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DIELECTRONIC RECOMBINATION RATE COEFFICIENTS FOR S^{q+} ($q = 1$–5) IONS

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ABSTRACT

We have calculated the total dielectronic recombination rate coefficient for S^{q+} ($q = 1$–5) ions, in the low-density limit. We tabulate results over the temperature range $T = 3 \times 10^4$–10^6 K. At electron temperatures ($\sim 10^5$ K) and densities ($\leq 10^4$ cm^{-3}) applicable to the Io plasma torus, these results differ substantially from existing data.

Subject headings: atomic processes — planets: Jupiter — planets: satellites — transition probabilities

1. INTRODUCTION

There is much interest (Shemansky 1989) in modeling the Io oxygen-sulfur plasma torus in Jupiter's magnetosphere so as to determine its energy transport properties (Shemansky 1988). There is strong evidence (Richardson & McNutt 1987; Southwood & Kivelson 1989) to suggest that the transport is nondiffusive in nature. It has been proposed (Shemansky 1987, 1988) that dielectronic recombination (DR) is in fact the dominant mechanism for energy loss from the hot outer region of the torus. Dielectronic recombination, the process of resonant electron capture followed by radiative stabilization (Burgess 1964), is the dominant electron-ion recombination mechanism in many laboratory and astrophysical non–LTE plasmas, and it is a major energy-loss mechanism in an optically thin plasma. Given that there are a number of possible sources of error in the modeling of the energy transport (Shemansky 1989), it is important to have a complete set of DR rate coefficients, accurate to $\pm 20\%$ say. Total DR rate coefficients have been calculated already for O^{q+} ($q = 1$–5) ions $T = 10^3$–10^7 K, in the low-density limit (see Nussbaumer & Storey 1983; Badnell 1988, 1989). However, sulfur ions have received less attention. Jacobs et al. (1979) have calculated the total DR rate coefficient for all ions of sulfur with an application to a magnetic fusion plasma in mind. In particular, they imposed a cutoff on the number of states through which recombination could take place, applicable to an electron density of 10^{10} cm^{-3}. Also, nondipole autoionizing transitions were neglected, and a single-configuration approximation was used to evaluate energies and transition rates. It is to be expected, and indeed we find it to be true for S^+ and S^{2+}, that these approximations may not be valid for atoms only a few times ionized. No such restrictions apply to the calculations reported here. We make use of the AUTOSTRUCTURE computer codes (Badnell 1986; Badnell & Pindzola 1989a) which have been highly successful in describing high-resolution merged electron-ion beams DR experiments (see Badnell, Pindzola, & Griffin 1990; Pindzola, Badnell, & Griffin 1990).

In § 2, we describe briefly the theoretical methods used in the present work and their application to the calculation of DR rate coefficients for S^{q+} ($q = 1$–5) ions. In § 3, we present our results and compare them with those due to Jacobs et al. (1979) as well as with those obtained from the widely used General Formula of Burgess (1965).

2. THEORY AND APPLICATION

The total dielectronic recombination rate coefficient for a given initial state i is given by (see, e.g., Burgess 1964)

$$\alpha_d(i;\,\mathrm{tot}) = \left(\frac{4\pi a_0^2 I_\mathrm{H}}{kT}\right)^{3/2} \sum_j \frac{\omega(j)}{2\omega(i)} \times \frac{\sum_f A_r(j \rightarrow f) \sum_l A_a(j \rightarrow i,\, E_c\, l) e^{-E_c/kT}}{\sum_h A_r(j \rightarrow h) + \sum_{m,l} A_a(j \rightarrow m,\, E_c\, l)} ,$$

where E_c is the energy of the continuum electron, which is fixed by the position of the resonances, $\omega(j)$ is the statistical weight of the $(N + 1)$–electron ion doubly-excited state, $\omega(i)$ is the statistical weight of the N-electron ion initial target state, and $(4\pi a_0^2 I_\mathrm{H}/k)^{3/2} = 4.1414 \times 10^{-16}$ cm^3 K$^{3/2}$. With respect to the radiative rates A_r, the sum over f is over all states which are stable against autoionization, while the sum over h is over all possible states. For the autoionization rates A_a, the sum over m includes all energetically accessible states of the N-electron ion. First-order many-body perturbation theory is used to evaluate energies and transition rates for the many intermediate states j, in LS coupling or intermediate coupling schemes, using the AUTOSTRUCTURE package (see Badnell 1986; Badnell & Pindzola 1989a). Full configuration mixing is retained at every stage through diagonalization of the N-electron and $(N + 1)$–electron Hamiltonians.

The set of N-electron configurations retained for each ion is given in Table 1. The set was chosen so as to allow for all of the important dielectronic recombinations over $T = 3 \times 10^4$–10^6 K, and to allow for all of the important configuration-mixing insofar as the DR was concerned. By this, we mean that, if an oscillator strength is small, we do not require it to a high degree of accuracy so long as it really is small. Second, if two or more upper levels are strongly mixed, then we only require the sum of the oscillator strengths to a given accuracy, in general, since we are interested in the total recombination and not that through a given particular level. A number of continuum orbitals and a Rydberg orbital (nl) were then coupled (separately) to each of the N-electron configurations in Table 1. Each nl was treated separately in the sum over j so that, in the $(N + 1)$–electron bound-state problem, virtually all of the configuration mixing is in the N-electron core. A few extra configurations were included to allow for outer electron stabilization.

TABLE 1

N-ELECTRON CONFIGURATIONS RETAINED FOR THE DIELECTRONIC RECOMBINATION OF S^{q+} (q = 1–5)

Ion	Configurations
S^{5+}.....	$3s$, $3p$, $3d$
S^{4+}.....	$3s^2$, $3s3p$, $3s3d$, $3p^2$, $3p3d$
S^{3+}.....	$3s^23p$, $3s^23d$, $3s3p^2$, $3s3p3d$, $3p^3$, $3p^23d$
S^{2+}.....	$3s^23p^2$, $3s^23p3d$, $3s^23p4s$, $3s3p^3$, $3s3p^23d$, $3s3p3d^2$
S^{+}.....	$3s^23p^3$, $3s^23p^23d$, $3s^23p^24s$, $3s^23p^24p$, $3s^23p^24d$, $3s^23p^25s$, $3s3p^4$, $3s3p^24p$

The sum over j was taken over n = 3–1000 and $l = 0$ to l_{max}, where l_{max} = 4–10 depending on the ion, so as to converge the sum. The only high-n approximation that we made was to extrapolate the Rydberg radial wavefunctions using quantum-defect theory (see Badnell & Pindzola 1989a). The radial wavefunctions were generated by solving for them in a local model potential, itself generated by Slater-type orbitals according to the prescription of Burgess, Mason, & Tully (1989). The bound functions were optimized by minimizing a weighted-sum of eigenenergies, by varying a radial scaling parameter on the model potential. Final energy-level corrections were made using the observed values in Martin, Zalubas, & Musgrove (1990). We can compare our resulting ground to excited-state oscillator strengths with those of a much more elaborate calculation by Ojha & Hibbert (1989) for S^+, and those of a similar level of calculation by Ho & Henry (1984) for S^{2+}. In both cases, the strong oscillator strengths agree to ~10% while the weak agree to ~20%. For S^{2+}, the 10% applies to the sum of the highly mixed $3d$ and $4s$ $^3P^o$ to ^3P ground transition rates. It has long been known that a single configuration calculation can overestimate the weak oscillator strengths by an order of magnitude (see Beck & Sinanoglu 1972), and this could give rise to a spurious nonnegligible contribution to the DR.

3. RESULTS

In Table 2, we present our results for the total DR rate coefficient for S^{q+} (q = 1–5) ions over $T = 3 \times 10^4$–10^6 K, obtained in the low-density limit. The results were obtained in the LS coupling scheme, except for the case of S^{5+}, where we present our intermediate coupling results. These are a factor 1.25 larger than the LS coupling results. By analogy with our results for oxygen ions (Badnell 1989; Badnell & Pindzola 1989b), we expect the effect of intermediate coupling to be negligible (< 1%) for S^{4+}, and small (~5%) for S^+, S^{2+}, and S^{3+}. A detailed discussion of the effects of intermediate coupling versus LS coupling schemes for DR may be found in the paper by Badnell & Pindzola (1989b). The results in Table 2 can be extended to higher temperatures by $T^{-3/2}$ scaling and, except perhaps for the case of S^{5+}, they will still be total rate coefficients as the DR due to higher energy core excitations should be small (see Jacobs et al. 1979; Badnell & Pindzola 1989b). We note that the temperature of most interest to the Io plasma torus (~10^5 K) lies at, or just below, the higher-temperature peak cross section, where all Rydberg states (n = 3–1000) are accessible. At lower temperatures, the Maxwellian starts to cutoff the contribution from high-n states exponentially. We do not tabulate results below $T = 3 \times 10^4$ K as they can become increasingly unreliable due to the influence of possible very low lying autoionizing levels ($E_c \sim 0.01$ Ryd). These can give rise to a rate coefficient comparable with that of the high-temperature peak, but peaked at ~10^3 K and affecting results at $T = 10^4$ K still. This problem has been discussed in detail by Nussbaumer & Storey (1983) and by Badnell (1988), who have calculated results for a number of oxygen ions. It is not easy to do a similar calculation for sulfur ions because of the high degree of accuracy required of the small relative energies E_c. These were obtained from the observed autoionizing energy levels in the oxygen case, but similar data is sparse for sulfur ions (see Martin et al. 1990).

If we make a direct comparison of the results of Jacobs et al. (1979) with those from Table 2, at the temperature of the peak cross section, we obtain the following ratios: 1.46, 0.54, 1.00, 1.26, and 0.71 for S^{q+}, q = 1–5, respectively. However, this is a misleading comparison since Jacobs et al. (1979) imposed a cutoff on n given by the Inglis-Teller formula, using a field strength determined by the Holtzmark formula for the microfield produced by a plasma with electron density of 10^{10} cm^{-3}. If we impose a similar n cutoff, we obtain the following ratios for the results of Jacobs et al. to those from Table 2: 2.75, 0.67, 1.38, 1.90, and 1.02, again for S^{q+}, q = 1–5, respectively. We now obtain very good agreement (1.02) for the simple Na-like

TABLE 2

DIELECTRONIC RECOMBINATION RATE COEFFICIENTS FOR SULFUR IONS[a]

log T(K)	S^+	S^{2+}	S^{3+}	S^{4+}	S^{5+}
4.5.....	1.50 (−12)	9.23 (−12)	2.90 (−11)	5.11 (−11)	4.69 (−11)
4.6.....	2.94 (−12)	2.06 (−11)	4.83 (−11)	6.48 (−11)	7.18 (−11)
4.7.....	4.85 (−12)	3.83 (−11)	7.68 (−11)	8.64 (−11)	9.98 (−11)
4.8.....	6.86 (−12)	5.94 (−11)	1.10 (−10)	1.10 (−10)	1.24 (−10)
4.9.....	8.51 (−12)	7.90 (−11)	1.38 (−10)	1.30 (−10)	1.39 (−10)
5.0.....	9.45 (−12)	9.27 (−11)	1.57 (−10)	1.41 (−10)	1.43 (−10)
5.1.....	9.60 (−12)	9.82 (−11)	1.62 (−10)	1.41 (−10)	1.37 (−10)
5.2.....	9.08 (−12)	9.59 (−11)	1.56 (−10)	1.32 (−10)	1.23 (−10)
5.3.....	8.10 (−12)	8.77 (−11)	1.41 (−10)	1.17 (−10)	1.05 (−10)
5.4.....	6.89 (−12)	7.61 (−11)	1.21 (−10)	9.94 (−11)	8.68 (−11)
5.5.....	5.65 (−12)	6.33 (−11)	1.00 (−10)	8.12 (−11)	6.94 (−11)
5.6.....	4.49 (−12)	5.10 (−11)	8.01 (−11)	6.44 (−11)	5.41 (−11)
5.7.....	3.49 (−12)	4.00 (−11)	6.25 (−11)	4.99 (−11)	4.14 (−11)
5.8.....	2.66 (−12)	3.07 (−11)	4.79 (−11)	3.80 (−11)	3.11 (−11)
5.9.....	2.00 (−12)	2.32 (−11)	3.61 (−11)	2.85 (−11)	2.31 (−11)
6.0.....	1.48 (−12)	1.73 (−11)	2.68 (−11)	2.11 (−11)	1.70 (−11)

NOTE.—1.50(−12) = 1.50×10^{-12}.

[a] In units of cm^3 s^{-1}.

ion S^{5+}. The uncoupled angular momentum representation used by Jacobs et al. (1979) is known to overestimate the DR rate for a low-charge Be-like ion by a factor of 1.5 (see Badnell 1987), and the same is to be expected for the Mg-like ion S^{4+}. We now look at the effect of the nondipole autoionizing transitions into excited states, which we included in our calculations but which were neglected by Jacobs et al. (1979). If we omit them from our calculations, our results increase by $\sim 1\%$ for S^{4+} and S^{5+}, 15% for S^{3+}, and 26% for S^{2+}. Thus, it is possible to account for the differences between our results and those of Jacobs et al. (1979) down to the 25% level for S^{3+}, S^{4+}, and S^{5+}. This is all that we can expect, given the use of different atomic structures; in particular, our allowance for configuration mixing in the core. However, the results of Jacobs et al. (1979) for S^{2+} are a factor of 2 smaller than our results that have the same n cutoff and which also neglect nondipole autoionizing transitions into excited states. For the case of S^{+}, we cannot separate out the effect of dipole and nondipole autoionizations into excited states, but we expect the dipole transitions to dominate. For example, if we omit all autoionizing transitions to excited states, our results for S^{+} increase by a factor of 3.44. This is a much larger effect than for S^{2+}, even though there are 16 possible excited states that the dominant $3s^2 3p^2(^3P)3d\ ^4Pnl$ recombining terms can autoionize to, 14 of them being due to nondipole transitions in the core, compared to 10 for S^{2+} (see also Martin et al. 1990). Thus, we cannot explain the results of Jacobs et al. (1979) to better than a factor of 2 for S^{+} and S^{2+}, except in terms of the different atomic structures that were used. We recall that, in § 2, we took care to ensure that the oscillator strengths that we used, and which dominate the DR of S^{+} and S^{2+}, were consistent with the results of other workers. Thus, we believe that the results of Table 2 are the most reliable DR rate coefficients, for S^{q+} ($q = 1$–5) ions, to be used for modeling a low-density plasma in the tabulated temperature range.

We finish by comparing the results of Table 2 with those of the General Formula (GF) of Burgess (1965), obtained using the same oscillator strengths. We find that the GF overestimates the rate coefficient by a factor of 6.1, 1.22, 1.09, 1.66, and 1.31 for S^{q+}, $q = 1$–5, respectively. The large error for S^{+} is due, of course, to the dipole autoionizing transitions into excited states, which are not modeled by the GF. If we omit them, then the overestimate is reduced to a factor of 1.8. In fact, the factor of 1.66 overestimate for S^{4+} is due, in part, to the GF modeling the uncoupled angular momentum representation, as discussed above.

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