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Dielectronic recombination cross section for Cl^{7+}

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The resonant dielectronic recombination cross section is estimated for a Cl^{7+} target interacting with incident electrons in the $10 \sim 20$-rydberg range. Cross sections averaged over energy bins of size $\Delta E = 0.1$ Ry are approximately $(1-3)\times 10^{-19}$ cm^2.

Dielectronic recombination (DR) of positive ions has been recognized as an important atomic process contributing to the radiative cooling of plasma and to the production of exotic resonance states in solar coronae. However, values of cross sections σ^{DR} and rate coefficients α^{DR} are presently scarce because of technical difficulties, both of an experimental and a theoretical nature. In recent years strenuous theoretical efforts have been made[1,2] to estimate the rate coefficients for a selected set of ions. Since the complexity of the process requires many simplifying approximations, the validity of which is not always well understood, further refinements of the theoretical procedures may be necessary. Meanwhile, it is essential that direct experimental measurement of σ^{DR} be made. So far, in spite of the effort by many experimental groups, no reliable data has yet been obtained. On the other hand, a fairly simple but detailed theoretical calculation of the rate α^{DR} and the cross section σ^{DR} is now possible, using the *same* theoretical approaches for both quantities α^{DR} and σ^{DR}. Obviously, it is crucial to adopt the same theoretical procedure in the evaluation of these quantities if a check on σ^{DR} is to be inferred from a reliable estimate of α^{DR}.

As the first in a series of calculations, we determine σ^{DR} for the Cl^{7+} (Ne-like) ground-state target ion

$$\underset{(i)}{e^- + \mathrm{Cl}^{7+}} \to \underset{(d)}{(\mathrm{Cl}^{6+})^{**}} \to \underset{(f)}{(\mathrm{Cl}^{6+})^{*}} + \gamma$$

in which the $d \to f$ process is complicated by competing Auger processes $d \to i'$, where

$$i_1' = i = (1s^2 2s^2)2p^6 + kl_c \ ,$$

$$i_2' = (1s^2 2s^2)2p^5 3s + k' l_c' \ ,$$

$$i_3' = (1s^2 2s^2)2p^5 3p + k'' l_c'' \ .$$

The theoretical procedure adopted here is that used in previous publications.[1,2] The cross section σ^{DR} is evaluated in the isolated resonance approximation for each individual intermediate resonance state d. This is justified especially for the low-lying (dominant) resonances as their widths are usually of the order of 10^{-2} Ry or less, while the distance between the resonances are typically of the order of a Rydberg or greater. The radiative and Auger transition probabilities A_r and A_a are evaluated using single configuration Hartree-Fock wave functions and a continuum function with full nonlocal exchange. The LS-coupling scheme has been adopted, as described in Ref. 1. Thus, we have the DR cross section averaged over an energy interval ΔE defined by

$$\bar{\sigma}^{\mathrm{DR}} \equiv \frac{1}{\Delta E} \int_{e_c - \Delta E/2}^{e_c + \Delta E/2} de_c' \, \sigma^{\mathrm{DR}} \ , \tag{1}$$

where

$$\sigma^{\mathrm{DR}}(d,i) = \frac{4\pi}{(k_c a_0)^2} [V_a(i \to d)\tau_0] \omega(d) \tilde{\delta}(\pi a_0^2) \ . \tag{2}$$

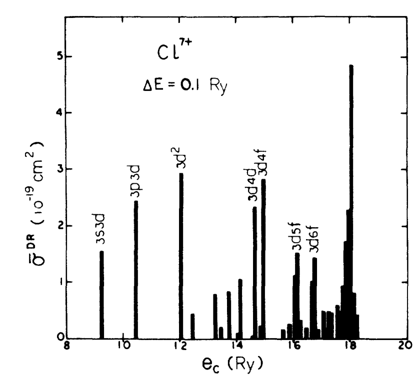

FIG. 1. Energy-averaged DR cross section $\bar{\sigma}^{\mathrm{DR}}$ for the system $e + Cl^{7+}$, with $2p^6 kl_c \to 2p^5 3dnl$ and the bin size $\Delta E = 0.1$ Ry. Select transitions of the type $2p^6 + kl_c \to 2p^5 3snl$ and $2p^6 + kl_c \to 2p^5 3pnl$ are also included, for $n \geq 4$, but excitations to $2p^5 3dnl$ dominate the cross section. For $e_c \gtrsim 18.2$ Ry, excitations to $2p^5 4dnl$ ($n \geq 4$) are possible, however, these make only small contributions to $\bar{\sigma}^{\mathrm{DR}}$.

In (1), the integration is over the continuum energy of the incoming electron e_c. We chose $\Delta E = 0.1$ Ry. The cross section (2) contains the fluorescence yield $\omega = \Gamma_r(d)/\Gamma(d)$, $\Gamma(d) \equiv \Gamma_r(d) + \Gamma_a(d)$; V_a is the radiationless capture probability as defined in Ref. 1 with the appropriate continuum function normalization. The widths Γ_r and Γ_a are, in turn, defined in terms of A_r and A_a, respectively. The atomic time unit is

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

and

$$\tilde{\delta} \equiv (\Gamma/2\pi)/[(E_i - E_d)^2 + \Gamma^2/4]$$

such that, with $E_i = e_i + e_c$,

$$\int de_c' \tilde{\delta} = 1 .$$

Equation (2) is to be compared with the corresponding DR rate coefficient α^{DR}, defined in the same approximation,

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

Except for the temperature dependence, (2) and (3) contain essentially the same theoretical quantities, V_a and ω.

TABLE I. Energy-averaged DR cross section for the specific transitions ($2p^6kl_c \rightarrow 2p^53dnl$) are listed for the bin size $\Delta E = 0.1$ Ry. The i' are the channels open to Auger decay from the intermediate state d, in addition to the initial state $1s^22s^22p^6 + kl_c$. Select transitions of the type $2p^6 + kl_c \rightarrow 2p^53snl$ and $2p^6 + kl_c \rightarrow 2p^53pnl$ are also included. Values of $\bar{\sigma}^{\mathrm{DR}}$ for $n \gtrsim 10$ are obtained approximately, by an extrapolation.[6]

d	e_c(Ry)	$\bar{\sigma}_{LS}^{\mathrm{DR}}$($10^{-19}$ cm^2)	i'
$2p^53d\,3s$	9.28	1.54	
$3d\,3p$	10.4	2.45	
$3d\,3d$	12.0	2.92	
$3s\,4d$	12.5	0.46	
$3p\,4d$	13.2	0.79	
$3s\,5d$	13.4	0.22	
$3d\,4s$	13.7	0.80	
$3d\,4p$	14.2	1.07	
$3d\,4d$	14.7	2.35	
$3p\,5d$	14.8	0.21	
$3d\,4f$	14.9	2.84	
$3d\,5s$	15.6	0.15	$2p^53s + kl_c$
$3d\,5p$	15.8	0.26	$2p^53s + kl_c$
$3d\,5d$	16.0	1.11	$2p^53s + kl_c$
$3d\,5f$	16.1	1.24	$2p^53s + kl_c$
$3d\,5g$	16.2	0.32	$2p^53s + kl_c$
$3d\,6s$	16.2	0.16	$2p^53s + kl_c$
$3d\,6p$	16.4	0.24	$2p^53s + kl_c$
$3d\,6d$	16.6	1.02	$2p^53s + kl_c$
$3d\,6f$	16.6	1.44	$2p^53s + kl_c$
$3d\,7s$	16.7	0.01	$2p^53s + kl_c, 2p^53p + kl_c$
$3d\,7p$	16.8	0.15	$2p^53s + kl_c, 2p^53p + kl_c$
$3d\,7d$	16.9	0.48	$2p^53s + kl_c, 2p^53p + kl_c$
$3d\,7f$	16.9	0.05	$2p^53s + kl_c, 2p^53p + kl_c$
⋮			⋮
$3d\,16d + \cdots 3d\,21d$	17.9 to 18.0	2.28	$2p^53s + kl_c, 2p^53p + kl_c$
$3d\,22d + \cdots 3d\,70d$	18.0 to 18.1	4.90	$2p^53s + kl_c, 2p^53p + kl_c$
$3d\,71d + \cdots 3d\,\infty d$	18.1 to 18.2	0.78	$2p^53s + kl_c, 2p^53p + kl_c$
$4d\,4d$	18.2	0.40	$2p^53s + kl_c, 2p^53p + kl_c$

The total rates are obtained by summing (3) over all possible states d, i.e., $\alpha^{\mathrm{DR}}(i)=\Sigma_d \alpha^{\mathrm{DR}}(i,d)$. On the other hand, since σ^{DR} is essentially a resonance cross section, it depends on the continuum energy and on the size of the bin, ΔE.

We restrict our study to the intermediate states d of the type $d=(1s^2 2s^2)2p^5 3dnl$ formed from the initial state $i=(1s^2 2s^2)2p^6+kl_c$ by $2p$-electron excitation. ($2p$ excitation nearly saturates the cross section; $2s$ and $1s$ excitation contribute very little.) This particular process is being studied experimentally.[3] As noted above, the magnitude of $\bar{\sigma}^{\mathrm{DR}}$ depends upon choice of bin size, ΔE, and upon the location of the resonances; i.e., $e_c=E_d-e_i$. In Fig. 1, we present the result of our calculation for the choice $\Delta E=0.1$ Ry in the full LS-coupling scheme. The specific transitions and the scattering energies are listed in Table I. Because our calculation of Γ_a includes, explicitly, Auger decays into all energetically accessible i', the observed dependence of $\bar{\sigma}^{\mathrm{DR}}(2p^5 3dnl)$ upon n, for fixed l, is more complicated than the familiar $1/n^3$. In general,[6]

$$\bar{\sigma}^{\mathrm{DR}}(2p^5 3dnl) \propto 1/(n^3+\mathrm{const}) ,$$

where $10^3 \lesssim \mathrm{const} \lesssim 10^6$ depending upon values of L, L_{ab}, S_{ab}, and the configuration. (L_{ab} and S_{ab} are the orbital and spin angular momenta of the active electron pair.) For a given configuration, summing $\bar{\sigma}^{\mathrm{DR}}(2p^5 3dnl)$ over n produces a value which may be greater than or less than the result deduced from a calculation which assumes a single $i'=i=1s^2 2s^2 2p^6+kl_c$.

Evidently, the DR cross sections are quite small, of the order of 10^{-19} cm^2 for a reasonable choice of $\Delta E/e_c \gtrsim 10^{-2}$, and n not too large ($n \lesssim 10$). Our theoretical estimate is expected to be reliable to about $\pm 30\%$, but a more direct check on its accuracy should come from experiments and from more detailed calculations including the relativistic effect and configuration mixing. Additional cross section for the Li-like ions[4] (S^{13+}, Si^{11+}, and C^{3+}), and for the Na-like ions[5] (Mg^{1+}, Ar^{7+}, Fe^{15+}, and Mo^{31+}) will be reported elsewhere.

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