Accurate Atomic Data for S I, S II, and S III

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1 Introduction

Prominent S I emission lines have been observed from Jupiter's satellite Io and the Io torus [1]. Absorption lines from neutral sulfur have been reported in the interstellar gas towards Oph [2]. S I emission features are also observed in the far-ultraviolet spectra of α Orionis [3] by the Goddard High Resolution Spectrograph (GHRS) on board the Hubble Space Telescope. Several S II and S III emission lines have been detected in ultraviolet (UV) spectra of the Io plasma torus in the magnetosphere of Jupiter by the Voyager ultraviolet spectrometers, the International Ultraviolet Explorer, and more recently by the high-resolution Hopkins Ultraviolet Telescope aboard Astro-1 and by the GHRS on board Hubble Space Telescope. The UV S III lines are important in temperature diagnostics of solar and stellar transition regions. Comprehensive laboratory analysis of S II [4] and S III [5] spectra are available. New S III lines from the $3p3d$ $^3F^0$, $3p4d$ $^3P^0$, $3p4p$ ^1S, ^1P, ^1D, $3p3d$ $^1P^0$, $^1D^0$, $^1F^0$, and $3p5d$ $^1P^0$ terms have been identified in the laboratory spectrum.

In order to give a correct interpretation of the observational data from the plasma, accurate values of oscillator strengths and electron excitation collision strengths of the constituent ions are needed. In recent years, we have carried out a program to calculate accurate atomic data for S I, S II, and S III. These studies are motivated not only because of the importance of atomic data in Io torus and stellar plasma modeling, but also to resolve existing discrepancies between the available calculations and between calculations and measurements. For example, our calculation resolved long-standing large discrepancies in f-values between theory and experiment for the $3p^4$ ^3P - $3p34s'$ $^3D^0$ transition in S I at 1479 Å [6], and most of the existing discrepancies between available calculations for f-values of S III were resolved [7]. Theoretical calculations of cross sections for electron impact excitation of S II [8] and S III [9] have been carried out in concert with the experimental measurements by A. Chutjian and his co-workers at the Jet Propulsion Laboratory [10]. The measurements are made using the electron energy-loss, merged-beams method. Good agreement between theory and experiment for available low-lying transitions provides us confidence in the accuracy of our calculations and the theoretical models used in these calculations.

2 Oscillator Strengths and Transition Probabilities

Oscillator strengths and transition probabilities of electric-dipole-allowed and intercombination transitions from fine-structure levels of the terms belonging to the $3s^23p^4$, $3s^23p^34s$, $3s^23p^35s$, $3s^23p^33d$, $3s^23p^34d$ configurations of S I, $3s^23p^3$, $3s3p^4$, $3s^23p^23d$, $3s^23p^24s$, and $3s^23p^24p$ configurations of S II, and $3s^23p^2$, $3s3p^3$, $3s^23p3d$, $3s^23p4s$, $3s^23p4p$, and $3s^23p4d$ configurations of S III are calculated using extensive configuration-interaction wave functions. Relativistic effects in intermediate coupling are incorporated by means of the Breit-Pauli Hamiltonian. Small adjustments to diagonal elements of the Hamiltonian matrices have been made so that the energy splittings are as close as possible to the experimental values. Our results of excitation energies, oscillator strengths, and transition probabilities are compared with other available calculations and with measurements to assess the quality of atomic data.

The atomic state wave functions are represented by the J-dependent CI expansions of the form

$$\Psi_i(JM_J) = \sum_{j=1}^{M} b_{ij} \ \phi_j(\alpha_j L_j S_j JM_J), \quad (1)$$

where each of the M single-configuration functions ϕ_j is constructed from one-electron functions, and α_j defines the coupling of angular momenta of the electrons. The sum over j includes all configurations in which the orbital L_j and spin S_j angular momenta couple to give the total angular momentum

$$J = Lj + Sj. \quad (2)$$

Each one-electron function is the product of a radial function, a spherical harmonic, and a spin function. The radial part of each orbital is expressed in analytic form as a sum of Slater-type-orbitals

$$P_{nl} = \sum_{j=1}^{k} c_{jnl} r^{I_{jnl}} exp\left(-\xi_{jnl} r\right), \quad (3)$$

where n and 1 are, respectively, the principal and orbital quantum numbers and c_{jnl}, ξ_{jnl}, and I_{jnl} are the expansion coefficients, exponents, and powers of r, respectively.

The 1s, 2*s*, 2*p*, 3*s*, and 3*p* radial functions are chosen as the Hartree-Fock functions of the $3s^23p^4\ ^3P$, $3s^23p^3\ ^4S^0$, and $3s^23p^2\ ^3P$ ground states of S I, S II, and S III, respectively, and other radial functions have been obtained with the computer code CIV3 [11]. We used flexible radial functions and included a large number of configurations in the configuration-interaction (CI) expansions to ensure convergence. The calculated energy levels are in close agreement with laboratory measurements. There is usually good agreement between the length and velocity forms of oscillator strength except for weak and a few other transitions. In cases of discrepancies between the length and velocity values, the length value is recommended because it normally remains stable with respect to the addition of more configurations.

3 Collision Strengths and Collision Rates

Electron collisional excitation strengths for inelastic transitions in S II and S III have been calculated using the R-matrix method in a 19-state ($3s^23p^3\ ^4S^0$, $^2D^0$, $^2P^0$, $3s3p^4\ ^4P$, ^2D, ^2S, $3s^23p^23d\ ^2P$, ^4F, ^4D, ^2F, ^4P, $^3s^23p^24s\ ^4P$, ^2P, $3s^23p^24p\ ^2S^0$, $^4D^0$, $^4P^0$, $^2D^0$, $^4S^0$, $^2P^0$) and a 17-state ($3s^23p^2\ ^3P$, ^1D, ^1S, $3s3p^3\ ^5S^0$, $^3D^0$, $^3P^0$, $^1P^0$, $^3S^0$, $^1D^0$, $3s^23p3d\ ^1D^0$, $^3F^0$, $^3P^0$, $^3D^0$, $^1F^0$, $^1F^0$, $^1P^0$, $3s^23p4s\ ^3P^0$, $^1P^0$) close-coupling approximations, respectively. Rydberg series of resonances converging to the excited state thresholds are explicitly included in the scattering calculations. Resonances are found to make substantial enhancements in collision strengths at low energies for several transitions. Cross sections in our 19-state calculation for S II [8] show very good agreement with the recent merged-beams energy loss experiment [10] for the forbidden $3s^23p^3\ ^4S^0$ - $3s^23p^3\ ^2D^0$, $3s^23p^3\ ^4S^0$ - $3s^23p^3\ ^2P^0$, and resonance $3s^23p^3\ ^4S^0$ - $3s3p^4\ ^4P$ transitions and also with the 18-state R-matrix calculation [12]. A similar multistate R-matrix calculation for electron impact excitation of inelastic transitions in neutral sulfur is planned.

Collision rates are obtained from the total collision strengths by integrating over a Maxwellian velocity distribution. Effective collision strengths are presented for electron temperatures from 5,000K to 100,000K, suitable for astrophysical applications, for all 136 inelastic transitions among 17-LS states of S III [9] and for all 171 inelastic transition transitions among 19-LS states of S II [8]. Our results are believed to be accurate to about 10% for transitions among low-lying excited states but may be less accurate for transitions involving higher excited states.

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