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Photoionization of S^{3+} using the Breit-Pauli *R*-matrix method

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ABSTRACT

Sulphur is one of the most abundant chemical elements in the universe and a large number of lines have been observed in the spectra of astrophysical object. The S IV and SV ions considered in this work have received much interest in the last decade. The main objective of the present work is to report on photoionization cross-sections of S IV using the Breit-Pauli *R*-matrix (BPRM) method. We have carried out extensive non-relativistic and relativistic calculations of the photoionization cross sections to focus on relativistic effects. The reliability of the atomic data presented here has been carefully tested. We have exploited the BPRM code to describe the atomic wavefunctions and generate the energy levels for the SV 81 fine-structure bound target states and the corresponding *A*-values for transitions between these levels. The partial and total cross sections for the photoionization of the Al-like S^{3+} ground and excited states are determined for photon energy ranging from the S^{4+} $3s^2$ threshold up to the S^{4+} 4s threshold. We present statistically weighted, level resolved ground photoionization cross sections for the S IV ion. Both resonance positions and the oscillator strengths are presented. Extensive comparison of the present calculated values with those obtained from direct theoretical scattering calculation is also presented. To the best of our knowledge, the work reported herein describes for the first time a detailed relativistic photoionization calculation for this system, and the results are relevant to the laboratory and astrophysical plasmas.

1. Introduction

The spectral lines associated with forbidden transitions of the Mg-like ions, in astrophysical low-density plasma regions, are sensitive to the density and temperature of the surrounding serving as tool for measurements of these quantities provided that the radiative decay rates (*A*-values) are known. Sulphur is one of the most abundant chemical element in the universe and a large number of lines have been observed in spectra of the Sun as well other astrophysical objects. The emission lines of Mg-like ions have been identified in spectra of laboratory plasmas. Particularly, the photoionization studies are of great theoretical and experimental interest because of the importance of the double-excited configurations which can perturb Rydberg series leading to drastic changes in the expected spectral pattern. Such perturbations have been reported for Mg-like chloride [1].

There have been a number of studies focused on essential atomic data for sulphur ions. These include transition oscillator strengths and transition rates in Li-like sulphur ion [2], energy levels and the K-shell excited sextet states in B-like S [3], fine-structure energy levels, oscillator strengths and radiative rates for S XIII spectrum [4], relativistic energy levels, lifetimes and radiative rates for Na-like to Ar-like sulphur ions [5], oscillator strengths and transition rates in S II [6], spontaneous radiative rates for E1, E2, M1 and M2 transitions in He-like sulphur ions [7] and S III [8,9].

Electron impact collision calculations have also been reported for some of these ions: S XIII [10], S VII [11], SV [12], S I [13,14], SV [15,16].

A few works have been dedicated to photoionization studies in sulphur ions [17–20]. These studies require different models and numerical methods, increasing in difficulty in the goal of assessing the accuracy of the recommended atomic data.

The S IV and SV ions considered in this work have received much interest in the last decade. Oscillator strengths for resonance transitions in S IV have received attention both experimentally as well as theoretically. In a series of papers [21–25] very extensive calculations, using independent procedures, focused on the oscillator strengths for transitions involving the ground state levels of S IV. The effect of inclusion of core-core, core-valence and valence-valence correlation in target representation has been considered for both SV [26,27] and S IV [28]. In our recent work [26], and references herein the energy levels, oscillator strengths, radiative dacay rates, lifetimes and electron collision strengths have been obtained for 567 fine-structure levels of SV. The calculations have

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been performed within the relativistic Flexible Atomic Code (FAC) framework and the distorted wave approximation (DW). The calculation included 96 configuration state functions (CSF) in the model reaching a total of 3147 fine-structure levels. This type of model calculation allowed for valence-valence and valence –core correlation effects. The collision calculation has also been performed and line intensities of dominant transitions between all of the 567 fine structure levels have been obtained. Following the above mentioned works, the inclusion of core-core correlation has only a small effect on the oscillator strengths, particularly in the case of length form. Its inclusion makes the agreement between length and velocity forms poorer, suggesting that larger number of configurations would be needed to stabilize the velocity value. In view of this uncertainty, the present results include only valence and core-valence correlation effects.

The main objective of the present work is to report on photoionization of S IV using the Breit-Pauli *R*-matrix method. The present calculation is based on the close-coupling (CC) method [29] in which an $(N+1)$-electron system is described in terms of its *N*-electron parent ion. The method is a powerful framework for the systematic studies of atomic spectra. The partial and total cross sections for the photoionization of the Al-like S^{3+} ion for photon energy ranges from the S^{4+} $3s^2$ threshold up to the S^{4+} 4s threshold are determined in the semi-relativistic *R*-matrix approach. Some important transitions for synthetic spectral modelling are discussed in Section 2. Section 3 presents the method of calculation and results. Section 4 gives our concluding remarks.

2. Important transitions for synthetic spectral modelling

The relevant emission lines in the SV spectrum have been recorded in astrophysical plasmas in 1996 between June 25 at 21:28 U.T. and June 26 at 02:46 U.T. at 21,000 km above the West Solar Limb by SUMER Instrument on Solar and Heliospheric Observatory [30]. We have theoretically studied [26] these emission lines in density (N_E) and temperature (T_E) domain corresponding to the SV maximum abundance, and the ratio between line intensities computed within the relativistic FAC code and those recorded in 1996, in the Log $N_E[cm{-}3] = 12 - 15$ density range, and at $\mathrm{Log}T_E[\mathrm{K}] = 5.2$ temperature value, has shown good agreement for the strongest 94 lines with wavelengths between 220 and 1560 Å. Some of transitions responsible for the intense emission lines recorded in cold plasma with $10^4\,\mathrm{K} < T_E < 3\times10^5\,\mathrm{K}$, are: $3s^2(^1S^e_0)$ – $3s3p(^1P^o_1)$, $3s3p\ (^3P^o_0)$ – $3p^2(^3P^o_1,\ ^3P^o_0)$, $3s3p\ (^3P^o_0)$ – $3s3d(^3D^e_1)$, $3s3p(^1P^o_1)$ – $3s3d\ (^3D^e_2)$.

The intensity ratio of the two fine structure components in the $3s^2\ 3p\ ^2P_J$ – $3s3p\ ^2S_{1/2}$ and $^2P_{1/2}$ resonance transitions has been measured in Al-like S IV using the beam-foil technique [31] and large deviations from *LS* ratios have been found, particularly in the ^2P – ^2S case. Besides the intrinsic atomic physics interest, the observed discrepancies between theory and experiment may also be important for many users of spectroscopic data. Some astrophysical examples where the plasma parameters, such as temperature and number densities, have been determined using SIV lines are discussed in Ref. [28]. The present article focuses initially on transitions that occur between discrete levels in our system SV. We first present detailed results from the current BPRM *ab initio* calculation on energy eigenvalues for this atomic system.

3. Photoionization of S^{3+} and electron – impact excitation of S^{4+} within the *R*-matrix method

3.1. Target description and bound state transitions

The first step in a close-coupling calculation is the construction of good target wavefunctions. Errors in the target wavefunctions enter the scattering matrix in first order. The theoretical basis for the present calculation has been described in detail by Burke, Hibbert and Robb [32], Burke and Robb [33], Berrington [34], Burke [35]. The $(N+1)$-electron Hamiltonian in the Breit-Pauli R-matrix (BPRM) method is:

$$H_{BP}^{N+1} = H_{NR}^{N+1} + H_{D1}^{N+1} + H_{mass}^{N+1} + H_{SO}^{N+1} \quad (1)$$

where the only the one-electron terms resulting from the reduction of the Dirac equation to Breit-Pauli form up to order α^2Z^4, are retained, i.e. the mass-correction term, the one-electron Darwin term and the spin-orbit term; implicitly accounted for are fine-structure two-electron contributions from closed sub-shells.

An initial calculation in LS-coupling has been performed in order to get the optimum model for target states description. Three LS-coupling calculations of varying accuracy have been carried out. The initial states wave function was constructed from the N-electron target states to include the main configurations, $3s^2$, 3s3p and $3p^2$ along with all single electron promotions out the 3s, 3p and the outer shell 3d along with double promotions of the type $3s^2$-$3p^2$ and $3p^2$-$3d^2$. Other possible two-electron promotions were omitted to balance the calculation. The first two calculations included transitions between all terms with $n \le 5$ while the correlation effects have been considered by allowing for the only $3s^2 - 3p^2$ two-electron promotions in the target descriptions. The third calculation retained the all terms with $n \le 4$, while the target wave functions included the $3s^2\ -3p^2$ and $3p^2$-$3d^2$ two-electron promotions. In summary, the first calculation (*model 1*) included the following configurations: ($1s^22s^22p^6$) $3s^2$, 3s3p, $3p^2$, 3s4s, 3p3d, 3s4p, 3s4d, 3p4s, 3s4f, 3p4d, 3p4p, 3d4d, 4s5s, 3p5p, 4p5p. In order to form the (N + 1) symmetries we considered all the total angular momenta $0 \le L \le 15$, including both, even and odd, parities for doublet and quartet multiplicity. The correlation effects have been considered by allowing for the $3s^2$–$3p^2$ two-electron promotions in the target description. An energy mesh with interval of 0.001 Z^2-scaled Rydbergs was used below the highest threshold and a coarser mesh of 0.01 scaled Rydbergs in the region of all channels open up to a maximum energy of 15 Ryd. The second calculation (*model 2*), included the configurations: ($1s^22s^22p^6$) $3s^2$, 3s3p, 3s3d, 3s4s, 3s4p, 3s4f, $3p^2$, 3p3d, 3p4s, 3p4p, 3p4d, 3p5p, 3d4d, 4s5s, and 4p5p. All these states were represented by multi-configuration interaction wave functions and included also the $3s^2$ –> $3p^2$ two-electron promotion in the target wave functions. The R-matrix radius has been calculated to be $a = 15au$, and for each angular momentum 20 Schmidt-orthogonalized continuum orbitals were included to give accurate results for the incident electron energies up to 8 Ryd. A total of 92 configurations corresponding to 30 symmetries with 1100 couplings, were included in this non-relativistic calculation. In this second calculation an energy mesh with an interval of 0.001 Z^2-scaled Rydbergs was used below the highest threshold. Finally, the third calculation (*model 3*) included all the terms from the lowest 15 *N*-electron configuration coupled to all of single-particle orbitals, both spectroscopic and correlation. We restrict ourselves to transitions between states with $n \le 4$, including the more puzzling $3d^2$ allowing for the $3s^2$–$3p^2$ and $3s^2$–$3d^2$ two-electron promotions in the target wave function. The following configurations $3s^2$, 3s3p, 3s3d, 3s4s, 3s4p, 3s4d, 3s4f, 3s5s, 3s5p, $3p^2$, 3p3d, 3p4s, 3p4p, 3p4d, $3d^2$ were included in the *R*-matrix expansion. An energy mesh with intervals of 0.0001 Z^2 –scaled Rydberg has been used over the entire energy range for each angular momentum 20 Schmidt-orthogonalized continuum orbitals were included to give accurate results for incident electron energies up to **7** Ryd. A total number 81configurations corresponding to 29 symmetries with 834 couplings were included in the non-relativistic calculation. In all the models above, eight spectroscopic orthogonal one-electron 1*s*, 2*s*, 2*p*, 3*s*, 3*p*, 3*d*, 4*s*, 4*p* orbitals, and four $\overline{4d}, \overline{4f}, \overline{5s}, \overline{5p}$ pseudo-orbitals were used both in