

Dielectronic recombination rate coefficients for Be-like ions: $Z = 6-42$

N R Badnell

Department of Applied Mathematics and Theoretical Physics, Silver Street, Cambridge,
CB3 9EW, UK

Received 30 September 1986

Abstract. We have calculated the total dielectronic recombination rate coefficient $\alpha_d(i; \text{tot})$ for the ground level of sixteen Be-like ions ranging from C^{2+} to Mo^{38+} . We express $\alpha_d(2^1\text{S}-2^3\text{P})$ in LS coupling allowing for configuration mixing in the initial and final states. We then use intermediate coupling core excitation energies ($w = 1$ and 3) and core radiative rates ($w = 1$) in the calculation of α_d . We also allow for the radiative stabilisation of the spectator electron. We calculate $\alpha_d(2-3)$ in multiconfiguration LS coupling and intermediate coupling using AUTOSTRUCTURE, as described in an earlier paper, allowing for $\Delta n_c = 0$ and $\Delta n_c > 0$ secondary autoionisation. We present tables of results for each core contribution to $\alpha_d(i; \text{tot})$ over a wide range of temperatures for each ion. Comparison is made with the results of other workers where possible.

1. Introduction

Dielectronic recombination is an important process governing the behaviour of plasmas not in local thermodynamic equilibrium and is thus of great interest, for example, in studies of the solar corona, laboratory plasmas and gaseous nebulae. The general formula (GF) of Burgess (1965) is widely used for high-temperature plasmas and thus it is of interest to look at effects not represented by the GF, e.g. non-dipole autoionising transitions, secondary autoionisation, radiative stabilisation of the spectator electron, configuration mixing of doubly excited states and various coupling schemes. Dielectronic recombination is also important at low temperatures, as found in gaseous nebulae, where capture takes place via core excitations of levels which lie below the first dipole excited level; this has been investigated by Nussbaumer and Storey (1983, 1984, 1986).

Recent work on the dielectronic recombination of Be-like ions includes that by Hahn and co-workers who have calculated dielectronic recombination rate coefficients for O^{4+} , Ar^{14+} , Fe^{22+} and Mo^{38+} in a single configuration LS -corrected angular momentum averaging scheme (see Hahn (1985) for a review of this work plus a general review of dielectronic recombination up to then). LaGattuta (1984) has made a detailed study of dielectronic recombination via 2-2 core transitions in C^{2+} , O^{4+} , Ar^{14+} and Fe^{22+} in LS coupling allowing for configuration mixing in the initial and final states. Jacobs *et al* (1977a, b, 1979, 1980) have calculated dielectronic recombination rate coefficients for Ne^{6+} , Mg^{8+} , Si^{10+} , S^{12+} , Ca^{16+} , Fe^{22+} and Ni^{24+} ; however, they include only dipole autoionising transitions and except for Ca^{16+} and Ni^{24+} do not allow for radiative stabilisation of the spectator electron. Also, they fail to exclude autoionisation into excited states that are energetically inaccessible. Finally, in their work on the dielectronic recombination of ions of C, N and O at low temperatures Nussbaumer and Storey (1983) have presented results for C^{2+} , N^{3+} and O^{4+} over $T = 10^3-6 \times 10^4$ K.

Recently we have developed AUTOSTRUCTURE, a general program for the calculation of multiconfiguration *LS* coupling and intermediate coupling autoionisation rates (see Badnell 1985) and have applied it to the calculation of dielectronic recombination rate coefficients α_d for 1-2 and 2-3 core transitions in Fe^{22+} and Fe^{21+} (see Badnell 1986b). In this paper we extend the calculation of $\alpha_d(2-3)$ to other members of the Be isoelectronic sequence as well as making a detailed *LS*-coupling calculation for the 2-2 core transitions. The theory and application to Be-like ions is outlined in § 2 and § 3 and our results are presented in tabular form in § 4 where we also make comparisons and discuss the results of other workers.

2. The dielectronic recombination rate coefficient

The total dielectronic recombination rate coefficient for a given initial state i is given by (see e.g. Burgess 1966)

$$\alpha_d(i; \text{tot}) = \left(\frac{4\pi a_0^2 I_H}{k_b T} \right)^{3/2} \sum_j \frac{\omega(j)}{2\omega(i)} \times \frac{\sum_k A_r(j \rightarrow k) \sum_l A_a(j \rightarrow i, E_r l) \exp(-E_r/k_b T)}{\sum_k [A_r(j \rightarrow k) + \sum_l A_a(j \rightarrow k, E_r l)]} \quad (2.1)$$

where E_r is the energy (in rydbergs) of the continuum electron, which is fixed by the position of the resonances. $\omega(j)$ is the statistical weight of the $(N+1)$ -electron doubly excited state, $\omega(i)$ is the statistical weight of the N -electron target ion and $(4\pi a_0^2 I_H/k_b)^{3/2} = 4.1414 \times 10^{-16} \text{ cm}^3$. Equation (2.1) assumes that the $(N+1)$ -electron level k is stable against autoionisation. When this is not so we replace $A_r(j \rightarrow k)$ in the numerator of (2.1) by

$$\frac{A_r(j \rightarrow k) \sum_f A_r(k \rightarrow f)}{\sum_f [A_r(k \rightarrow f) + \sum_{l'} A_a(k \rightarrow f, E_{r'} l')] } \quad (2.2)$$

and this in turn assumes that the $(N+1)$ -electron level f is stable against autoionisation.

3. Application to Be-like ions

We define n_0 to be the largest value of n ($\forall l$) for which a given core transition is stable against autoionisation. In table 1 we present the values of n_0 for each ion for each

Table 1. Values for n_0 (as defined in the text).

Ion	2 ¹ S-2 ³ P	2 ¹ S-2 ¹ P	3 ¹ S-3 ¹ P	3 ¹ S-3 ¹ D	Ion	2 ¹ S-2 ³ P	2 ¹ S-2 ¹ P	3 ¹ S-3 ¹ P	3 ¹ S-3 ¹ D
O ⁴⁺	4	3	9	5	Ti ¹⁸⁺	10	7	18	12
Ne ⁶⁺	5	4	11	7	Cr ²⁰⁺	10	8	19	13
Mg ⁸⁺	6	4	12	8	Fe ²²⁺	11	8	19	13
Si ¹⁰⁺	7	5	14	9	Ni ²⁴⁺	11	8	19	13
S ¹²⁺	8	6	15	10	Zn ²⁶⁺	11	8	19	14
Ar ¹⁴⁺	9	6	16	11	Se ³⁰⁺	11	9	19	14
Ca ¹⁶⁺	9	7	17	12	Mo ³⁸⁺	11	9	18	14

core transition considered in § 3.1 and § 3.2. These values were determined by $n_0 = \text{Integer Part}(z/\sqrt{\Delta E})$ where z is the residual charge of the target ion and ΔE is the core excitation energy. The values of n_0 for 2-2 core transitions obtained using ΔE from SUPERSTRUCTURE (see Eissner *et al* 1974) are the same as those obtained with ΔE from Edlén (1983).

3.1. 2-2 core transitions

We consider

$$1s^2 2s^2 + E_f l_f \rightleftharpoons 1s^2 2s 2p n l \begin{cases} \nearrow 1s^2 2s^2 n l + h\nu_1 \\ \searrow 1s^2 2s 2p n' l' + h\nu_2 \end{cases} \quad l' = l \pm 1, 2 \leq n' \leq n_0$$

where $2s^2 = \varepsilon_{2s} 2s^2 + \varepsilon_{2p} 2p^2$ and ε_{2s} and ε_{2p} are the mixing coefficients for the 1S term obtained from SUPERSTRUCTURE. The values of n_0 are given in table 1.

In *LS* coupling we obtain for the autoionisation rate

$$A_a = \left(\frac{8I_H}{\hbar} \right) \frac{2(2s_c + 1)}{3(2l_f + 1)} l_{>} \delta_{s,1/2} \delta_{l,l_f} \left[\left(\varepsilon_{2s} - \frac{\varepsilon_{2p}}{\sqrt{3}} \right) \delta_{s_c,0} R_1(2s, E_f l_f; 2p, n l) - \frac{3}{2} \left(\frac{\varepsilon_{2s} R_f(2s, E_f l_f; n l, 2p)}{(2l+1)} - \frac{(-1)^{s_c} \varepsilon_{2p} R_f(2p, E_f l_f; n l, 2s)}{(2l_f+1)\sqrt{3}} \right) \right]^2 \quad (3.1)$$

where $(8I_H/\hbar) = 1.653\,66 \times 10^{17} \text{ s}^{-1}$, $l_{>} = \max(l, l_f)$ and s_c is the spin of the $(2s_c+1)P$ parent. The no-mixing case was derived in detail in Badnell (1986a). We note that equation (3.1) differs by the factor $(-1)^{s_c}$ on the R_f Slater integral from equation (17) of LaGattuta (1984).

We obtain for the radiative rate for the core electron

$$A_{rc} = \left(\frac{\alpha^3}{6\tau_0} \right) \frac{2(\Delta E)^3}{3} \left(\varepsilon_{2s} - \frac{\varepsilon_{2p}}{\sqrt{3}} \right)^2 \delta_{s,1/2} \delta_{s_c,0} \left| \int_0^\infty P_{2s} r P_{2p} dr \right|^2 \quad (3.2)$$

where $(\alpha^3/6\tau_0) = 2.6775 \times 10^9 \text{ s}^{-1}$. We note the expected symmetry of the mixing coefficients in (3.2) with those in the direct term of (3.1). LaGattuta (1984, equation (16)) gives a different form for the mixing in A_{rc} , using typical values for the mixing coefficients ($\varepsilon_{2s} = 0.971$ and $\varepsilon_{2p} = 0.240$) this difference amounts to about 5% for A_{rc} .

One-electron radiative rates (A_{rs}) were used for the spectator electron when $n' > 2$. For $n' = 2$ the three-electron spin factors of Badnell (1986a) were introduced and screening by only one of the $n = 2$ electrons was assumed for the final state.

If we use the Coulomb-Bethe (cBe) approximation for A_a for the singlet parent ($s_c = 0$) we obtain

$$\frac{(2l_f+1)A_a}{A_a + A_{rc}R} = \frac{(2l_f+1)l_{>} \Delta E \left| \int_0^\infty P_{nl} r F dr \right|^2}{l_{>} \Delta E \left| \dots \right|^2 + 2.5906 \times 10^{-7} (2l_f+1)R} \quad (3.3)$$

where $R = [1 + (\sum A_{rs})/A_{rc}]$ and we note that we have converted the dipole acceleration integral to a dipole length integral. We then use the intermediate coupling results of SUPERSTRUCTURE for A_{rc} and for the core excitation energy (ΔE) in (3.3) and (2.1). Additionally, we introduce correction factors on $|\dots|^2$ which are the ratio of Coulomb-exchange distorted-wave (see Badnell 1984)† to cBe collision strengths evaluated just

† Due to a printer's error equation (3.10) of Badnell (1984) contains an incorrect sign and should read $(4l_{>}^2 - 1)$.

above threshold to correct for the overestimation by the CV_e approximation for the few lowest l_f . For all but the few lowest n , the sum over n in (2.1) was converted to an integral which was evaluated up to $n = 500$ using Simpson's rule. The dipole length integral in (3.3) was evaluated at each integration node ($\forall l$) using a subroutine due to Burgess which is based on a recast form of the recurrence relations of Burgess (1964).

For the case of the triplet parent ($s_c = 1$) equation (3.1) was evaluated in the Coulomb-Oppenheimer approximation for the few lowest n before using

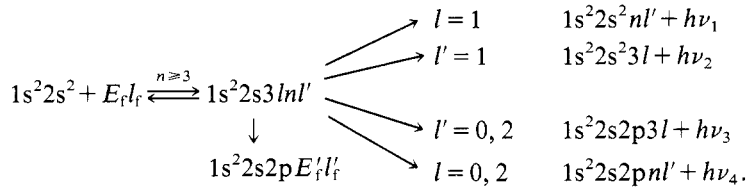
$$\int_N^\infty B(n) e^{b/n^2} dn = \frac{a_1}{2b} (e^{b/N^2} - 1) + \frac{a_2}{2b^2} [e^{b/N^2} (b/N^2 - 1) + 1] \quad (3.4)$$

where $B(n) = a_1/n^3 + a_2/n^5$ and $b = z^2/kT$, to complete the sum over n in (2.1). This was also used to complete the sum over n for the case of the singlet parent.

Since there is no core fine structure, LS coupling can be expected to be a good approximation for dielectronic recombination via the singlet parent (for which the full Rydberg series contributes). The same is not true for the triplet parent; the mixing of non-autoionising LS terms with autoionising LS terms due to core fine structure means that in intermediate coupling (or pair coupling) a factor of 4.5 more radiative channels are accessible. We return to this point again in § 4.2.

3.2. 2-3 core transitions

We consider



Using these configurations, LS coupling and intermediate coupling autoionisation transition rates were evaluated in first-order perturbation theory using *AUTOSTRUCTURE* (see Badnell 1985) which also incorporates *SUPERSTRUCTURE* (see Eissner *et al* 1974) and so calculates the radiative transition rates at the same time. Explicit calculations were carried out up to $n = 8$ (as described in detail in Badnell 1986b); any contributions from $n > 8$ were evaluated using the n^{-3} asymptotic dependence of A_a and $A_r(n \rightarrow 2)$, $A_r(3 \rightarrow 2)$ being independent of n .

The $1s^2 2s 2p n l'$ configuration is not stable against autoionisation to $1s^2 2s^2 + E_f l_f$ for $n > n_0$. In table 1 we list (i) the values of n_0 for the singlet-singlet parent transition. We also list (ii) the values of n_0 for which the $1s^2 2s 3 l n l'$ configurations ($l = 1, 2$) are subject to autoionisation to $1s^2 2s 3s + E_f l_f$ for $n > n_0$. Case (i) introduces the factor (2.2) for $n > n_0$, sample calculations that we have done show that $A_r(k \rightarrow f) \ll A_a(k \rightarrow h, E_f l_f)$ for all but the highest z (see § 4.3) and we conclude (as in Badnell 1986b) that in general it is a good approximation to truncate the sum over n for this path. Case (ii) introduces additional autoionisation rates in the denominator of (2.1). Calculations we have done and the work of Jacobs *et al* (1977) show that the new autoionising channels dominate over radiative stabilisation and again we conclude that it is a good approximation to truncate the sum over n for these paths. Of course the sum may already have been truncated by case (i). All configurations are retained in the calculation up to $n = 8$ even though they may now only contribute through mixing.

The error due to the neglect of 1- n ($n > 2$) and 2- n ($n > 3$) core transitions is negligible (see Badnell 1986b) while that due to 1-2 core transitions can be expected to amount to no more than about 15% of $\alpha_d(i; \text{tot})$ at the highest temperatures for which we tabulate results.

4. Results and discussion

In table 2 we present our results for each ion for $\alpha_d(2^1S-2^wP)$, for $w = 1$ and 3, $\alpha_d(2-3)$ and $\alpha_d(2^1S; \text{tot})$. For C^{2+} and N^{3+} we give only $\alpha_d(2^1S-2^1P)$, $\alpha_d(2-3)$ being negligible at all temperatures (see e.g. the O^{4+} results). $\alpha_d(2^1S-2^3P)$ starts to become important for $T < 10^5$ K and has been calculated in *LS* coupling by Nussbaumer and Storey (1983) for C^{2+} , N^{3+} and O^{4+} . At the lowest temperature that we tabulate we estimate $\alpha_d(2^1S-2^3P)$ to be about 15% of $\alpha_d(2^1S-2^1P)$ for these ions. Our approximate treatment of A_{rs} cannot be expected to be reliable for the few lowest z and so we only present results for $\alpha_d(2^1S-2^3P)$ from Ne^{6+} onwards.

4.1. $\alpha_d(2^1S-2^1P)$

We use $E_f = \Delta E(2^1S-2^1P) - (z/n)^2$ to evaluate the energy of the continuum electron for use in (2.1). Since the lowest energetically accessible n has E_f just greater than zero, small errors in $\Delta E(2^1S-2^1P)$ can produce large errors in E_f and this puts a lower limit on the temperature for which we can give reliable results. We thus tabulate results for $kT > \Delta E(2^1S-2^1P)/5$.

Our results for $\alpha_d(2^1S-2^1P)$ for C^{2+} lie 10% below those of Seaton and Storey (1976), who used the UCL-DW code to obtain A_a by extrapolating the excitation collision strengths, and 20% below those of LaGattuta (1984) for both C^{2+} and O^{4+} . Our results for Ar^{14+} and Fe^{22+} differ by less than 10% from those of LaGattuta (1984) at temperatures above the peak of $\alpha_d(2^1S-2^1P)$. However, LaGattuta (1984) used $n_0 = 8$ and 10 for Ar^{14+} and Fe^{22+} while we use $n_0 = 6$ and 8 respectively; consequently our results for $\alpha_d(2^1S-2^1P)$ remain larger at lower temperatures.

The importance of configuration interaction in the initial and final states was pointed out by Eissner (see Seaton and Storey 1976) and LaGattuta (1984) gives results with and without configuration interaction to illustrate this. It is not surprising then that the single configuration results in Hahn (1985) for $\alpha_d(2^1S-2^1P)$ for Fe^{22+} and Mo^{38+} are 25% and 35% larger than ours (they only give results well above the peak); the use of intermediate coupling A_{rc} is also important for Mo^{38+} .

Seaton and Storey (1976) pointed out that the Burgess G_F (1965) overestimates $\alpha_d(2^1S-2^1P)$ by 50% for C^{2+} due to its averaging over incident angular momenta. However, as z increases so does the contribution from radiative stabilisation of the spectator electron which is not allowed for by the G_F . The two errors start to cancel out and the 'overestimate' is a factor of 1.5, 1.3, 1.1 and 1.0 for C^{2+} , Mg^{8+} , Ar^{14+} and Fe^{22+} respectively. With reference to table 2 we see that the inclusion of $\alpha_d(2^1S-2^3P)$ further reduces this factor although it is temperature dependent.

The results of Jacobs *et al* (1977b, 1979, 1980) for Be-like ions overestimate $\alpha_d(2^1S-2^1P)$ by a factor of 1.5 due to their averaging over incident angular momenta; this applies even to their results for Ca^{16+} and Ni^{24+} since they allowed the spectator electron to radiate.

Table 2. Partial and total dielectronic recombination rate coefficients for Be-like ions ($\text{cm}^3 \text{s}^{-1}$).

C^{2+}				N^{3+}			
$\log T(\text{K})$		${}^1\alpha_d(2-2)$		$\log T(\text{K})$		${}^1\alpha_d(2-2)$	
4.8		2.43	-11	5.0		4.03	-11
5.0		3.02	-11	5.2		3.94	-11
5.2		2.70	-11	5.4		3.06	-11
5.4		1.95	-11	5.6		2.03	-11
5.6		1.23	-11	5.8		1.22	-11
5.8		7.16	-12	6.0		6.83	-12
6.0		3.94	-12	6.2		3.68	-12
6.2		2.09	-12	6.4		1.93	-12
6.4		1.09	-12	6.6		9.95	-13
6.6		5.58	-13	6.8		5.08	-13
6.8		2.84	-13	7.0		2.57	-13

O^{4+}				Ne^{6+}									
$\log T(\text{K})$	${}^1\alpha_d(2-2)$	$\alpha_d(2-3)$		$\log T(\text{K})$	${}^3\alpha_d(2-2)$	${}^1\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$					
5.0	3.39	-11		5.0	1.17	-11	3.14	-11	4.31	-11			
5.2	3.98	-11	3.01	-13	5.2	6.98	-12	4.52	-11	1.68	-13	5.24	-11
5.4	3.45	-11	5.81	-13	5.4	3.97	-12	4.55	-11	6.19	-13	5.01	-11
5.6	2.44	-11	7.05	-13	5.6	2.17	-12	3.57	-11	1.26	-12	3.92	-11
5.8	1.53	-11	6.26	-13	5.8	1.15	-12	2.38	-11	1.63	-12	2.66	-11
6.0	8.80	-12	4.53	-13	6.0	5.99	-13	1.43	-11	1.53	-12	1.64	-11
6.2	4.81	-12	2.86	-13	6.2	3.08	-13	8.05	-12	1.16	-12	9.51	-12
6.4	2.55	-12	1.66	-13	6.4	1.57	-13	4.34	-12	7.54	-13	5.25	-12
6.6	1.32	-12	9.16	-14	6.6	7.92	-14	2.27	-12	4.47	-13	2.80	-12
6.8	6.78	-13	4.87	-14	6.8	3.99	-14	1.17	-12	2.49	-13	1.46	-12
7.0	3.45	-13	2.54	-14	7.0	2.01	-14	5.99	-13	1.34	-13	7.53	-13
					7.2	1.01	-14	3.04	-13	6.98	-14	3.84	-13
					7.4	5.07	-15	1.53	-13	3.60	-14	1.94	-13
					7.6	2.54	-15	7.72	-14	1.83	-14	9.81	-14

Mg^{8+}				Si^{10+}									
$\log T(\text{K})$	${}^3\alpha_d(2-2)$	${}^1\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$	$\log T(\text{K})$	${}^3\alpha_d(2-2)$	${}^1\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$				
5.0	1.65	-11	5.06	-11			6.72	-11					
5.2	1.00	-11	5.47	-11			6.48	-11					
5.4	5.81	-12	5.46	-11	3.41	-13	6.08	-11					
5.6	3.23	-12	4.48	-11	1.03	-12	4.91	-11					
5.8	1.73	-12	3.11	-11	1.90	-12	3.48	-11					
6.0	9.10	-13	1.93	-11	2.38	-12	2.26	-11					
6.2	4.70	-13	1.11	-11	2.20	-12	1.37	-11					
6.4	2.40	-13	6.04	-12	1.65	-12	7.94	-12					
6.6	1.22	-13	3.20	-12	1.07	-12	4.40	-12					
6.8	6.15	-14	1.66	-12	6.36	-13	2.36	-12					
7.0	3.10	-14	8.50	-13	3.54	-13	1.24	-12					
7.2	1.56	-14	4.32	-13	1.90	-13	6.37	-13					
7.4	7.82	-15	2.18	-13	9.93	-14	3.25	-13					
7.6	3.93	-15	1.10	-13	5.11	-14	1.65	-13					

Table 2. Continued

S^{12+}					Ar^{14+}				
$\log T(K)$	${}^3\alpha_d(2-2)$	${}^1\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$	$\log T(K)$	${}^3\alpha_d(2-2)$	${}^1\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$
5.2	1.88-11	4.55-11		6.43-11	5.2	2.12-11	7.51-11		9.63-11
5.4	1.20-11	5.59-11		6.80-11	5.4	1.45-11	7.19-11		8.64-11
5.6	7.18-12	5.40-11	5.16-13	6.17-11	5.6	9.10-12	6.51-11	3.08-13	7.45-11
5.8	4.05-12	4.21-11	1.76-12	4.80-11	5.8	5.30-12	5.08-11	1.25-12	5.73-11
6.0	2.19-12	2.82-11	3.98-12	3.44-11	6.0	2.93-12	3.44-11	3.19-12	4.05-11
6.2	1.16-12	1.70-11	5.98-12	2.41-11	6.2	1.57-12	2.10-11	5.63-12	2.82-11
6.4	5.98-13	9.59-12	6.31-12	1.65-11	6.4	8.18-13	1.19-11	6.94-12	1.97-11
6.6	3.06-13	5.18-12	5.16-12	1.06-11	6.6	4.21-13	6.49-12	6.36-12	1.33-11
6.8	1.55-13	2.72-12	3.54-12	6.42-12	6.8	2.14-13	3.43-12	4.73-12	8.37-12
7.0	7.86-14	1.41-12	2.17-12	3.65-12	7.0	1.09-13	1.77-12	3.05-12	4.94-12
7.2	3.96-14	7.18-13	1.23-12	1.99-12	7.2	5.48-14	9.08-13	1.80-12	2.76-12
7.4	1.99-14	3.64-13	6.71-13	1.06-12	7.4	2.76-14	4.61-13	9.98-13	1.49-12
7.6	1.00-14	1.84-13	3.54-13	5.48-13	7.6	1.39-14	2.33-13	5.34-13	7.81-13
7.8	5.02-15	9.26-14	1.83-13	2.81-13	7.8	6.95-15	1.17-13	2.79-13	4.03-13
8.0	2.52-15	4.66-14	9.38-14	1.43-13	8.0	3.49-15	5.90-14	1.43-13	2.06-13
8.2	1.26-15	2.34-14	4.76-14	7.22-14	8.2	1.75-15	2.96-14	7.31-14	1.04-13
Ca^{16+}					Ti^{18+}				
$\log T(K)$	${}^3\alpha_d(2-2)$	${}^1\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$	$\log T(K)$	${}^3\alpha_d(2-2)$	${}^1\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$
5.2	3.66-11	5.36-11		9.02-11	5.4	2.33-11	8.58-11		1.09-10
5.4	2.36-11	6.28-11		8.65-11	5.6	1.53-11	7.83-11		9.37-11
5.6	1.44-11	6.41-11	1.62-13	7.87-11	5.8	9.25-12	6.40-11	6.61-13	7.40-11
5.8	8.33-12	5.37-11	8.87-13	6.29-11	6.0	5.26-12	4.55-11	2.19-12	5.30-11
6.0	4.60-12	3.81-11	2.61-12	4.53-11	6.2	2.86-12	2.89-11	4.92-12	3.67-11
6.2	2.45-12	2.39-11	5.44-12	3.18-11	6.4	1.51-12	1.69-11	8.10-12	2.65-11
6.4	1.28-12	1.39-11	8.00-12	2.32-11	6.6	7.85-13	9.34-12	9.59-12	1.97-11
6.6	6.60-13	7.64-12	8.48-12	1.68-11	6.8	4.02-13	4.98-12	8.59-12	1.40-11
6.8	3.36-13	4.06-12	6.98-12	1.14-11	7.0	2.04-13	2.60-12	6.30-12	9.10-12
7.0	1.70-13	2.11-12	4.82-12	7.11-12	7.2	1.03-13	1.34-12	4.03-12	5.47-12
7.2	8.59-14	1.08-12	2.97-12	4.14-12	7.4	5.21-14	6.81-13	2.36-12	3.09-12
7.4	4.33-14	5.51-13	1.70-12	2.29-12	7.6	2.62-14	3.45-13	1.31-12	1.68-12
7.6	2.17-14	2.79-13	9.24-13	1.22-12	7.8	1.32-14	1.74-13	6.97-13	8.84-13
7.8	1.09-14	1.41-13	4.88-13	6.40-13	8.0	6.60-15	8.75-14	3.63-13	4.57-13
8.0	5.48-15	7.08-14	2.53-13	3.29-13	8.2	3.31-15	4.40-14	1.87-13	2.34-13
8.2	2.75-15	3.56-14	1.29-13	1.68-13	8.4	1.66-15	2.21-14	9.51-14	1.19-13
Cr^{20+}					Fe^{22+}				
$\log T(K)$	${}^3\alpha_d(2-2)$	${}^1\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$	$\log T(K)$	${}^3\alpha_d(2-2)$	${}^1\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$
5.4	3.25-11	6.36-11		9.61-11	5.4	2.69-11	8.30-11		1.10-10
5.6	2.10-11	6.94-11		9.04-11	5.6	1.93-11	8.23-11		1.02-10
5.8	1.26-11	6.29-11	4.01-13	7.59-11	5.8	1.24-11	7.29-11	2.40-13	8.55-11
6.0	7.19-12	4.76-11	1.64-12	5.64-11	6.0	7.38-12	5.54-11	1.30-12	6.41-11
6.2	3.92-12	3.13-11	3.93-12	3.92-11	6.2	4.13-12	3.69-11	3.54-12	4.46-11
6.4	2.08-12	1.87-11	7.04-12	2.79-11	6.4	2.23-12	2.23-11	6.83-12	3.14-11
6.6	1.08-12	1.05-11	9.34-12	2.09-11	6.6	1.17-12	1.26-11	9.77-12	2.36-11
6.8	5.54-13	5.67-12	9.24-12	1.55-11	6.8	6.04-13	6.83-12	1.04-11	1.78-11
7.0	2.82-13	2.98-12	7.28-12	1.05-11	7.0	3.08-13	3.60-12	8.62-12	1.25-11
7.2	1.42-13	1.54-12	4.90-12	6.57-12	7.2	1.56-13	1.86-12	6.02-12	8.04-12
7.4	7.18-14	7.84-13	2.96-12	3.82-12	7.4	7.90-14	9.51-13	3.73-12	4.76-12
7.6	3.61-14	3.98-13	1.67-12	2.11-12	7.6	3.98-14	4.83-13	2.15-12	2.67-12
7.8	1.81-14	2.01-13	9.06-13	1.12-12	7.8	2.00-14	2.44-13	1.17-12	1.44-12
8.0	9.11-15	1.01-13	4.76-13	5.86-13	8.0	1.00-14	1.23-13	6.21-13	7.54-13
8.2	4.57-15	5.08-14	2.46-13	3.01-13	8.2	5.04-15	6.17-14	3.22-13	3.89-13
8.4	2.29-15	2.55-14	1.26-13	1.54-13	8.4	2.53-15	3.10-14	1.65-13	1.99-13

Table 2. Continued.

Ni ²⁴⁺					Zn ²⁶⁺				
log T(K)	³ $\alpha_d(2-2)$	¹ $\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$	log T(K)	³ $\alpha_d(2-2)$	¹ $\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$
5.6	2.34-11	9.95-11		1.23-10	5.6	2.73-11	1.22-10		1.49-10
5.8	1.52-11	8.45-11		9.98-11	5.8	1.78-11	9.81-11		1.16-10
6.0	9.10-12	6.41-11	9.35-13	7.41-11	6.0	1.08-11	7.36-11	6.14-13	8.50-11
6.2	5.14-12	4.30-11	2.83-12	5.10-11	6.2	6.16-12	4.97-11	2.25-12	5.82-11
6.4	2.79-12	2.62-11	5.60-12	3.46-11	6.4	3.36-12	3.06-11	4.80-12	3.88-11
6.6	1.47-12	1.49-11	8.49-12	2.49-11	6.6	1.78-12	1.76-11	7.70-12	2.71-11
6.8	7.60-13	8.13-12	9.74-12	1.86-11	6.8	9.24-13	9.61-12	9.46-12	2.00-11
7.0	3.89-13	4.30-12	8.66-12	1.34-11	7.0	4.74-13	5.10-12	8.96-12	1.45-11
7.2	1.97-13	2.23-12	6.35-12	8.78-12	7.2	2.41-13	2.65-12	6.88-12	9.77-12
7.4	9.98-14	1.14-12	4.08-12	5.32-12	7.4	1.22-13	1.36-12	4.56-12	6.04-12
7.6	5.03-14	5.79-13	2.39-12	3.02-12	7.6	6.14-14	6.91-13	2.73-12	3.48-12
7.8	2.53-14	2.93-13	1.33-12	1.64-12	7.8	3.09-14	3.49-13	1.54-12	1.92-12
8.0	1.27-14	1.48-13	7.09-13	8.69-13	8.0	1.55-14	1.76-13	8.28-13	1.02-12
8.2	6.37-15	7.42-14	3.70-13	4.51-13	8.2	7.79-15	8.86-14	4.34-13	5.31-13
8.4	3.20-15	3.73-14	1.90-13	2.31-13	8.4	3.91-15	4.45-14	2.24-13	2.73-13
8.6	1.60-15	1.87-14	9.69-14	1.17-13	8.6	1.96-15	2.23-14	1.14-13	1.39-13

Se ³⁰⁺					Mo ³⁸⁺				
log T(K)	³ $\alpha_d(2-2)$	¹ $\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$	log T(K)	³ $\alpha_d(2-2)$	¹ $\alpha_d(2-2)$	$\alpha_d(2-3)$	$\alpha_d(\text{tot})$
5.6	3.33-11	8.14-11		1.15-10	5.8	2.36-11	8.34-11		1.07-10
5.8	2.22-11	8.24-11		1.05-10	6.0	1.62-11	8.39-11		1.00-10
6.0	1.38-11	7.19-11	2.70-13	8.60-11	6.2	1.03-11	7.21-11	4.48-13	8.29-11
6.2	8.07-12	5.36-11	1.48-12	6.32-11	6.4	6.08-12	5.31-11	2.01-12	6.12-11
6.4	4.48-12	3.52-11	3.73-12	4.34-11	6.6	3.40-12	3.45-11	4.37-12	4.23-11
6.6	2.40-12	2.11-11	6.38-12	2.99-11	6.8	1.83-12	2.05-11	6.63-12	2.90-11
6.8	1.26-12	1.18-11	8.64-12	2.17-11	7.0	9.62-13	1.15-11	8.16-12	2.06-11
7.0	6.47-13	6.39-12	9.16-12	1.62-11	7.2	4.97-13	6.19-12	8.16-12	1.48-11
7.2	3.30-13	3.36-12	7.76-12	1.14-11	7.4	2.54-13	3.24-12	6.68-12	1.02-11
7.4	1.67-13	1.73-12	5.51-12	7.41-12	7.6	1.29-13	1.67-12	4.66-12	6.47-12
7.6	8.45-14	8.85-13	3.47-12	4.44-12	7.8	6.50-14	8.54-13	2.90-12	3.82-12
7.8	4.25-14	4.49-13	2.01-12	2.50-12	8.0	3.27-14	4.33-13	1.67-12	2.14-12
8.0	2.14-14	2.27-13	1.11-12	1.36-12	8.2	1.65-14	2.19-13	9.18-13	1.15-12
8.2	1.07-14	1.14-13	5.89-13	7.14-13	8.4	8.26-15	1.10-13	4.87-13	6.05-13
8.4	5.38-15	5.74-14	3.06-13	3.69-13	8.6	4.15-15	5.53-14	2.53-13	3.13-13
8.6	2.70-15	2.88-14	1.57-13	1.89-13	8.8	2.08-15	2.78-14	1.30-13	1.60-13

We end this section by noting that at $T=10^7$ K our results for $\alpha_d(2-2)$ for Fe^{22+} differ by less than 5% from the GF value we used in our previous paper (Badnell 1986b).

4.2. $\alpha_d(2^1S-2^3P)$

At sufficiently low temperatures $\alpha_d(2^1S-2^3P)$ dominates the total dielectronic recombination rate coefficient. However, the total recombination rate for high- z ions is dominated by radiative recombination at temperatures below the peak of $\alpha_d(2^1S-2^1P)$

and so is insensitive to errors in $\alpha_d(2^1S-2^3P)$. The same is not true for ions only a few times ionised; here radiative recombination only begins to become important at temperatures below the peak of $\alpha_d(2^1S-2^3P)$.

The main source of error in using *LS* coupling for $\alpha_d(2^1S-2^3P)$ is the neglect of core fine structure. LaGattuta (1984) calculated $\alpha_d(2^1S-2^3P)$ in *LS* coupling but used pair-coupling statistical weights whenever the core fine-structure splitting was greater than the term splitting. However, this is not necessarily the relevant quantity since one also needs to consider the ratio A_a/A_{rs} . For example, $A_a/A_{rs} \sim 10^4$ for O^{3+} and $\alpha_d(2^1S-2^3P)$ is sensitive to even small deviations from *LS* coupling since this can produce strong new autoionising channels. Correspondingly, even though *LS* coupling can be regarded as a poor description for Fe^{21+} , since the core fine-structure splitting is greater than the term splitting, $\alpha_d(2^1S-2^3P)$ is relatively insensitive to new autoionising channels because $A_a \sim A_{rs}$. We can illustrate this by calculating $\alpha_d(2^1S-2^3P)$ using *LS*-averaged autoionisation rates; this allows access to all radiative channels. When $A_a \ll A_{rs}$ *LS*-averaged coupling, *LS* coupling and intermediate coupling should give similar results for $\alpha_d(2^1S-2^3P)$. If $A_{rs} \ll A_a$ (\forall levels in intermediate coupling) then the *LS*-averaged and intermediate coupling results would be about 4.5 times the *LS*-coupling results.

For the ratio ${}^{(LS)}\alpha_d(2^1S-2^3P)/{}^{LS}\alpha_d(2^1S-2^3P)$ we obtain 4.5, 3.6, 2.5 and 1.4 for O^{4+} , Ar^{14+} , Fe^{22+} and Mo^{38+} targets respectively. In practice, preliminary intermediate coupling calculations with *AUTOSTRUCTURE* for $O^{4+}+e^-$ show $A_a \sim A_{rs}$ for *LS*-forbidden A_a , thus the increase is less than the factor of 4.5 indicated by *LS* averaging.

4.3. $\alpha_d(2-3)$

Our results for $\alpha_d(2-3)$ were calculated as described in § 3.2 except for Mo^{38+} . Due to the z^4 dependence of A_{rs} , $(A_{rc} + A_{rs}) > A_a(2-2)$ for Mo^{38+} and so we kept the factor (2.2) set equal to unity until the $3^1D \rightarrow 3^1S$ autoionising channel became open. This only resulted in a 5% increase in $\alpha_d(2-3)$ and if we were to have kept the factor (2.2) equal to unity $\forall n$ it would have resulted in a further increase of only 5%. This is due of course to the fact that $(A_{rc} + A_{rs}) > A_a(2-3)$ as well and hence dielectronic recombination is dominated by capture to the few lowest n and soon falls off like n^{-3} .

We carried out sample calculations for O^{4+} , Si^{10+} and Fe^{22+} and found that the effect of intermediate coupling was less than 10% as was that of including the configurations $1s^2 2p^2 E_i l_f$ and $1s^2 2p 3l n l'$ which contribute only through mixing. For $E_f(3)/kT \approx 4$ the uncertainty in position of the lowest-lying resonances puts a lower limit on the temperature for which we can give reliable results; however, $\alpha_d(2-3)$ contributes less than 1% to $\alpha_d(i; \text{tot})$ by then.

As we discussed previously (Badnell 1986b) Jacobs *et al* (1977a, b, 1979, 1980) do not allow for the $2s \rightleftharpoons 3d \rightarrow 2p$ process which contributes up to two thirds of $\alpha_d(2-3)$ and so we do not consider their results for $\alpha_d(2-3)$ any further. The results given by Hahn (1985) for Fe^{22+} and Mo^{38+} at temperatures above the peak of $\alpha_d(2-3)$ are 20% and 15% respectively larger than our results. However, as z decreases the effect of our cut-off due to $\Delta n_c = 0$ secondary autoionisation becomes increasingly important. Hahn's (1985) results for $\alpha_d(2-3)$ are a factor of two greater than ours for Ar^{14+} and a factor of three for O^{4+} . The affect on $\alpha_d(i; \text{tot})$ is small for O^{4+} since it is dominated by $\alpha_d(2-2)$ at all temperatures but for Ar^{14+} it means that Hahn's (1985) results for $\alpha_d(i; \text{tot})$ are a factor of 1.5 larger than ours at $T = 3 \times 10^6$ K and a factor of two at $T = 2 \times 10^7$ K.

5. Conclusions

(i) It is important to take account of both $\Delta n_c = 0$ and $\Delta n_c > 0$ secondary autoionising transitions in the calculation of dielectronic recombination rate coefficients for $\Delta n_c > 0$ core transitions.

(ii) Radiative stabilisation of the spectator electron can contribute significantly to dielectronic recombination via $\Delta n_c = 0$ core transitions.

(iii) The effects of core fine structure on dielectronic recombination at low temperatures should be the subject of further investigation.

Acknowledgments

This work has benefited from conversations with Dr Alan Burgess and was supported by the SERC.

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