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Electron Impact Excitation and Ionization Rate Coefficients and Population Densities of Excited States in Lithium-like Si XII and S XIV

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Abstract

Absolute excitation and ionization rate coefficients have been evaluated for arbitrary excited states at certain electron temperatures kT_e and electron densities N_e of the Lithium-like ions Si XII and S XIV.

The populations of the chosen excited levels are calculated for the doublet state of the Li-like ions. The calculations have been carried out by using the coupled rate simultaneous equations in which the monopole and quadruple transitions have been introduced in the calculations in addition to the dipole transitions .

A theoretical population model has been developed to study the influence of the different processes that might contribute to the population of the different levels at the plasma parameters. The population densities of these different levels were then derived from these rate coefficients.

For most levels the theoretical excitation rate coefficients were found to be in good agreement with the available theoretical and experimental data.

The other calculations were found to be in fair agreement with available ones in literature.

Key words: Lithium-like ions, Rate coefficients, Population densities.

Introduction

Atomic processes are of great importance from astrophysical and controlled thermonuclear fusion research point of views. Especially the low energy recombination cross sections and rate coefficients are required for understanding fusion and astrophysical plasmas[1].

The demand for reliable rate coefficients for highly ionized multi-electron atoms by electron collisions has considerably increased during the last decade and can only be met by theory. However, cross-checking the different theoretical approaches by experimental results is still necessary.

Rate coefficients for ionization, recombination and excitation of highly charged multi-electron atoms by electron collisions are needed in many areas of physics. Now further steps towards the study of the heavier elements Silicon and Sulfur have been made[2-4].

In particular, recombination plays a significant role in astrophysics because it is the dominant electron-ion recombination process for most ions in low density, photo-ionized and electron-ionized cosmic plasmas.

A detailed knowledge of the different rate coefficients is needed in the study of high temperature plasmas[5-7], ionization balance, thermal structure and line emission of cosmic plasmas in astrophysics and in controlled thermo-nuclear fusion research. Only if these and the transition probabilities are known the radiation emitted by a non-equilibrium plasma can be quantitatively described by a theoretical population model. For electron – induced ionization, recombination, excitation and de-excitation, mainly from excited atomic states, a detailed analysis is presented for the dependence of the rate coefficients on the electron energy, the temperature and the atomic parameters.

More recently the use of heavy-ion accelerators and electron coolers of ion storage rings has greatly advanced the experiment[8]. Rate coefficients for various ions have been measured at electron energies from threshold to hundreds of electron volts (eV) [9,10].

The ion Si XII which has been studied in this work is the heaviest ion for which it has been possible to prove that a rapid recombination scheme does work to develop a VUV or soft X-ray laser.

A series of calculations of atomic data of various sulfur ions were motivated mainly by the recent observations of ultraviolet emission lines from the plasma torus for determining the composition and nature of the interstellar medium.

In the present work, the absolute electron impact excitation, ionization, recombination and de-excitation rate coefficients of about 13 configurations for the doublet state are considered for lithium-like ions Si XII and S XIV.

Oscillator strengths for allowed and forbidden transitions including relativistic effects in Breit-Pauli approximation were calculated by using the Cowan code and also by using the available results. These oscillator strengths are used in the calculations of the rate coefficients.

The level populations are calculated as functions of the electron density and the plasma temperature for the configurations $1s^2 2s$, $1s^2 2p$, $1s^2 3s$, $1s^2 3p$, $1s^2 3d$, $1s^2 4s$, $1s^2 4p$, $1s^2 4d$, $1s^2 4f$, $1s^2 5s$, $1s^2 5p$, $1s^2 5d$ and $1s^2 5f$ for each ion.

The theory is presented in section 2. Section 3 displays the results of the present calculations. Finally a conclusion is given in the last section.

Theory

Rate Coefficients

We consider the electronic $|p\rangle \rightarrow |n\rangle$ and $|p\rangle \rightarrow |i\rangle$ transitions in an atom, where p and n are the (effective) principal quantum numbers of initial and final states $|p\rangle$ and $|n\rangle$, and $|i\rangle$ denotes the ion ground state [7]. The following notation is used : E_{pi} and $E_{pn} = E_n - E_p$ are the ionization, excitation (for $E_n > E_p$) and de-excitation ($E_n < E_p$) energies, E_e and E are the incident electron and the energy transfer to the atom, respectively.

Ionization rate

The ionization rate coefficient is given by [11]:

$$K_{pi} = \frac{9.56\times10^{-6}\left(kT_e\right)^{-1.5}\exp\left(-\varepsilon_{pi}\right)}{\varepsilon_{pi}^{2.33} + 4.38\varepsilon_{pi}^{1.72} + 1.32\varepsilon_{pi}} \quad cm^3 s^{-1} \tag{1}$$

Where, ε_{pi} is the transfer energy ($\varepsilon_{pi} = E_{pi}/kT_e$) and kT_e is expressed in eV.

Recombination rate

The recombination rate coefficient is given by:

$$K_{ip} = \frac{3.17\times10^{-27}\left(kT_e\right)^{-3}\left(g_p/g_i\right)}{\varepsilon_{pi}^{2.33} + 4.38\varepsilon_{pi}^{1.72} + 1.32\varepsilon_{pi}} \quad cm^6 s^{-1} \tag{2}$$

Where g_p and g_i are the statistical weights of level $|p\rangle$ and of the ion ground state $|i\rangle$.

Excitation rate

An empirical formula which represents the numerical rate coefficients for the excitation rate with transfer energy ε_{pn} is:

$$k_{pn} = \frac{1.6\times10^{-7}\left(kT_e\right)^{0.5}\ \exp\left(-\varepsilon_{pn}\right)}{kT_e + \Gamma_{pn}} \times \left[A_{pn}\ \ln\left(\frac{0.3kT_e}{R} + \Delta_{pn}\right) + B_{pn}\right] \quad cm^3 S^{-1} \tag{3}$$

Where, kT_e is in eV , R (Rydberg energy) in eV and $\varepsilon_{pn} = E_{pn}/kT_e$.

$$\Gamma_{pn} = R\ \ln\left(1 + \frac{p^3 kT_e}{R}\right)\left[3 + 11\left(\frac{s}{p}\right)^2\right] \times \left(6 + 1.6ns + \frac{0.3}{s^2} + 0.8\frac{n^{1.5}}{s^{0.5}}\left|s - 0.6\right|\right)^{-1}$$

$$R = 13.595, \quad p = z_{eff} \times \sqrt{R/E_{pi}}, \quad n = z_{eff} \times \sqrt{R/E_{ni}}, \quad s = \left|n - p\right|$$

$$A_{pn} = \left(2R/E_{pn}\right) f_{pn} \tag{4}$$

f_{pn} being the absorption oscillator strength.

$$\Delta_{pn} = \exp\left(-\frac{B_{pn}}{A_{pn}}\right) + \frac{0.06s^2}{np^2}$$

where $B_{pn} = \frac{4R^2}{n^3}\left(\frac{1}{E_{pn}^2} + \frac{4E_{pi}}{3E_{pn}^3} + b_p \frac{E_{pi}^2}{E_{pn}^4}\right)$ and $b_p = \frac{1.4\ln p}{p} - \frac{0.7}{p} - \frac{0.51}{p^2} + \frac{1.16}{p^3} - \frac{0.55}{p^4}$

De-excitation rate

The de-excitation rate is given by:

$$k_{pn} = \frac{1.6\times10^{-7}\left(kT_e\right)^{0.5}\, g_n/g_p}{kT_e + \Gamma_{np}} \times \left[A_{np}\ \ln\left(\frac{0.3kT_e}{R} + \Delta_{np}\right) + B_{np}\right] \tag{5}$$

Where Γ_{np} and Δ_{np} are obtained from Γ_{pn} and Δ_{pn} by interchanging *p* and *n.* g_p and g_n are the statistical weights of level $|\,p\rangle$ and $|\,n\rangle$.

Population Densities

Level population can be calculated by solving the steady-state rate equations[11]

$$N_j\left[\sum_{i<j} A_{ji} + N_e\left(\sum_{i>j} C_{ji}^d + \sum_{i>j} C_{ji}^e\right)\right] = N_e\left(\sum_{i<j} N_i C_{ij}^e + \sum_{i>j} N_i C_{ij}^d\right) + \sum_{i>j} N_i A_{ij} \tag{6}$$

where N_j is the population of level j , A_{ji} is the spontaneous decay rate from level j to level i (transition probabilities), C_{ji}^e is the electron collisional excitation rate coefficient, C_{ji}^d is the collisional de-excitation rate coefficient.

The population of the j th level is obtained from the identity

$$N_j = \left(\frac{N_j}{N_I}\right)\left(\frac{N_I}{N_T}\right)\left(\frac{N_T}{N_e}\right) N_e \tag{7}$$

where N_I is total number density of all the levels of the ion under consideration , and N_T is the total number density of all ionization stages. Since the populations calculated from Equation (6) are normalized such that

$$\sum_{j=1}^{n}\left(\frac{N_j}{N_I}\right) = 1 \tag{8}$$

where n is the number of all the levels of the ion under consideration, the quantity actually obtained from Equation (6) is the fractional or reduced population N_j / N_I . We calculated the population densities and rate coefficients by using the method given by Vriens[12] and by Feldman[13-15].

Results and discussion

Excitation, Ionization and recombination rate coefficients

Energy levels and transition probabilities were calculated using the Cowan code. For the evaluation of electron impact ionization, excitation, de-excitation and recombination rates, for excited atomic states in Si XII and S XIV, the rate coefficients have been evaluated by using an empirical formula which is published by Vriens[12]. The calculations were carried out by using a computer program (CRMO code)[16]. The calculations include all forbidden and allowed transitions that are necessary for the calculations. Therefore, in addition to the dipole transitions we have introduced the monopole and quadrupole transitions in the calculations.

The rate coefficients are determined for $2s^22s$ ($^2S_{1/2}$), $2s^22p$ ($^2P_{1/2}$), $2s^23s$ ($^2S_{1/2}$), $2s^23p$($^2P_{1/2}$), $2s^23d$ ($^2D_{3/2}$), $2s^24s$ ($^2S_{1/2}$), $2s^24p$ ($^2P_{1/2}$), $2s^24d$ ($^2D_{3/2}$), $2s^24f$ ($^2F_{5/2}$-), $2s^25s$ ($^2S_{1/2}$), $2s^25p$ ($^2P_{1/2}$), $2s^25d$ ($^2D_{3/2}$) and $2s^25f$ ($^2F_{5/2}$) excited atomic states in Si XII and S XIV. The calculations were carried out at different electron temperatures (in eV).

The ionization rates for all the levels are drawn versus the electron temperature (kT_e) as shown in figures (1-2) for Si XII and S XIV ions. The curves show the usual behavior for ionization trend.

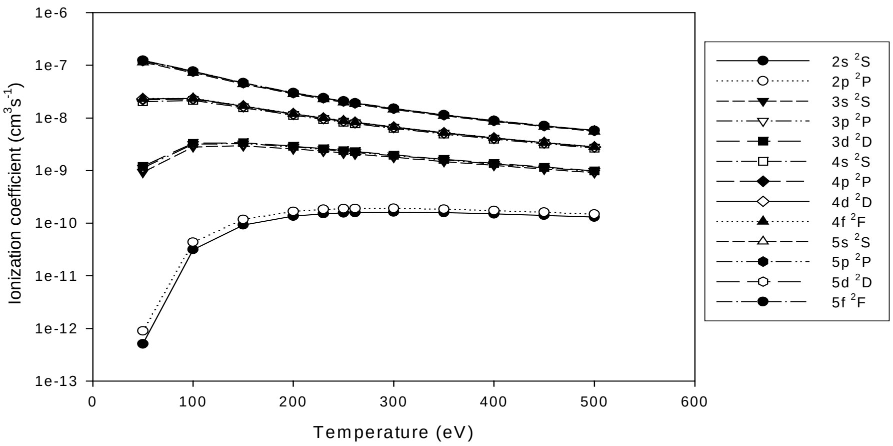


Fig. 1. Ionization rate coefficients for Si XII ion.

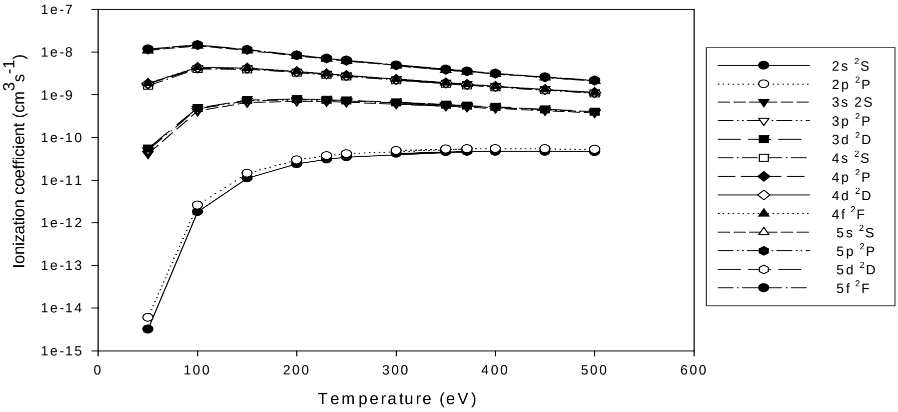
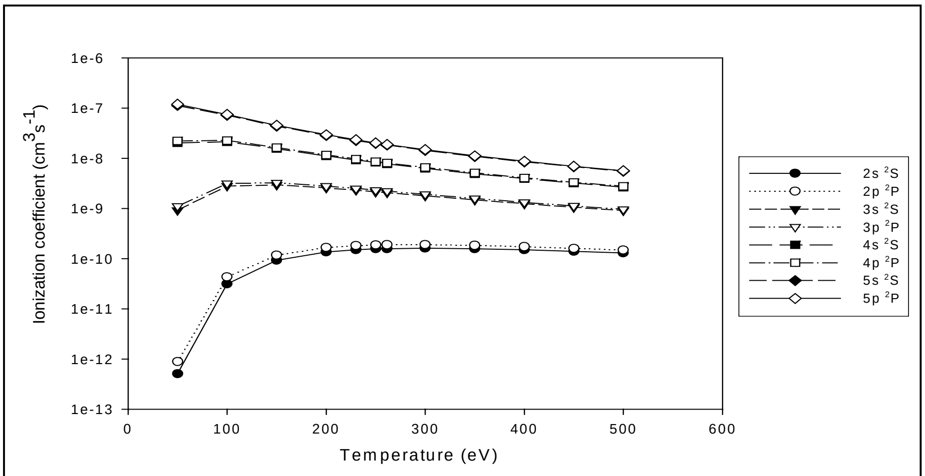


Fig. 2. Ionization rate coefficients for S XIV ion.

The ionization rates for the levels ns (^2S) and np (^2P), where n = 2-5 are drawn versus the electron temperature (kT_e) as shown in figures (3-4) for Si XII and S XIV ions.



ig. 3. Ionization rate coefficients for $1s^2ns$ ($^2S_{1/2}$) and $1s^2np(^2P_{1/2})$ transitions in Si XII ion.

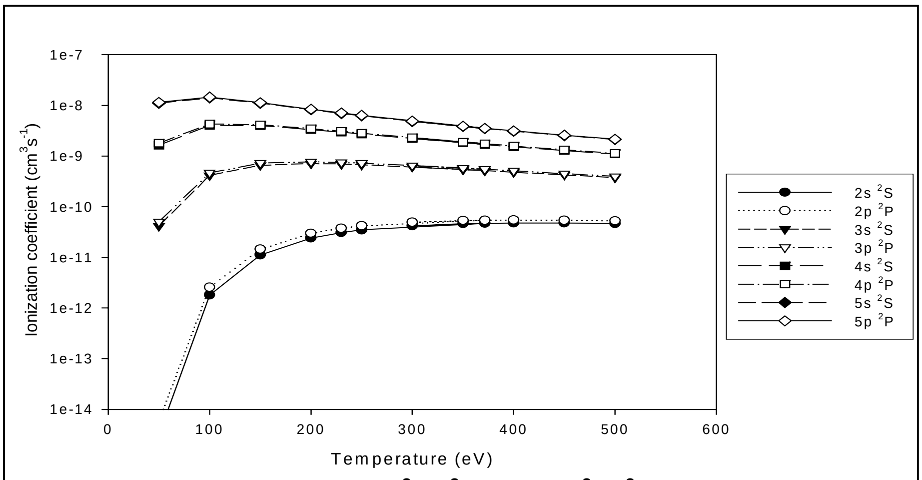


Fig. 4. Ionization rate coefficients for $1s^2ns$ ($^2S_{1/2}$) and $1s^2np(^2P_{1/2})$ transitions in S XIV ion

Figures (3-4) show that the curves are divided into groups according to the principle quantum number "n", that is as n decreases the coupling between the electrons and the nucleus getting larger. When n =2 and by increasing the temperature the behavior of the energy states shows saturations. This phenomenon might be referred to the filment of the electrons in these ionization states by increasing the temperature. When n increases, the ionization rate coefficients are decreasing by increasing the temperature because they are far from the nucleus.

The excitation rate coefficients are drawn versus the electron temperature kT_e in (in eV) as shown in figures (5-6) for some multipole transitions for Lithium-like Si XII and S XIV ions.

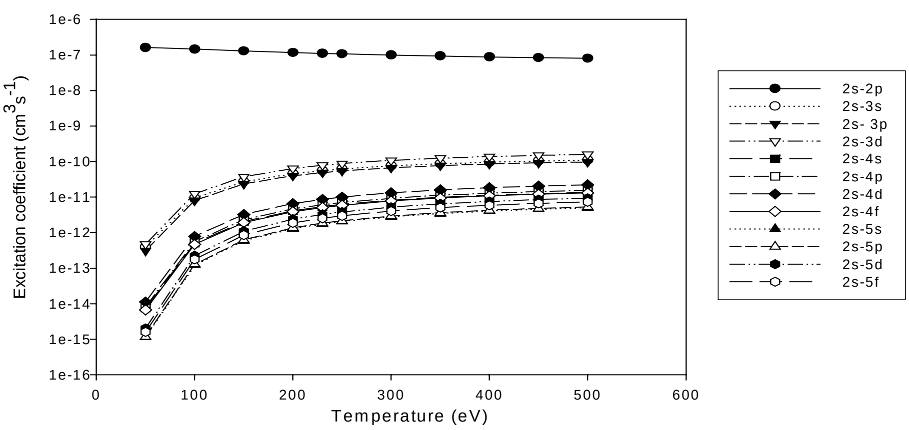


Fig. 5. Excitation rate coefficients for Si XII ion.

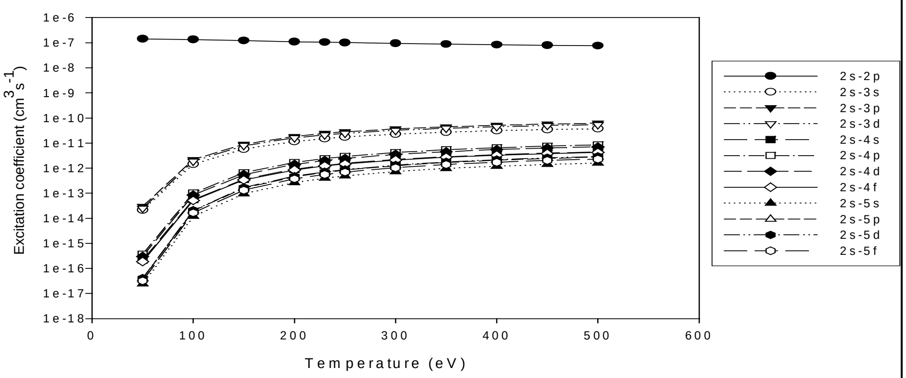


Fig. 6. Excitation rate coefficients for S XIV ion.

A detailed study of both dipole and multipole radiative and forbidden transitions showed a comparable behavior with respect to both the theoretical and experimental work as shown in figures (7-13) in case of Si XII ion for $\Delta n=2$ and 3.

For most levels the theoretical excitation rate coefficients of this work were found to be in good agreement with available theoretical and experimental data as shown in figures (8-10 and 12). The rate coefficients that were calculated by using the Coulomb-Born Oppenheimer approximation[17,19] are comparable with this work.

The other calculations[18] were found to be in fair agreement with those available in literature.

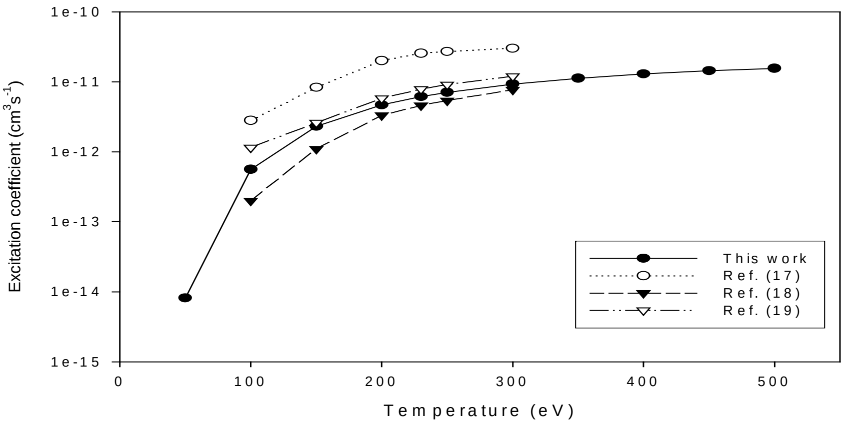


Fig. 7. Excitation rate coefficients for 2s - 4p transition for Si XII ion.

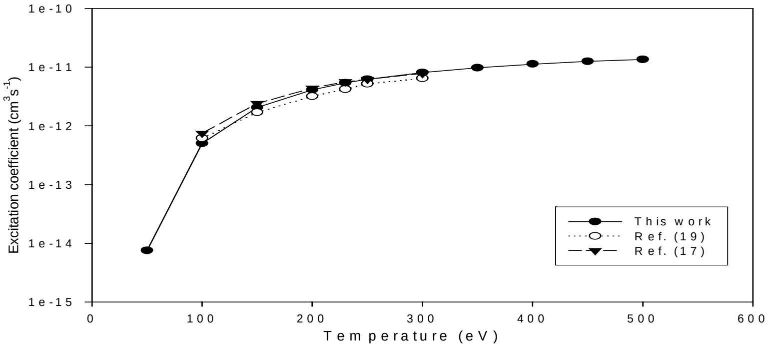


Fig. 8. Excitation rate coefficients for 2s - 4s transition for Si XII ion.

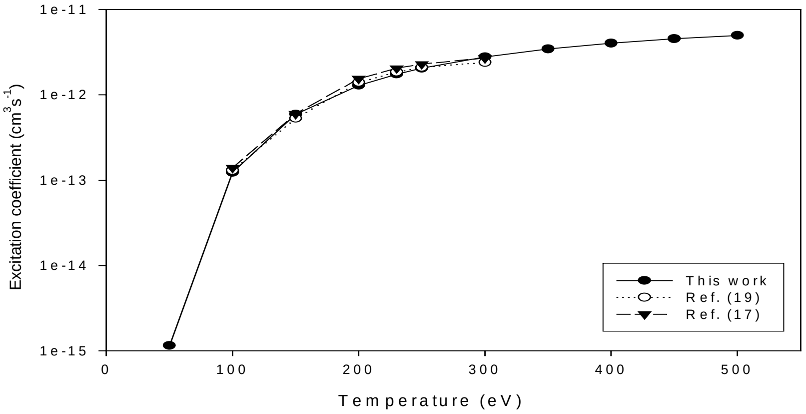


Fig. 9. Excitation rate coefficients for 2s - 5s transition for Si XII ion.

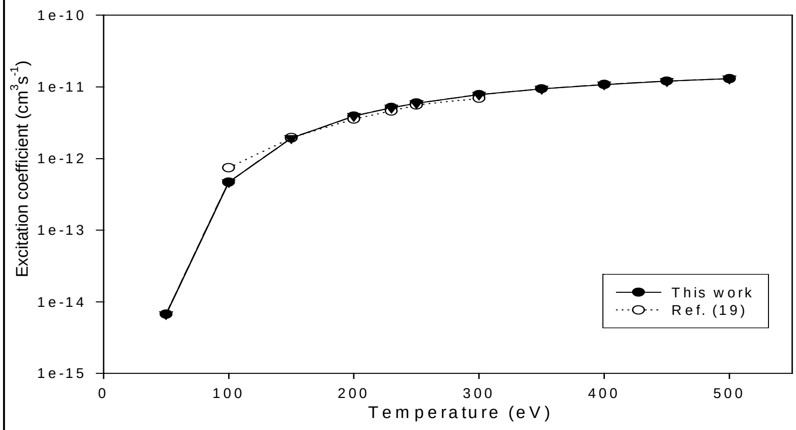
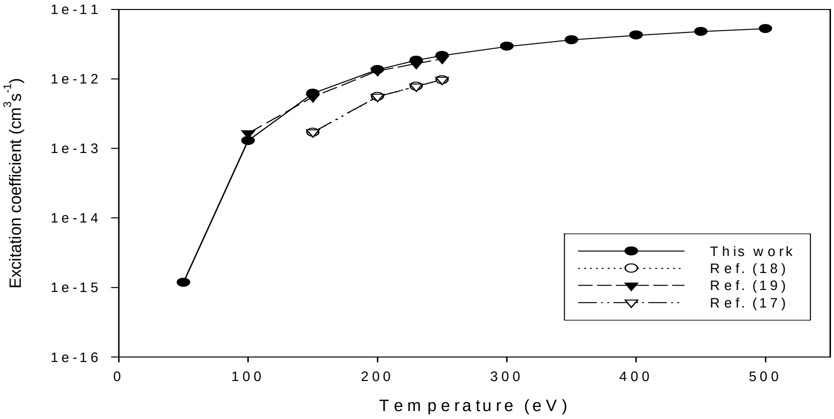


Fig. 10. Excitation rate coefficients for 2s - 4f transition for Si XII ion.



ig.11. Excitation rate coefficients for 2s - 5p transition for Si XII ion.

The Population Density of the Exited Levels

The level populations N_j are calculated by solving the 13 coupled rate equations (6) belonging to the configurations $2s^22s$ ($^2S_{1/2}$), $2s^22p$ ($^2P_{1/2}$), $2s^23s$ ($^2S_{1/2}$), $2s^23p$($^2P_{1/2}$), $2s^23d$ ($^2D_{3/2}$), $2s^24s$ ($^2S_{1/2}$), $2s^24p$ ($^2P_{1/2}$), $2s^24d$ ($^2D_{3/2}$), $2s^24f$ ($^2F_{5/2}$), $2s^25s$ ($^2S_{1/2}$), $2s^25p$ ($^2P_{1/2}$), $2s^25d$ ($^2D_{3/2}$) and $2s^25f$ ($^2F_{5/2}$) excited atomic states in Si XII and S XIV ions. Fractional populations are obtained by the aid of equations (7) and (8) using the CRMO code[16]. Calculations are performed at electron temperatures 230 eV in the case of Si XII ion[2] and 371.37 eV (1/2 the ionization potential) in case of S XIV ion[13].

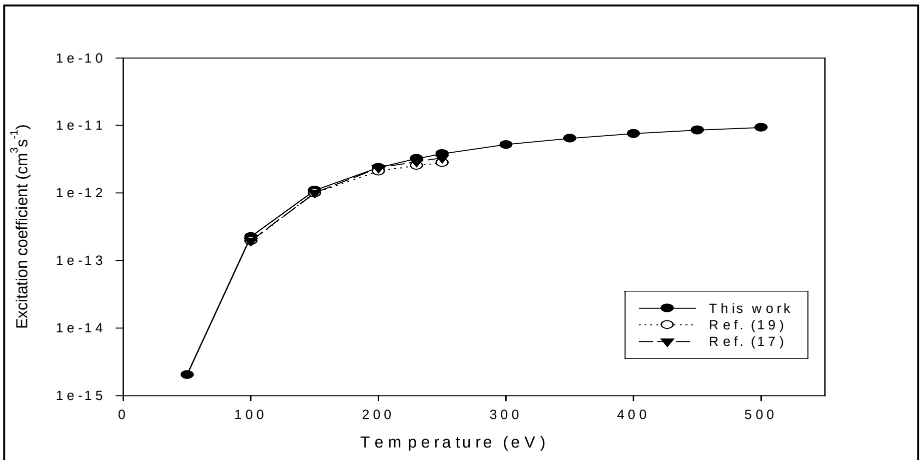


Fig.12. Excitation rate coefficients for 2s - 5d transition for Si XII ion.

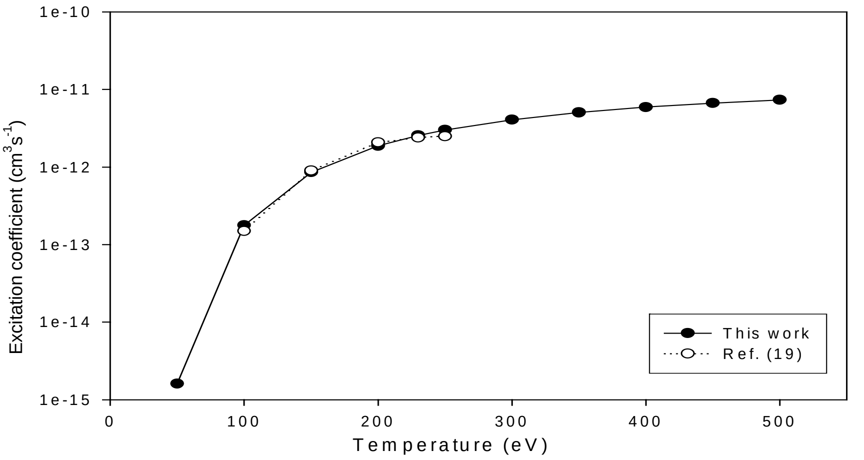


Fig.13. Excitation rate coefficients for 2s - 5d transition for Si XII io

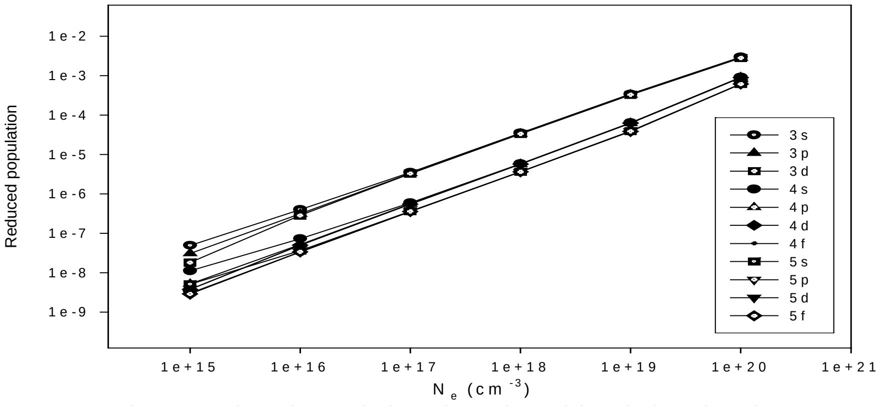


Fig.14. Reduced populations for selected levels for Si XII ion at an electron temperature 230 eV.

The calculated reduced populations (fractional level populations per unit statistical weight N_j/g_jN_i) as a function of electron densities ($N_e = 10^{15}$-10^{20} cm^{-3}) are drawn in figures (14-15) for Si XII and S XIV ions, respectively. The behavior of level populations of the Si XII and S XIV ions can be explained as follows: at low electron densities the reduced populations increase. This is due to the increase in the collisional excitation rates with density[13-15]. At high electron densities ($N_e \geq 10^{18}$-10^{20} cm^{-3}) where the collisional excitation rates exceed the radiative decay rates, the reduced populations are equal for levels with equal n.

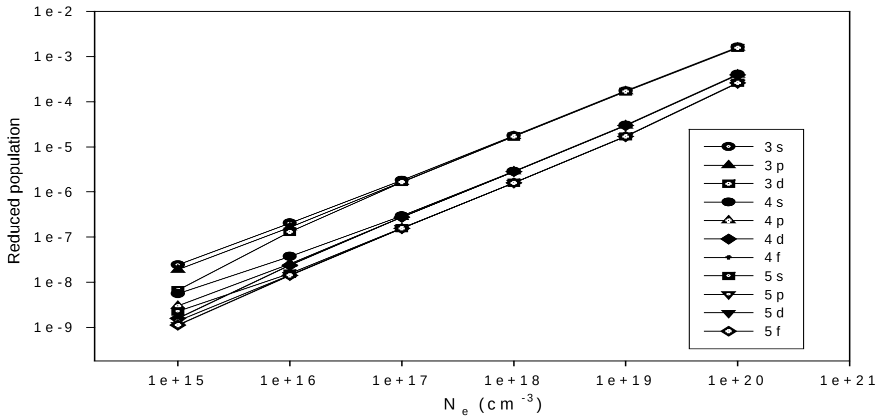


Fig.15. Reduced populations for selected levels for S XIV ion at an electron temperature 1/2 of the ionization potential.

The Conclusion

The ionization, recombination and excitation rates are calculated for 13 levels up to n = 5 in Si XII and S XIV ions. The rate coefficients were comparable with the available data.

The population density for each level is calculated and hence the reduced populations were determined.

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