | 1.911[−21] | 1.909[−21] | 1.946[−21] | 1.917[−21] | 1.91[−21] |

^a These entries were obtained by Hagelstein [1].

^b These entries were obtained by Sampson *et al* [3]. Note that the energy above threshold was 1016.8 eV, which is slightly larger than 1000 eV chosen for the present calculations.

largest five discrepancies are 9% for transition 2–13, a factor of 4 for 2–83, 26% for 2–109, 16% for 2–110, and 16% for 2–113. (3) In ‘Comparison C’, the following transitions have large discrepancies (per cent is given in parentheses if >20%): transition from level 2 to levels 6, 13 (26%), 29, 30, 36 (21%), 70, 71 (20%), 81, 85, 87, 91, 109 (46%), 111, and 112 (60%). (4) ‘Comparison D’ also reveals that about half of all the transitions have discrepancies greater than 10%. Nearly one-fifth of all the transitions have discrepancies of more than 100%. For the transitions 2–81, 2–83, 2–87, the differences run into several orders of magnitude.

Next we investigate table 4. (1) When ‘Comparison A’ is made, the conclusion is the same as in tables 2–3. The discrepancies are greater than 1% for transitions from level 3 to levels 7, 28–30, 35, 42–44, 49, 54, 55, 65, 68, 72, 75, 94, and 106. (2) For ‘Comparison B’ the differences are larger than those in the previous two tables. Notably, these are 12% for transitions 3–8, 18% for 3–25, 10% for 3–26, 32% for 3–34, 11% for 3–35, 21% for 3–36, 12% for 3–45, 11% for 3–48, 23% for 3–50, 28% for 3–51, 21% for 3–53, 16% for 3–56 and 3–57, and 14% for 3–108. These discrepancies are due to the fact that cross sections for these transitions are generally relatively very small, except for transition 3–108 whose collision strength is as large as 2.16×10^{-2} . (3) As to ‘Comparison C’, the conclusion is greatly different from those in the previous two tables. For transitions from level 3 to levels 4–58 (except levels 7, 13, 14, 19, 21, 24, 33, 56), level 63 and level 64, respectively, the differences are vast (about a few factors). However, once again, most of the collision strengths for these transitions are small ($<10^{-4}$). These differences are attributed to the different atomic structures used and will be analysed in detail below. For the transitions from level 3 to levels 59–113 (except levels 63 and 64), the agreement is fairly good because the cross sections for these transitions are large. This supports the conclusion drawn in the previous two tables. (4) ‘Comparison D’ also shows that in about half of all the transitions the discrepancies are very much larger than those in the previous two tables. There are 13 transitions whose differences are of several orders of magnitude. They are the transitions from level 3 to levels 29, 32, 35, 37, 42, 43, 47, 49, 52 and 54–57.

The above detailed investigations for the agreement and disagreement of ‘Comparison C’ and ‘Comparison D’ of tables 2–4 can be reflected in the atomic structure used. This suggests that the bound orbital wavefunctions may play a crucial role in the calculation. The main reason for the discrepancies in ‘Comparison D’ as well as in ‘Comparison C’ is most likely due to the different atomic structures used in the calculations. Strong correlation effects have been known for F-like selenium for configurations $2s2p^6$ and $2s^22p^5$. These are exhibited

not only in the discrepancies in the energy levels, but also in the gauge dependence of the transition rates to the ground configuration $2s^22p^5$. Although most of the correlation effects in energies was caught by the calculation of Hagelstein, both Hagelstein [1] and Sampson *et al* [3] used the mean configuration in determining potential instead of the more realistic MCDF potential in their atomic structure calculations. These approximations should have some influence on the atomic structure, especially for small transitions which are strongly influenced by the bound wavefunctions. Use of the GRASP² code to provide atomic structure should enhance the reliability and accuracy of the present cross sections. In addition, in computing the collisions section, there are several detailed considerations in the present RDWB calculational procedures. It is hoped that the present sets of data would be of use in the development of XUV lasers and other fields involving highly stripped ions.

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