

Rate coefficients for electron impact excitation of S XV

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Abstract. Collision strengths for electron impact excitation of S XV are calculated in a close-coupling approach. The nineteen lowest LS states are included in the calculation. Rate coefficients are obtained for transitions from the ground $1s^2\ ^1S_0$ state to the fine-structure levels of all excited states of $1s2\ell$ ($\ell = 0, 1$) and $1s3\ell$ ($\ell = 0, 1, 2$) configurations. The resulting effective collision strengths are fitted to a polynomial function of $\log(T_e/K)$, and rate coefficients are presented in the temperature range between $1\ 10^6$ K and $1\ 10^8$ K.

Key words: atomic data

1. Introduction

The intensities of emission lines arising from transitions in He-like ions are frequently used to determine the electron temperature and density of a plasma. The knowledge of the electron impact excitation of the He-like ions is required to analyze such emissions.

The Bragg Crystal Spectrometer on board the YOHKOH satellite (Culhane et al. 1991) detects soft X-rays from S XV in the solar corona to provide information of the coronal plasma. Sampson et al. (1983) and Zhang & Sampson (1987) obtained cross sections for excitation of S XV by electron impact in the Coulomb-Born approximation with including the electron exchange and resonance effects approximately. Keenan et al. (1987) estimated the rate coefficients for S XV with an interpolation of the rate coefficients for other He-like ions. Nakazaki et al. (1993) calculated cross sections for the excitation of S XV in a close-coupling approach using the R-matrix method. In their calculation the nineteen lowest LS states were included and the complicated resonance structure in the energy range near the threshold was fully

accounted for. They reported effective collision strengths “ \mathcal{Y} ” for the transitions from the ground $1s^2\ ^1S$ state to all LS states of $1s2\ell$ ($\ell = 0, 1$) and $1s3\ell$ ($\ell = 0, 1, 2$) configurations. However, the analysis of the satellite data requires collision data between fine-structure levels.

In the present paper, the calculation with the R-matrix method (Nakazaki et al. 1993) is repeated with parameters changed a little to improve the result. The calculation includes the same nineteen target terms as the previous calculation by Nakazaki et al. (1993). From the results, fine-structure cross sections are calculated with Saraph’s (1978) program JAJOM, which transforms the LS coupled reactance matrices to those for intermediate coupling with the term-coupling coefficients. Finally effective collision strengths \mathcal{Y} for the fine-structure levels are obtained from the corresponding cross sections and fitted to a polynomial function of $\log(T_e/K)$. They are compared with the previous works mentioned above. Recently, to analyze emission spectra from laboratory plasmas and solar plasmas, Harra-Murnion et al. (1996) used the effective collision strengths of S XV which were calculated by Norrington et al. (1998) using the Dirac R-matrix method. The present results are compared with those of relativistic calculations to confirm the reliability of the former.

2. Theory

2.1. Target wavefunctions

The nineteen lowest LS states of the target ion, i. e. $1s^2\ ^1S$, $1s2s\ ^1,^3S$, $1s2p\ ^1,^3P$, $1s3s\ ^1,^3S$, $1s3p\ ^1,^3P$, $1s3d\ ^1,^3D$, $1s4s\ ^1,^3S$, $1s4p\ ^1,^3P$, $1s4d\ ^1,^3D$ and $1s4f\ ^1,^3F$, are included in the expansion of the wavefunction in the R-matrix calculation. Each state is represented by a configuration interaction wavefunction. Ten basis orbitals $1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f$ are used. The radial part of the orbital is expressed in the Slater form

$$P_{nl}(r) = \sum_{j=1}^K C_j r^{p_j} \exp(-\xi_j r). \quad (1)$$

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Table 1. Configurations mixed for each target symmetry

State	Configurations
¹ S	1s ² , 1s2s, 1s3s, 1s4s, 2s ² , 2s3s, 2s4s
³ S	1s2s, 1s3s, 1s4s, 2s3s, 2s4s
¹ P	1s2p, 1s3p, 1s4p, 2s2p, 2s3p, 2s4p
³ P	1s2p, 1s3p, 1s4p, 2s2p, 2s3p, 2s4p
¹ D	1s3d, 1s4d, 2s3d, 2s4d
³ D	1s3d, 1s4d, 2s3d, 2s4d
¹ F	1s4f, 2s4f
³ F	1s4f, 2s4f

The coefficients C_j and the parameters p_j and ξ_j for all the orbitals are the same as those of Nakazaki et al. (1993). The excitation energies were obtained from Hibbert's (1975) CIV3 program and have been already presented by Nakazaki et al. (1993). The resulting energies are in fair agreement with the experimental values determined by Martin et al. (1990) and the oscillator strengths obtained agree with those of other calculations (Lin et al. 1977; Drake 1979). Table 1 gives a list of the configurations included in our calculation.

2.2. Collision calculations

The total wavefunction representing the electron-ion collision system is expanded in a sphere with radius r_a as follows:

$$\Psi_k = \mathcal{A} \sum_{ij} c_{ijk} \Phi_i(1, \dots, N, \hat{\mathbf{r}}_{N+1}, \sigma_{N+1}) u_{ij}(r_{N+1}) + \sum_j d_{jk} \phi_j(1, \dots, N+1), \quad (2)$$

where \mathcal{A} is the anti-symmetrization operator, Φ_i the channel function representing the target state coupled with the spin and angular functions for the scattered electron, u_{ij} the continuum basis orbitals for the scattered electron, and ϕ_j three-electron bound configurations formed from the ten bound orbitals. The coefficients c_{ijk} and d_{jk} are determined by diagonalizing the total Hamiltonian of the whole system with the basis set expansion defined by Eq. (2).

We use the computer code of Berrington et al. (1995) to calculate the R-matrix on the boundary of the sphere ($r_a = 4.9$ a.u.). We include 39 continuum orbitals for each angular momentum l to ensure convergence in the energy range considered. The calculations are made for all the partial waves with total angular momentum $L = 0$ up to 14. In the outer region of the sphere, a set of close-coupling equation is solved using the asymptotic code STGFJJ of Seaton. STGFJJ computes reactance matrices K by matching the solutions in the inner and the outer regions at the boundary $r = r_a$. The collision calculation is carried out over the energy range from the

1s2s ³S threshold to 480 Ryd. The LS coupled K -matrices are transformed to those for intermediate coupling using the code JAJOM (Saraph 1978), which yields collision strengths between fine-structure levels. The term-coupling coefficients are constructed from the unitary matrices that diagonalize the non-relativistic Hamiltonian and the Breit-Pauli Hamiltonian including the one-body mass-correction, Darwin and spin-orbit terms. Contributions from the partial waves higher than $L = 14$ are taken into account with an extrapolation.

2.3. Calculation of rate coefficients

Rate coefficients for a transition from level i to level f are defined as

$$C(i \rightarrow f) = \frac{8.629 \cdot 10^{-6}}{g_i \sqrt{T_e/K}} \exp(-\Delta E_{if}/kT_e) \mathcal{Y}(i \rightarrow f) \text{ cm}^3 \text{ s}^{-1}, \quad (3)$$

where g_i is the statistical weight of the initial level i , ΔE_{if} the respective transition energy, T_e the electron temperature, and k Boltzmann's constant. Assuming a Maxwellian electron velocity distribution, the effective collision strength $\mathcal{Y}(i \rightarrow f)$ is defined as

$$\mathcal{Y}(i \rightarrow f) = \int_0^\infty \Omega(i, f) \exp(-\varepsilon_f/kT_e) d(\varepsilon_f/kT_e), \quad (4)$$

where ε_f is the energy of the electron after the collision, and $\Omega(i, f)$ is the collision strength. It should be noted that \mathcal{Y} is symmetric over the transition $i \rightarrow f$ and $f \rightarrow i$. To obtain the rate coefficient at high temperature, we fit the present collision strengths in the non-resonance region to either of the following two analytic functions

$$\Omega(i, f) = A + B/X + C/X^2 + D/X^3 + E \ln X, \quad (5)$$

and

$$\Omega(i, f) = F_0/X^2 + \sum_{j=1}^4 F_j \exp(-j\alpha X), \quad (6)$$

where $X = k_i^2/(\Delta E_{if})$, where k_i^2 is the incident energy in Ryd and ΔE_{if} is given in Ryd. For a dipole-allowed transition, the first one (5) is used with $D = 0$ and $E = 4g_i f_{if}/\Delta E_{if}$, where f_{if} is the oscillator strength for $i \rightarrow f$. The form (5) with $E = 0$ is used for optically forbidden cases, unless the spin changes. For the spin-forbidden cases, the second one (6) is employed. The parameters A , B , C , D , F_j ($j = 0 - 4$) and α are determined by the least square method. Thus the effective collision strength is evaluated with the collision strengths calculated in the resonance region and those fitted above that.

3. Results and discussion

Effective collision strengths are calculated for transitions from the ground 1s² ¹S₀ state to all fine-structure levels of the excited states of 1s2 ℓ ($\ell = 0, 1$) and 1s3 ℓ ($\ell = 0, 1, 2$)

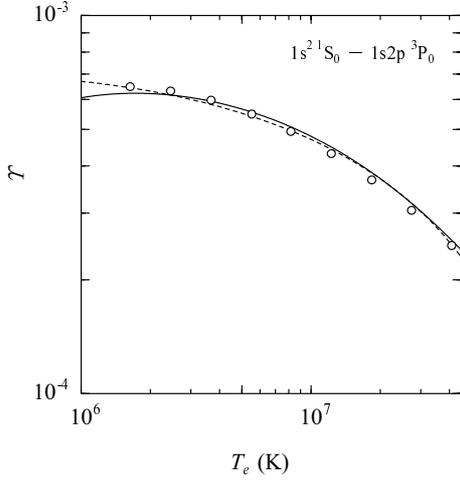


Fig. 1. Effective collision strengths of the $1s^2\ ^1S_0 - 1s2p\ ^3P_0$ excitation for S xv as a function of temperature (in K). — present, - - - Keenan et al. (1987), \circ Zhang & Sampson (1987)

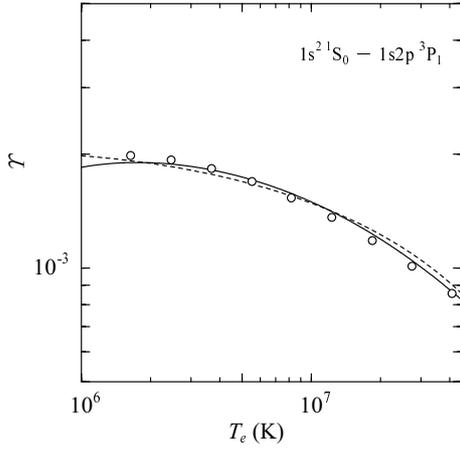


Fig. 2. Effective collision strengths of the $1s^2\ ^1S_0 - 1s2p\ ^3P_1$ excitation for S xv as a function of temperature (in K). — present, - - - Keenan et al. (1987), \circ Zhang & Sampson (1987)

configurations. They are obtained for a temperature range $T_e = (1\ 10^6 - 1\ 10^8)$ K. This is the range of the largest fractional abundance of S xv, if they are in ionization equilibrium (Arnaud & Rothenflug 1985). The resulting effective collision strengths are analytically fitted to the form

$$\Upsilon(i \rightarrow f) = \sum_{j=1}^5 a_j (\log(T_e/\text{K}))^{j-1}. \quad (7)$$

The fitting coefficients a_j are presented in Table 2. Equation (7) with these coefficients reproduces the present effective collision strengths within 2%. It should be noted here that fitting is valid only in the temperature range $6.0 \leq \log(T_e/\text{K}) \leq 8.0$.

As mentioned in the Introduction two groups (Zhang & Sampson 1987; Keenan et al. 1987) reported effective collision strengths for S xv. A comparison is made

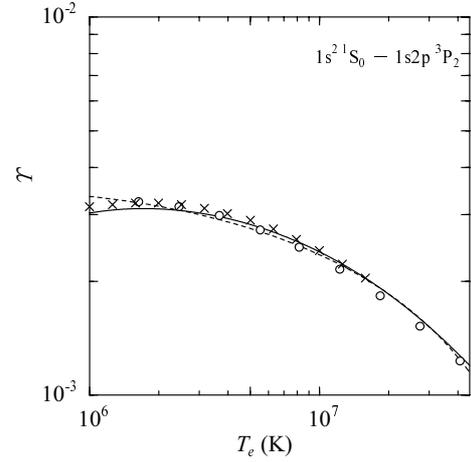


Fig. 3. Effective collision strengths of the $1s^2\ ^1S_0 - 1s2p\ ^3P_2$ excitation for S xv as a function of temperature (in K). — present, - - - Keenan et al. (1987), \circ Zhang & Sampson (1987), \times Norrington et al. (1998)

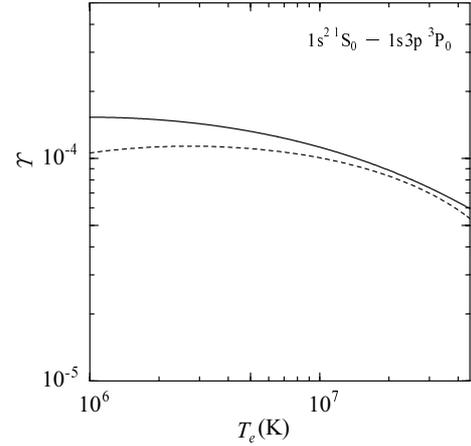


Fig. 4. Effective collision strengths of the $1s^2\ ^1S_0 - 1s3p\ ^3P_0$ excitation for S xv as a function of temperature (in K). — present, - - - Keenan et al. (1987)

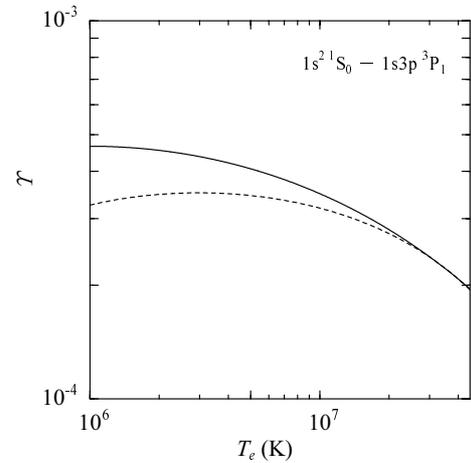
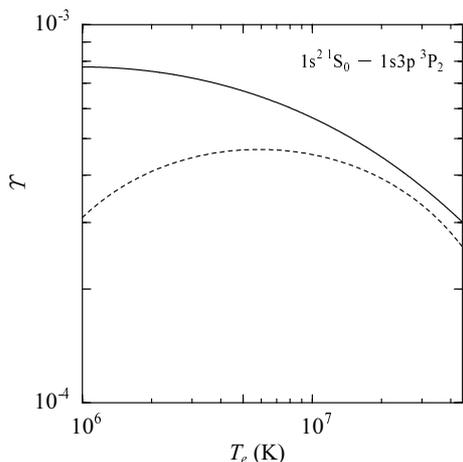


Fig. 5. Effective collision strengths of the $1s^2\ ^1S_0 - 1s3p\ ^3P_1$ excitation for S xv as a function of temperature (in K). — present, - - - Keenan et al. (1987)

Table 2. The coefficients a_j for representing effective collision strengths in the Eq. (7)

Transition	a_1	a_2	a_3	a_4	a_5
$1s^2\ ^1S_0 \rightarrow$					
1s2s 3S_1	-3.33705-1	1.77776-1	-3.48207-2	2.98916-3	-9.52407-5
1s2p 3P_0	6.97347-3	-9.42094-3	3.26111-3	-4.23881-4	1.87625-5
1s2p 3P_1	-3.87011-2	7.51109-3	1.76968-3	-4.77642-4	2.69621-5
1s2p 3P_2	2.91278-2	-4.37873-2	1.55922-2	-2.05178-3	9.14270-5
1s2s 1S_0	-3.31623-1	1.89505-1	-4.01002-2	3.74264-3	-1.29723-4
1s2p 1P_1	-1.11639+0	6.09708-1	-1.20523-1	1.00895-2	-2.90431-4
1s3s 3S_1	-1.66879-2	8.61416-3	-1.58238-3	1.24605-4	-3.58347-6
1s3s 1S_0	-5.67084-2	3.35671-2	-7.34784-3	7.08562-4	-2.53421-5
1s3p 3P_0	4.42035-3	-3.30288-3	8.97563-4	-1.02955-4	4.22531-6
1s3p 3P_1	8.05612-3	-6.66147-3	1.93747-3	-2.31257-4	9.70766-6
1s3p 3P_2	2.25231-2	-1.67952-2	4.55738-3	-5.22231-4	2.14181-5
1s3d 3D_1	-8.23698-3	4.64345-3	-9.46943-4	8.38753-5	-2.74378-6
1s3d 3D_2	-2.18444-2	1.25583-2	-2.64003-3	2.42410-4	-8.23008-6
1s3d 3D_3	-1.90254-2	1.07170-2	-2.18296-3	1.93064-4	-6.30414-6
1s3d 1D_2	-5.63991-2	3.32276-2	-7.23355-3	6.91053-4	-2.44324-5
1s3p 1P_1	-2.14083-1	1.20097-1	-2.44723-2	2.12954-3	-6.50267-5

**Fig. 6.** Effective collision strengths of the $1s^2\ ^1S_0 - 1s3p\ ^3P_2$ excitation for S xv as a function of temperature (in K). — present, - - - Keenan et al. (1987)

between the present result and the previous data. Figures 1 – 6 show the comparison for the excitation of the levels $1s2p\ ^3P_J$ and $1s3p\ ^3P_J$ with $J = 0, 1, 2$. For other transitions the comparison is essentially the same as shown in the previous paper (Nakazaki et al. 1993) and not repeated here. From the figures, it is found that the values of Zhang & Sampson (1987) are in good agreement with the present ones. Zhang & Sampson (1987), however, reported their result only for the excitation to $n = 2$ levels. The result of Keenan et al. (1987) agrees with that of the present calculation for all the transitions but the excitations to $1s3s\ ^1S_0$ and $1s3p\ ^3P_J (J = 0, 1, 2)$ levels. The difference in the latter transitions may be ascribed to an inadequate number of states included in the R-matrix calculation which they used for their interpolation. All the

R-matrix calculations include 11 lowest LS states, while the present calculation takes into account 19 LS states. Note that Keenan et al. (1987) reported no result for the excitation of the levels of $1s3d$ configuration.

In Fig. 3, we show a typical comparison between the present results and those of Dirac R-matrix calculation by Norrington et al. (1998). Figure 3 shows that the present result agrees very well with the fully-relativistic calculation except in the region of low temperature. Comparisons for other transitions (not shown here) have the same conclusion. This confirms the validity of the present method of the calculation of fine-structure transitions. In the region of low temperature, a small difference is seen between the two results. This may be ascribed to the difference in the resonance structure in the two sets of collision strength. Norrington et al. (1998) took account of only the states up to $n = 3$. The present calculation includes the states with $n = 4$. As for the resonance structure, therefore, the present calculation should be more accurate.

In conclusion the present paper presents the rate coefficients for excitation from the ground $1s^2\ ^1S_0$ state to all the fine-structure levels of $1s2\ell$ ($\ell = 0, 1$) and $1s3\ell$ ($\ell = 0, 1, 2$) configurations of S xv. In this sense the present calculation gives the most comprehensive data on the rate coefficients for the electron impact excitation of S xv. The result may be of significance in application, e. g. to high temperature plasma in astronomy or laboratory.

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