J. Phys. B: At. Mol. Opt. Phys. **23** (1990) L565-L569. Printed in the UK

LETTER TO THE EDITOR

On the dielectronic recombination of Li-like Al

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Received 23 July 1990

Abstract. We have calculated dielectronic recombination rate coefficients for Al^{10+} using the AUTOSTRUCTURE code. Our high-temperature zero-density results are in good agreement (30%) with those obtained from the general formula of Burgess and are a factor of 3.6 larger than the recent R-matrix results of Terao and Burke. There are two reasons for this discrepancy. Firstly, we obtain a non-negligible contribution from high angular momentum ($l > 6$) states, 40% of our total, unlike Terao and Burke. Secondly, our allowance for outer electron stabilization, which was neglected by Terao and Burke, increases our results by a factor of 1.65. The discrepancy increases to a factor of 10, or more, when dielectronic recombination is dominated by low-lying states as found in a high-density or low-temperature plasma.

The demonstration of soft x-ray amplification in a laser-produced recombining aluminium plasma by Carillon *et al* (1990) has stimulated interest in the governing atomic processes. Recently, Terao and Burke (1990) calculated dielectronic recombination (DR) rate coefficients for Al^{10+}. They obtained autoionization rates by fitting K matrices calculated using the R-matrix method (see Burke and Robb 1975), while the radiative rates and DR rate coefficients were calculated using perturbation theory. Terao and Burke (1990) obtained the surprising result that their high-temperature zero-density DR rate coefficients were about a factor of three smaller than those due to the general formula (GF) of Burgess (1965). We will show that this is due to an apparent error and an omission in the calculations carried out by Terao and Burke (1990) and that their results underestimate the DR rate coefficient by a factor of ten, or more, for a high-density or low-temperature plasma.

The main dielectronic capture and autoionization transition is

$$1s^2 2s + kl_c \rightleftarrows 1s^2 2p nl \qquad l_c = l \pm 1$$

which becomes energetically possible at $n = 8$. Depopulation is also possible via

$$1s^2 2p_{3/2} nl \rightarrow 1s^2 2p_{1/2} + kl$$

for $n > 43$, but this only has a small effect ($\sim 2\%$) on the total DR rate coefficient. The only radiative stabilization transition considered by Terao and Burke (1990) was

$$1s^2 2p nl \rightarrow 1s^2 2s nl + h\nu.$$

However,

$$1s^2 2p nl \rightarrow 1s^2 2p n'l' + h\nu$$

also contributes to the recombination for all $n' < 8$ and $l' < n'$ and we will show that this contribution is non-negligible. We will also evaluate the contribution from 2-3 core excitations which can be important at high temperatures ($T \sim 10^6$ K).

0953-4075/90/180565+05$03.50

We use first-order many-body perturbation theory to evaluate both the radiative and autoionization transition rates in *LS* coupling and intermediate coupling schemes. The calculations are carried out using the AUTOSTRUCTURE package (Badnell 1986, Badnell and Pindzola 1989), which is an extensive development of the SUPERSTRUCTURE atomic structure code of Eissner *et al* (1974), and which makes use of quantum defect theory to solve the high-n problem.

In table 1 we compare the l dependence of our 2-2 DR rate coefficients with those due to Terao and Burke (1990), both sets of calculations use *LS* coupling and neglect outer electron stabilization. We see that there is good agreement for $l = 0$-5 but that the results of Terao and Burke (1990) fall off rapidly thereafter while we obtain 40% of our total result from $l > 6$. We may examine this discrepancy more closely by comparing threshold 2s-2p partial collision strengths Ω and these are given in table 2 for the spin-triplet only, the spin-singlet results follow the same pattern. In addition to our distorted-wave results obtained from AUTOSTRUCTURE, we have also carried out a two-state R-matrix calculation (see Berrington *et al* 1987) using the same 1s, 2s, 2p Thomas-Fermi-Dirac-Amaldi (TFDA) radial functions and the results are also shown in table 2. The differences at low L, which are small in general, may be attributed to coupling effects and these decrease rapidly as L increases. The R-matrix results of Terao and Burke (1990) are also shown in table 2 for $L \leqslant 7$, contributions from $L \geqslant 7$ were found to be negligible. They were obtained from quantum defect theory and the

Table 1. Partial *LS*-coupling dielectronic recombination rate coefficients, neglecting outer electron stabilization, at $T = 1$ Ryd and in units of $cm^3\ s^{-1}$.

l	AUTOSTRUCTURE[a]	R-matrix[b]	l	AUTOSTRUCTURE[a]	R-matrix[b]
0	7.20 (−13)	7.25 (−13)	8	3.31 (−12)	1.35 (−13)
1	1.16 (−12)	1.12 (−12)	9	2.52 (−12)	—
2	2.35 (−12)	2.37 (−12)	10	1.81 (−12)	—
3	3.17 (−12)	3.55 (−12)	11	1.18 (−12)	—
4	4.01 (−12)	4.24 (−12)	12	5.85 (−13)	—
5	4.36 (−12)	4.38 (−12)	13	1.81 (−13)	—
6	4.33 (−12)	1.71 (−12)	14	4.07 (−14)	—
7	4.00 (−12)	5.69 (−13)	15	8.40 (−15)	—

[a] This work.
[b] Terao and Burke (1990).

Table 2. Threshold partial collision strengths $\Omega(2s\text{-}2p: {}^3L)$.

L	AUTOSTRUCTURE[a]	R-matrix[a]	R-matrix[b]	L	AUTOSTRUCTURE[a]	R-matrix[a]
0	6.69 (−2)	6.41 (−2)	6.69 (−2)	8	1.15 (−1)	1.15 (−1)
1	8.68 (−2)	8.19 (−2)	8.78 (−2)	9	6.32 (−2)	6.32 (−2)
2	1.25 (−2)	1.52 (−2)	1.81 (−2)	10	2.98 (−2)	3.00 (−2)
3	3.66 (−2)	2.38 (−2)	2.44 (−2)	11	1.23 (−2)	1.22 (−2)
4	2.11 (−1)	2.01 (−1)	2.18 (−1)	12	4.41 (−3)	4.44 (−3)
5	2.69 (−1)	2.63 (−1)	3.22 (−1)	13	1.40 (−3)	1.41 (−3)
6	2.41 (−1)	2.38 (−1)	2.69 (−1)	14	3.91 (−4)	3.99 (−4)
7	1.81 (−1)	1.80 (−1)	1.83 (−4)	15	9.75 (−5)	1.00 (−4)

[a] This work.
[b] Terao and Burke (1990).

resonance fitting program of Bartschat and Burke (1986) and we converted them to Ω using

$$\Omega_{LS}(\text{threshold}) = \pi(2S+1)(2L+1)\gamma_{LS}/2z^2$$

where $z = 10$ is the residual charge of the ion and the γ_{LS} were taken from table 2 of Terao and Burke (1990). Since we find that our results obtained using the *R*-matrix code agree with those from AUTOSTRUCTURE for high partial-wave collision strengths, it would appear that the problem with the results of Terao and Burke (1990) lies in the fitting of the resonances for high L. The differences between the two sets of *R*-matrix results due to the choice of bound orbitals, TFDA versus CIV3, should be no larger for high L than for low L. We note that the agreement between theory and experiment for the DR of light Li-like ions and metastable He-like ions (see Griffin *et al* 1989, Badnell *et al* 1990) confirms that the high angular momentum ($L > 6$) states are important.

In figure 1 we present our intermediate coupling DR results for 2-2 core excitations, both with and without outer electron stabilization, and compare them with the results

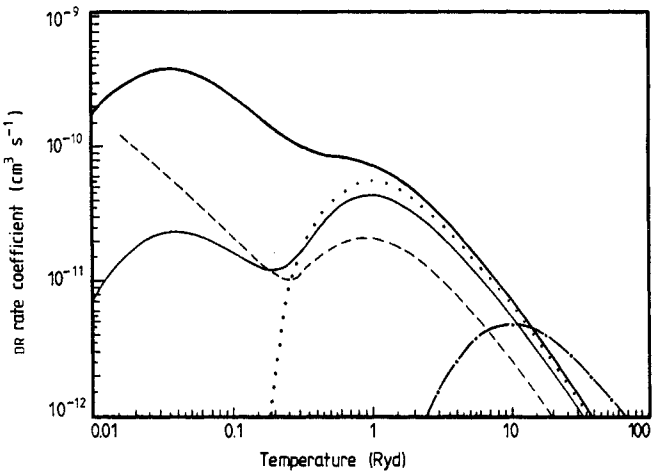

Figure 1. Dielectronic recombination rate coefficients for Al^{10+}...., Burgess GF (1965); ——, intermediate coupling both with and without outer electron stabilization, this work; — — —, intermediate coupling, Terao and Burke (1990), all 2-2 core excitations; —·—, 2-3 core excitations, *LS* coupling, this work.

of the Burgess GF (1965) and the intermediate coupling results of Terao and Burke (1990). At $T = 1$ Ryd, our results that allow for outer electron stabilization are a factor of 1.65 larger than our results that neglect it. The results of the Burgess GF (1965) now only differ by ±30% from our results, while the results of Terao and Burke (1990) are a factor of 3.6 smaller than our maximum results. We note that is not possible to z scale our O^{5+} results (Badnell and Pindzola 1989) to Al^{10+}. As a further check on these calculations we computed DR cross sections for Li-like Fe and they agree at the 1% level with the results of Griffin and Pindzola (1987) who used a completely independent set of programs based on Cowan's structure code. Also, we see that dielectronic recombination via 2-3 core excitations becomes dominant above $T = 10$ Ryd.

The low temperature peak of the results of Terao and Burke (1990) is at a lower temperature than ours. This position is determined by the position of the $2p_{1/2,3/2}8l$ resonances of Al^{9+} relative to the $2s_{1/2}$ level of Al^{10+} and thus ultimately by the $2s_{1/2}$-$2p_{1/2,3/2}$ splittings in Al^{10+}. Terao and Burke (1990) obtain $E(2p_{1/2}-2s_{1/2}) = 171\,966\ cm^{-1}$ and $E(2p_{3/2}-2s_{1/2}) = 177\,135\ cm^{-1}$ which are somewhat smaller than the observed values from Kelly (1982) of $E(2p_{1/2}-2s_{1/2}) = 176\,010\ cm^{-1}$ and $E(2p_{3/2}-2s_{1/2}) = 181\,180\ cm^{-1}$ while we obtain $E(2p_{1/2}-2s_{1/2}) = 175\,960\ cm^{-1}$ and $E(2p_{3/2}-2s_{1/2}) = 181\,760\ cm^{-1}$. The discrepancy between our results and those of Terao and Burke (1990) increases to a factor of 10 or more when DR is dominated by low-lying states as found in a low-temperature plasma (figure 1) or a high-density plasma (figure 2) since outer electron stabilization becomes more important. We present our intermediate coupling results with various n cut-offs in figure 2. The actual densities for which the cut-offs may represent the collision limit can only be deduced from the solution of the collisional dielectronic population rate equations (see Burgess and Summers 1969, Jacobs and Davis 1978) but the limit is likely to lie no higher than $n = 30$ for an electron density of $10^{19}\ cm^{-3}$ (see Carillon *et al* 1990). We see that even with a cut-off of $n = 8$ our 2-2 DR rate coefficient still dominates over radiative recombination for $T < 2$ Ryd, thereafter DR via 2-3 core excitations (which is dominated by $n < 10$) becomes dominant. Thus, it may not be justified to neglect DR in determining the ionization balance of a laser-produced aluminium plasma (see Carillon *et al* 1990, Pert 1990). However, the DR of Al^{10+} ($1s^2 2s + e^- \rightarrow 1s^2 2ln'l'$) only has an indirect effect on the level population of a Li-like recombination system ($1s^2 + e^- \rightarrow 1s^2 nl$).

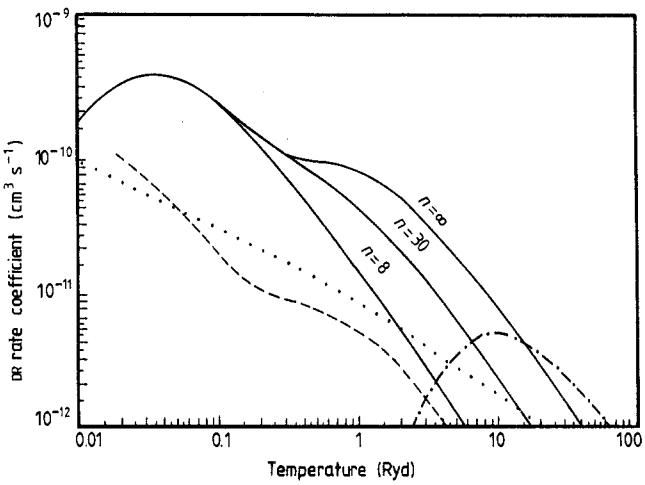

Figure 2. Recombination rate coefficients for Al^{10+}. ——, 2-2 dielectronic recombination summed to $n = 8$, 30 and infinity, this work; —·—, 2-3 dielectronic recombination, all n, this work; - - -, 2-2 dielectronic recombination summed to $n = 30$, Terao and Burke (1990); ····, radiative recombination, Terao and Burke (1990).

In conclusion, we have shown that the Burgess GF (1965) is accurate to 30% for the DR of Al^{10+} in a high-temperature low-density plasma and that the factor of 3.6 discrepancy between the results of our calculations and those of Terao and Burke (1990) is due to an apparent error and an omission in the calculations of the latter. We find that DR is still likely to dominate over radiative recombination for Al^{10+} in a high-density or low-temperature plasma.

I would like to thank Dr P J Storey for his help in implementing the *R*-matrix code. This work was supported by the Office of Fusion Energy, US Department of Energy, under Contract No DE-FG05-86ER53217 with Auburn University.

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