Dielectronic recombination cross section for C^{3+}

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Cross sections for the resonant collisional excitation $2s \rightarrow 2p(\Delta n = 0)$ accompanied by the capture of the incident electron to a Rydberg state, and subsequent decay of this state by radiation emission, are estimated for the C^{3+} target ion. They are typically of the order of $1 \sim 2 \times 10^{-18}$ cm^2 when averaged over an energy-bin size of $0.01 \lesssim \Delta e_c \lesssim 0.03$ Ry, dominated by the high-Rydberg-state contribution.

Radiative capture of projectile electrons by ionic targets is an important process affecting the behavior of plasmas in astrophysical environments and in laboratory devices. The first-order radiative recombination involves the capture of the continuum electron directly to one of the bound orbitals of the target ion with the emission of radiation, and has been satisfactorily treated[1,2] theoretically. The higher-order dielectronic recombination (DR) process is often the dominant mode of capture but is much more difficult to analyze theoretically,[3–5] mainly because there are many intermediate resonance states, all of which are to be treated individually. The DR proceeds by the projectile electron collisionally exciting the target ion to form a compound intermediate state d, which subsequently decays by emission of stabilizing radiation to a state f. The state f may not be stable against Auger-electron emission, in which case further cascade processes[3] should be incorporated. We present here a theoretical estimate of the DR cross section for the $e + C^{3+}$ system. Many simplifying approximations are introduced in the course of this analysis, the validity of which is being investigated. A preliminary study indicates that the method adopted here and in eariler reports[3–5] should be reliable enough to yield the cross sections which can be meaningfully compared with forthcoming experimental data. The details of the effects of configuration mixing and intermediate coupling will be reported elsewhere.

At present, experimental results on the DR rate are not available for direct comparison with theoretical data, except in the case[6,7] of Fe^{24+}. Several attempts[8–11] are being made to measure the DR cross sections for some light ions. Thus, the Li-like Si^{11+} and S^{13+} target systems were considered[8] in the (Si, S) + Ar reactions, where the K x rays were detected in coincidence with the Si^{10+} and S^{12+} formation, but without examining the energy variation of the cross section. As part of our study of the DR process for the Li-isoelectronic sequence,[5] the theoretical cross section $\bar{\sigma}^{DR}$ for this system with the initial 1s electron excitation ($\Delta n \neq 0$) was found[12] to be of the order of 10^{-20} cm^2, when averaged over an energy-bin size of 1 Ry. This seems to be consistent with the experiment, but because of the ambiguity of the Ar system as an electron beam source, proper interpretation cannot be given at present. The $e + Cl^{7+}$ system is also being studied both experimentally[9] and theoretically,[13] in which one of the $2p$ electrons of Cl^{7+} is excited ($\Delta n \neq 0$). For a bin size of $\Delta e_c \approx 0.1$ Ry, the theoretical $\bar{\sigma}^{DR}$ is found[13] to be $1 \approx 3 \times 10^{-19}$ cm^2. Additional experiments on the $e + Mg^+$ system[10] (with $\Delta n = 0$) and on the $e + C^+$ system[11] (with $\Delta n = 0$) are being carried out.

In this report, we present the energy-averaged DR cross section $\bar{\sigma}^{DR}$ for the $e^- + C^{3+}$ system, in which the $2s \rightarrow 2p$ electronic transition ($\Delta n = 0$) of the target and the capture of the projectile electron to a high Rydberg state (nl) is involved. That is,

$$\underset{(i)}{e_c^-(k_c l_c) + C^{3+}(1s^2 2s)} \leftrightarrow \underset{(d)}{C^{2+}(1s^2 2pnl)^{**}} \rightarrow \underset{(f)}{C^{2+}(1s^2 n_a l_a n_b l_b)} + \gamma , \quad (1)$$

where the resonance condition $E_d = E_i$ requires that $n \geq 4$, while $n_a l_a$ in the final state f should be either $2s$ or $2p$. Since the total widths $\Gamma(d)$ for the resonance states d of $(C^{2+})^{**}$ are typically of the order $< 10^{-2}$ Ry, we estimate the DR cross section averaged over an energy-bin size $\Delta e_c \sim 0.01$ and 0.03 Ry. The cross sections $\bar{\sigma}^{DR}$ for larger bin sizes can readily be obtained from the result presented here.

The theoretical procedure adopted is exactly the same as that employed in our previous work[3-5] on the DR rates. That is, we employ the full LS coupling scheme throughout, and the radial matrix elements for the radiative and Auger probabilities, A_r and A_a, respectively, are obtained using the single-configuration nonrelativistic Hartree-Fock wave functions. The continuum wave function is also generated using the Hartree-Fock potential with nonlocal exchange. The intermediate states d are treated as isolated resonances, although some overlap is expected for the high Rydberg states. The configuration mixing, relativistic corrections, and possible density effect on the high Rydberg states are neglected. For the calculational details, we refer to our eariler series of publications[3-5] on the DR rates $\alpha^{\rm DR}$. Important from the theoretical point of view is the fact that we use the *same* calculational procedure in evaluating $\bar{\sigma}^{\rm DR}$ as in the rate $\alpha^{\rm DR}$, so that comparison of $\bar{\sigma}^{\rm DR}$ with experiments could be a test of the approximations used in the evaluation of $\alpha^{\rm DR}$.

The DR cross section is defined in the isolated resonance approximation by

$$\sigma^{\rm DR}(d,i) = \frac{4\pi{\rm Ry}}{(k_c a_0)^2}[V_a(i\to d)\tau_0]\omega(d)\tilde{\delta}(e_c)(\pi a_0^2) , \quad (2)$$

where k_c is the wave number of the incident electron which is to be captured (with $k_c^2 = e_c$ in Ry), V_a is the radiationless capture probability (in $\sec^{-1}$) given[3-5] in terms of the Auger probability $A_a(d\to i)$ by detailed balance, as

$$V_a(i\to d) = \frac{g_d}{2g_i}A_a(d\to i)$$

with the appropriate statistical factors g, and the atomic unit for the time scale is

$$\tau_0 = a_0/v_0 = 2.42\times 10^{-17}\ \sec .$$

The fluorescence yield $\omega(d)$ is defined as usual by

$$\omega(d) = \Gamma_r(d)/\Gamma(d) ,$$

$$\Gamma(d) = \Gamma_r(d) + \Gamma_a(d) ,$$

where $\Gamma_r(d)$ and $\Gamma_a(d)$ are the radiative and Auger widths of the state d. Finally, the Lorentzian factor $\tilde{\delta}$ is defined as

$$\tilde{\delta}(E_i = e_c + e_i) = \frac{\Gamma}{2\pi}\frac{1}{(E_i - E_d)^2 + \Gamma^2(d)/4}$$

such that $\int \tilde{\delta}\, de_c = 1$. For narrow resonances with $\Gamma < 10^{-2}$ Ry, we may define an energy-averaged cross section

$$\bar{\sigma}^{\rm DR}(d,i) \equiv \frac{1}{\Delta e_c}\int_{e_c - \Delta e_c/2}^{e_c + \Delta e_c/2} de_c'\, \sigma^{\rm DR}(e_c') , \quad (3)$$

where Δe_c is the bin size with $\Delta e_c \gtrsim 10^{-2}$ Ry. We arbitrarily choose here $\Delta e_c = 0.01$ and 0.03 Ry. Combining (2) and (3), we finally have

$$\bar{\sigma}^{\rm DR}(d,i) = \frac{\rm Ry}{\Delta e_c}\frac{4\pi}{(k_c a_0)^2}[V_a(i\to d)\tau_0]\omega(d)(\pi a_0^2) . \quad (4)$$

It is of interest to compare (4) with the expression for the DR rate

$$\alpha^{\rm DR}(d,i) = \left[\frac{4\pi\ {\rm Ry}}{k_B T}\right]^{3/2} a_0^3 V_a(i\to d)\omega(d) e^{-e_c/k_B T} . \quad (5)$$

Except for the temperature-dependent factors (involving $k_B T$), the essential contents of (4) and (5) are the same; for both cases the dynamical information is contained entirely in V_a and $\omega(d)$. [In most applications of $\alpha^{\rm DR}$, however, we use

$$\alpha^{\rm DR}(i) = \sum_d \alpha^{\rm DR}(d,i) .$$

This could make $\alpha^{\rm DR}(i)$ less sensitive to the various approximations made in evaluating each $\alpha^{\rm DR}(d,i)$, and thus the study of $\bar{\sigma}^{\rm DR}$ may be a more stringent test of the reliability of the theory.]

We limit our discussion of the theoretical result to the energy region $0.02 < e_c < 0.60$ Ry, in which case only the $2s\to 2p$ excitation ($\Delta n = 0$) in (1) is possible. The $2s$ excitation to higher shells ($\Delta n \neq 0$) requires $e_c \gtrsim 1$ Ry, while the $1s$ excitation is possible for $e_c \gtrsim 5$ Ry. Table I contains the value of $\bar{\sigma}^{\rm DR}$ for the bin size $\Delta e_c = 10^{-2}$ Ry and for the various intermediate states d, and the result is plotted in Fig. 1. The dotted line in the figure corresponds to $\bar{\sigma}^{\rm DR}$ for $\Delta e_c = 0.03$ Ry. (In some cases, $\Delta e_c = 10^{-2}$ Ry may be of the same magnitude as $\Gamma(d)$ and some dependence on the actual resonance shape may be relevant.) The cross sections are evaluated explicitly for $4 \le n \le 11$, and the contribution from $n \ge 12$ is estimated using a special fit.[14] Sizable contributions come from $n \lesssim 400$, as shown by the large peaks in the figure near $e_c \approx 0.60$ Ry. Of course, these large-n effects are much more difficult to detect experimentally, as they are very sensitive to stray fields and to collision effects; the low-lying peaks in the range $0.02 \lesssim e_c \lesssim 0.45$ Ry may be more tractable

TABLE I. Dielectronic recombination cross section $\bar{\sigma}^{DR}$, averaged over a bin size $\Delta e_c = 0.01$ Ry, is given in units of 10^{-19} cm^2 for different intermediate resonance states $d = 1s^2 2pnl$. High-n contribution is estimated by fitting the low-n ($n \leq 11$) results with the formula given in Ref. 14. Only the $2s \to 2p$ (with $\Delta n = 0$) transitions are considered for the system $C^{3+} + e$.

e_c(Ry)	$nl(d = 1s^2 2pnl)$	$\bar{\sigma}^{DR}(10^{-19}\ \text{cm}^2)$
0.02–0.03	4*d*	33.4
0.03–0.04	4*f*	17.6
0.18–0.19	5*s*	0.43
0.20–0.21	5*p*	1.22
0.22–0.23	5*d*	1.78
0.23–0.24	5*f*	1.44
	5*g*	1.27
0.31–0.32	6*s*	0.22
0.32–0.33	6*p*	0.44
0.33–0.34	6*d*	1.76
0.34–0.35	6*f*	0.70
	6*g*	0.67
	6*h*	0.69
0.38–0.39	7*s*	0.13
0.39–0.40	7*p*	0.27
0.40–0.41	7*d*	1.00
	7*f*	0.47
	7*g*	0.60
	7*h*	0.50
	7*i*	0.53
0.43–0.44	8*s*	0.10
0.44–0.45	8*p*	0.20
0.45–0.46	8*d*	0.65
	8*f*	0.36
	8*g*	0.46
	8*h*	0.40
	8*i*	0.46
	8*j*	0.37
0.47–0.48	9*s*	0.08
	9*p*	0.19
	9*d*	0.48
0.48–0.49	9*f*	0.30
	9*g*	0.38
	9*h*	0.37
	9*i*	0.41
	9*j*	0.32
	9*k*	0.25
0.50–0.51	10	2.48
0.51–0.52	11	2.23
0.52–0.53	12	2.05
0.53–0.54	13	2.01
0.54–0.55	14	1.96
0.55–0.56	$n = 15,16$	3.6
0.56–0.57	$n = 17-20$	6.7
0.57–0.58	$n = 21-27$	10
0.58–0.59	$n = 28-67$	55
0.59–0.60	$n = 68-\infty$	143

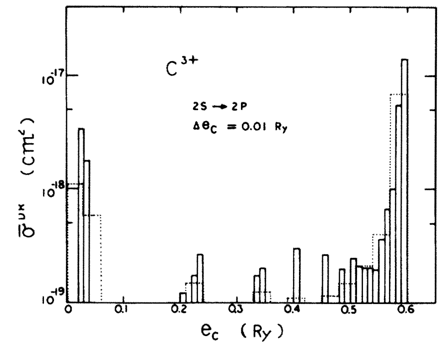

FIG. 1. DR cross section $\bar{\sigma}^{DR}$, averaged over a bin size $\Delta e_c = 0.01$ Ry, is given as it corresponds to the values in Table I. Dotted line is for the bin size $\Delta e_c = 0.03$ Ry.

experimentally. We estimate that the accuracy of our $\bar{\sigma}^{DR}$ is approximately $\pm 30\%$ for larger Δe_c.

Since the dominant part of $\bar{\sigma}^{DR}$ comes from the region $0.56 \lesssim e_c \lesssim 0.60$ Ry, it is possible to make a rough estimate of the DR rate $\alpha^{DR}(i)$ by using the similarity between formulas (4) and (5). By adding all the $\bar{\sigma}^{DR}$ values in Table I, we have, for $\Delta e_c = 0.01$ Ry,

$$\sum_d \bar{\sigma}^{DR}(d,i) \approx 2.3 \times 10^{-17}\ \text{cm}^2 .$$

For $k_B T = 2.48$ Ry and

$$\bar{e}_c = \bar{k}_c^2 a_0^2 = 0.595\ \text{Ry} ,$$

we then have

$$\bar{\alpha}^{DR}(i) \approx 6.7 \times 10^{-12}\ \text{cm}^3/\text{sec} ,$$

which compares well with the earlier explicit calculation[15]

$$\alpha^{DR} = 6.5 \times 10^{-12}\ \text{cm}^3/\text{sec} .$$

A series of recent theoretical investigations[12,13] of the DR cross sections for various target ions indicates that, when Δe_c is chosen appropriately, $\bar{\sigma}^{DR}$ is generally of the order of 10^{-20} cm^2 for the K-shell excitation, 10^{-19} cm^2 for the L-shell excitation, and 10^{-18} cm^2 for the M-shell excitation, all for the $\Delta n \neq 0$ target transitions. On the other hand, for the DR processes in which the $\Delta n = 0$ transitions are involved, $\bar{\sigma}^{DR}$ seems to be as large as 10^{-17} cm^2, most of which comes from the capture to high Rydberg states. To obtain $\bar{\sigma}^{DR}$ to an accuracy better than a factor of two, however, a much more detailed calculation such as that presented here is required.

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