Scaling properties of the dielectronic recombination rate

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Detailed theoretical calculation of the dielectronic recombination rate coefficient $\alpha^{\rm DR}$ has been carried out for the Be and Ne sequences, and the scaling properties of $\alpha^{\rm DR}$ in the nuclear core charge are examined. Based on these results an improved semiphenomenological formula is then constructed.

Dielectronic recombination (DR), which describes the electron capture by an ionic target via initial excitation of inner-shell electrons as the projectile electron goes into an excited orbital, is known to contribute significantly to radiation cooling of hot plasma, and competes with the direct radiative capture (RC) process. While several experimental attempts were made recently to directly measure the (DR) cross section, most of the available information on the DR rate coefficient $\alpha^{\rm DR}$ has thus far come from various theoretical estimates. Thus, we recently reported[1] a detailed study of the Ne sequence, which showed some remarkable deviation in the scaling behavior of $\alpha^{\rm DR}$ from the previous formula.[2,3] An extensive calculation of the $\alpha^{\rm DR}$ for the Be sequence has now been completed,[4] which further suggests modifications of the existing formula. Based on these two studies, we propose an improved formula for $\alpha^{\rm DR}$ with more realistic Z_C (and N) dependences, where Z_C is the nuclear core charge and N is the number of electrons in the initial target ion, although the N dependence is much less certain at present.

The DR rate coefficient $\alpha^{\rm DR}$ is defined as the thermal average of the product of electron velocity v and the DR cross section $\sigma^{\rm DR}$, and, in the nonoverlapping resonance approximation, assumes the form

$$\alpha^{\rm DR}(i) \equiv \langle v\sigma_i^{\rm DR}\rangle \approx \left(\frac{2\pi}{kT}\right)^{3/2}\sum_{l_c}\sum_{d} e^{-e_c/kT}V_a(i,l_c\to d)\omega(d), \qquad (1)$$

where the collisional-excitation, radiationless-capture probability V_a and the fluorescence yield ω for the intermediate states d are expressed as

$$V_a(i,l_c\to d)=\frac{2\pi}{\hbar}\,|\langle d|V|i,l_c\rangle|^2, \qquad (2a)$$

$$\omega(d)=\Gamma_r(d)/[\Gamma_r(d)+\Gamma_a(d)]\ , \qquad (2b)$$

and where l_c is the angular momentum of the continuum electron. In (2b), Γ_a and Γ_r are the Auger and radiative decay widths, respectively, of the state d. [The total DR rate may be obtained by summing (i) over all the initial ionic configurations.] The cascade effect[5] has been neglected in (1) for simplicity, but is included in the actual numerical calculation.

The scaling property of the quantities V_a, ω, and $\alpha^{\rm DR}$ may be discussed first for a purely Coulombic case, so that the scale-breaking behavior can then be studied as a function of N and Z_C. As noted earlier,[1] for an effective charge Z with $Z_I \le Z \le Z_C$ and $Z_I = Z_C - N$, we have the typical behavior for the dominant $\Delta n \ne 0$ transitions

$$V_a \sim Z^0,\ \ \Gamma_a\sim Z^0,\ \ \Gamma_r \sim Z^4\ ,$$

so that

$$\omega\sim\begin{cases} Z^0 \ \text{ for }\ \Gamma_r \gg \Gamma_a \ \text{ and }\ \omega\approx 1,\\ Z^4 \ \text{ for }\ \Gamma_r \ll \Gamma_a \ \text{ and }\ \omega \ll 1.\end{cases}$$

By taking the kT values to scale like Z^2 and $e_c = E_d - E_i \sim Z^2$ by the resonance condition, we have

$$\exp(-e_c/kT)\sim Z^0,$$

in which case Eq. (1) gives

$$\alpha^{\rm DR}\sim\begin{cases} Z^{-3}\ \text{ for }\ \omega\approx 1,\\ Z^{+1}\ \text{ for }\ \omega\ll 1.\end{cases} \qquad (3)$$

The behavior (3) will of course break down as the number of electrons N in the initial ion increases.

Calculation of A_a and A_r, whose sums correspond to Γ_a and Γ_r, has been carried out for both the Ne sequence ($N=10$) and the Be sequence ($N=4$). The actual procedure adopted involves two simplifying steps. Firstly, a complete set of transitions are calculated in the simple angular momentum-averaged (AMA) scheme[1] so as to be able to cover as many intermediate states d as possible. This provides a crude estimate of the total $\alpha^{\rm DR}$, and also allows us to select a small number of dominant transitions for a more detailed analysis. The second step is to recalculate the contribution of the dominant transitions using a more realistic coupling scheme (LS coupling in the present case). The final $\alpha^{\rm DR}$ is then estimated by proportionately scaling the AMA result. The

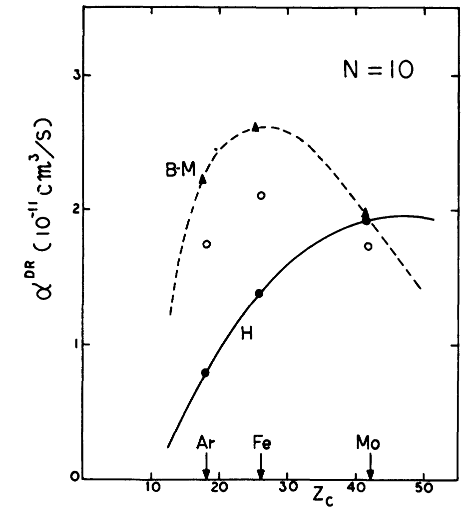

FIG. 1. Dielectronic recombination rate coefficient $\alpha^{\rm DR}$ for ten-electron ions are plotted for different ionic species. The solid curve is obtained by a detailed calculation, as given in Ref. 1, and coincides with the result of (6). The dashed curve is the prediction of Burgess-Merts formula. The kT values are scaled as Z^2, and taken to be 1 keV for Fe^{16+}. The values denoted by open circles are obtained with a different estimate of the oscillator strength, indicating the magnitude of inaccuracy involved. The Z dependence is still similar to the BM curve.

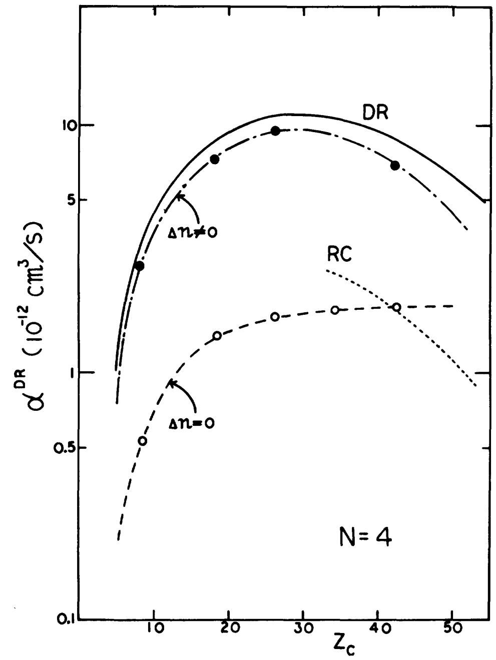

FIG. 2. Dielectronic recombination rate coefficient $\alpha^{\rm DR}$ for four-electron ions. Both the $\Delta n = 0$ and $\Delta n \neq 0$ contributions are given explicitly. Solid curve (DR) is the total sum. The temperature kT is scaled here as Z^2, with $kT = 1$ keV for Fe^{22+}. The direct radiative capture contribution is given by the dotted curve (RC).

cascade effect can be easily included in the AMA scheme.

Figure 1 shows the dependence of $\alpha^{\rm DR}$ for $N=10$ on Z_C when kT is scaled as Z^2, with the effective charge Z taken here to be roughly $Z \approx (Z_I + Z_C)/2$ and $kT = 1$ keV for Fe^{16+}. Of course only the $\Delta n \neq 0$ transitions are possible in this case; in particular, the $2p$ electron excitations to $3dnd$ and $3dnf$ configurations are some of the dominant transitions. The variation in Z is given by

$$\alpha^{\rm DR} \sim Z^{\gamma}, \tag{4}$$

with $\gamma \approx \frac{2}{3}$ for this case, being rather close to the limit (3) for $\omega \ll 1$. The curve BM is the result of a semiphenomenological formula of Burgess[2] as modified by Merts.[3] (There are some ambiguities in the input data used in generating these points, but the general Z_C dependence is not affected by them.) The case with $N=4$ is plotted in Fig. 2, where the $\Delta n \neq 0$ and $\Delta n = 0$ contributions are both given. The total $\alpha^{\rm DR}$ is then compared with the radiative capture rate (RC). Again the fit for $Z_C \lesssim 35$ indicates that $\gamma \approx 1$, thus nearly saturating the limit (3), although the relation (3) is obtained in the purely Coulombic limit. Apparently, the $\Delta n = 0$ contribution becomes quite large as Z_C increases, perhaps exceeding the $\Delta n \neq 0$ value for $Z_C \gtrsim 60$. However, the $\Delta n \neq 0$ contribution remains dominant for most cases. Details of these calculations will be published elsewhere.[1,4]

Based on the results of explicit calculations for the $N=4$ and 10 sequences, we proposed here a modified form of the semiphenomenological formula with an improved Z dependence. Following the original parametrization by Burgess[2] and a later modification by Merts[3] for the case $\Delta n \neq 0$, we set

$$\alpha^{\rm DR} \approx \alpha^{\rm DR}_{\rm BM}(A''/A'), \tag{5}$$

where $\alpha^{\rm DR}_{\rm BM}$ is the Burgess-Merts formula, where[3]

$$A' = 0.5x^{1/2}(1 + 0.21x + 0.03x^2)^{-1},$$
$$x = (Z+1)(n_i^{-2} - n_m^{-2}).$$

The new adjustment factor we introduced in (5) is

$$A''/A' \approx x[0.39\exp(-\sqrt{N}/3)]. \tag{6}$$

Note especially that A'' has a *different* x dependence from A', while the N dependence in (6) should *not* be taken seriously as it is obtained using only two data points at $N=4$ and 10. The formula (5) fits our calculated results very well, both for the $N=4$ and $N=10$ cases, but deviates considerably from the BM values. Of course the form

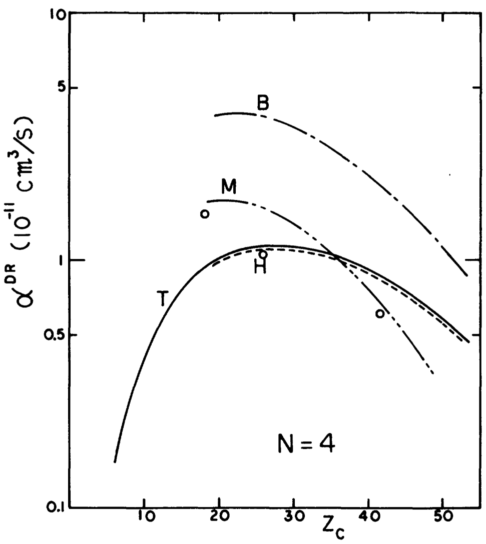

FIG. 3. Dielectronic recombination rate coefficient α^{DR} for four-electron ions. The theoretical calculation is given by curve T, and the formulas (6) and (5) give curve H. Curves B and M are the results of the Burgess and Merts formula. The kT is scaled as Z^2, with $kT=1$ keV for Fe^{22+}. Note again the Z dependence of the curves T and H. The values denoted by the open circles are obtained with a slightly different estimate of the oscillator strength.

(5) should be checked further by comparing it with additional theoretical calculations for other sequences with different N (including both open- and closed-shell ions), and also possibly with some experimental results. Just as in the original BM formula, the form (5) should be regarded as an empirical fit to the calculated values, specifically in the range $Z_C \leq 42$. Figure 3 contains comparison of the various formulas for the case $N=4$ and $kT=1$ keV for Fe^{22+}. The curve B is obtained from the Burgess formula for $\Delta n=0$, and the curve M from the Merts modification using A' for the $\Delta n \neq 0$ transitions. Apart from the overall magnitudes, the Z dependence is again seen to be quite different from the calculated values given by the curve T. The modification (5) with A'' is given by the curve H. The N dependence in (6) is approximately derived from the result for $N=4$ and 10 only. Extensive theoretical investigations of other systems with larger N various corrections to the DR rates are in progress.

As is well known, the DR process discussed above often dominates over the direct radiative capture[1] in the overall electron capture reaction involving highly stripped ions. Such an enhancement of higher-order effects is also seen in Auger ionization[6-8] and in the photo-Auger effect[9] (which is the inverse DR). This important dynamical property of heavy ions is probably caused by a disproportionately heavy concentration of transition strength to low-lying discrete orbitals and by the Pauli exclusion effect. The Z_C dependence of the screening effect also plays an important role. More study is needed, however, to understand this peculiar property.[10]

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