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Resonant electron capture to high Rydberg states of Ca II

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The dielectronic recombination cross section for the Ca II ion is calculated for the process in which the $4s$ electron is excited to the $4p$ state as the projectile electron is captured to a high Rydberg state (nl). The cross section, averaged over a bin size of 0.3 eV, exhibits a peak of 1.8×10^{-17} cm^2, while a cutoff for $n\leq80$ reduces this to 2.3×10^{-18} cm^2. The recent crossed-beam experiment gives a cross section of 1.8×10^{-17} cm^2 which is at least seven times larger than the theoretical value.

Electron capture by ionic targets via intermediate resonance states, followed by stabilizing radiation emission, is known as the dielectronic-recombination (DR) process. It is an important mode by which hot plasmas of electrons and ions can rapidly lose energy. The process may also be used as a diagnostic tool in the study of solar corona, stellar environments, and laboratory plasmas.

Because of various technical difficulties, experimental study of DR was not possible until recently, and most of the available information on DR has been obtained theoretically. Since DR describes higher-order processes involving many resonant intermediate states, theoretical calculation necessarily requires numerous drastic approximations.

During the past year, several measurements were reported[1-4] which could be used to test the theory.[5-8] Unfortunately, the DR cross sections seem to be extremely sensitive[9] to a small (electric) field which may be present in the interaction region either as a part of the experimental setup or accidentally as a stray field, especially when high Rydberg states (HRS) are involved.[1-3] More recently, a measurement of the DR cross section for the $Ca^{1+}+e^-$ system was reported,[10] which adopted a procedure very similar to that of Ref. 1 for $Mg^{1+}+e^-$, but presumably without any stray electric field (<0.3 V/cm) in the interaction region. Williams obtained a cross-section peak value of 1.8×10^{-17} cm^2 with $n\leq80$ and a width of about $0.3\sim0.5$ eV.

We present here a theoretical calculation of the DR cross section for the process ($\Delta n_t=0$, which means $4s\rightarrow4p$ with $n_t=4$)

$$\begin{array}{ccccc} e^-+\mathrm{Ca}^{1+} & \underset{A_a}{\overset{V_a}{\rightleftharpoons}} & (\mathrm{Ca}^{0+})^{**} & \xrightarrow{\Gamma_r} & (\mathrm{Ca}^{0+})^{*}+\gamma \\ k_cl_c+4s & & 4pnl & & 4snl,\ldots \\ (i) & & (d) & & (f) \end{array} \qquad (1)$$

(Explicit reference to the core electrons of Ca^{1+} is omitted for simplicity.) Other modes of collisional excitation capture (denoted by the probability V_a) are also possible, in which the $4s$ electron may be excited to the $3d$ state or to other higher states, and excitation of the core electrons may occur as well ($3p,3s$, etc.). They generally require higher threshold energies; although the threshold for the $4s\rightarrow3d$ transition is lower than that of (1), its principal decay mode is by Auger emission, thus making the DR cross section very small. The present study does not include these excitation modes nor the effect of external fields.

The theoretical procedure adopted here is similar to that employed earlier in the study of the e^-+Mg^{1+} and e^-+B^{2+} systems;[5,7] all the bound orbitals needed in the evaluation of the radiative and Auger transition probabilities, A_r and A_a, respectively, are generated by the nonrelativistic, single-configuration Hartree-Fock code; the continuum orbitals in A_a are calculated in the distorted-wave approximation; simple LS coupling is used. The cross section is evaluated in the isolated resonance approximation, neglecting possible overlaps between the resonance states; the effect of which becomes important only for very high $n\gtrsim300$.

Since the resonance peaks are very sharp and isolated for $n<80$, we represent the data by averaging σ^{DR} over a small energy bin of size Δe_c, which is chosen arbitrarily but with the requirement that it be small compared with the actual experimental beamwidth. Thus we define $(i\equiv4s)$

$$\bar{\sigma}^{DR}(i\rightarrow d)\equiv\frac{1}{\Delta e_c}\int_{e_c-\Delta e_c/2}^{e_c+\Delta e_c/2}\sigma^{DR}de_c'$$
$$=\left(\frac{\mathscr{R}_\infty}{\Delta e_c}\right)\frac{4\pi}{(k_ca_0)^2}[\tau_0V_a(i\rightarrow d)]\omega(d)(\pi a_0^2), \quad (2)$$

where e_c is the incident electron energy, $\tau_0=2.42\times10^{-17}$ sec, $\omega(d)=\Gamma_r(d)/\Gamma(d)$ with $\Gamma(d)=\Gamma_r(d)+\Gamma_a(d)$ and where $\mathscr{R}_\infty=13.6$ eV; they are given in units of sec^{-1} by

$$\Gamma_a(d)=\sum_{i'}A_a(d\rightarrow i'),\quad i'=4s\text{ and }3d\ ,$$
$$\Gamma_r(d)=\sum_{f'}A_r(d\rightarrow f')\ . \quad (3)$$

The important difference between the $Ca^{1+}+e^-$ case under discussion and the earlier case $Mg^{1+}+e^-$ is the presence of an additional Auger channel in (3), i.e., $i_1'=i=4s$ and $i_2'=3d$. As will be shown below, this has a serious effect on σ^{DR} especially on the $l=1$ intermediate states.

We briefly discuss the general structure of the cross section using the scaling properties of A_a and A_r. This will further clarify the theoretical calculation presented later. For $n\gtrsim8$, we expect that both $A_a(d\rightarrow i_1'=i)$ and $\Gamma_a=A_a(d\rightarrow i_1')+A_a(d\rightarrow i_2')$ will scale as n^{-3} for each fixed l. On the other hand, Γ_r will have a contribution $A_r(d=4pnl\rightarrow f_1'=4snl)$ and a small part $A_r(d=4pnl\rightarrow f_2'=3dnl)$ which are essentially independent of n, and the remaining part which approximately scales as n^{-3}. Thus for $n\lesssim n_m=300$, where $A_r(d\rightarrow f_1')\approx\Gamma_r$, we have $\Gamma_a>>\Gamma_r$ and

$$\bar{\sigma}^{DR}(i\rightarrow d)\approx\left(\frac{\mathscr{R}_\infty}{\Delta e_c}\right)\frac{4\pi}{(k_ca_0)^2}\frac{g_d}{2g_i}$$
$$\times\tau_0A_r(4p\rightarrow4s)\frac{A_a(d\rightarrow i)}{\Gamma_a(d)}(\pi a_0^2). \quad (4)$$

In (4), $V_a=(g_d/2g_i)A_a(d\rightarrow i)$ is used with the statistical factors g_d and g_i for the states (d) and (i), respectively. Note that the expression (4) is nearly independent of n, that is $\overline{\sigma}^{\rm DR}$ is constant for all n until n reaches n_m. On the other hand, for $n > n_m$, $A_r \approx \Gamma_r >> \Gamma_a$ so that $\omega \rightarrow 1$ and

$$\overline{\sigma}^{\rm DR}(i\rightarrow d)\approx\left[\frac{\mathcal{R}_\infty}{\Delta e_c}\right]\frac{4\pi}{(k_c a_0)^2}\tau_0\frac{g_d}{2g_i}A_a(d\rightarrow i)(\pi a_0^2)\ , \qquad (5)$$

which varies as n^{-3}, independent of $A_a(d\rightarrow i_2')$. This part of the contribution is generally small. Note that this is the region where the overlap problem arises.

The high-Rydberg-state contribution is estimated either by an extrapolation from low $n \lesssim 10$, or by the quantum defect method.[11]

We present in Fig. 1 the energy averaged cross section $\overline{\sigma}^{\rm DR}$ for an energy bin size of $\Delta e_c = 0.01$ Ry. The general structure is quite similar to that obtained for the Mg^{1+} and B^{2+} cases.[5,7] The l dependence of the cross section is studied by first summing $\sigma^{\rm DR}$ over n for $n < 80 \equiv n_c$. This result is exhibited in Fig. 2. The contribution from $l > 7$ is negligible. A drastic reduction in the $l=1$ contribution is found, which is caused by a sudden drop in the $A_a(d\rightarrow i_1'=i)$ due to cancellation in the matrix element. We note that relative values of the A_a's are such that

$$A_a(d\rightarrow i_1')\lesssim A_a(d\rightarrow i_2')\quad \text{for } l\neq 1\ , \qquad (6a)$$

but

$$A_a(d\rightarrow i_1')\approx 0.1 A_a(d\rightarrow i_2')\quad \text{for } l=1\ . \qquad (6b)$$

This means in turn that, in Eq. (4),

$$\begin{aligned} &A_a/\Gamma_a \approx 0.3 \sim 0.5,\quad l\neq 1\ ;\\ &A_a/\Gamma \approx 0.09,\quad l=1\ . \end{aligned} \qquad (7)$$

Finally, the n dependence of $\sigma^{\rm DR}$ for each fixed l is given roughly by Eq. (4) for $n < n_m$. This makes the summation over n up to $n=n_c << n_m$ very simple;

$$\sum_n^{n_c}\overline{\sigma}^{\rm DR}(i\rightarrow d)\approx\left[\frac{\mathcal{R}_\infty}{\Delta e_c}\right]\frac{4\pi}{(k_c a_0)^2}\frac{g_d}{2g_i}\frac{A_a}{\Gamma_a} \times A_r(4p\rightarrow 4s)n_c(\pi a_0^2)\ . \qquad (8)$$

Now compare our result with the recent experiment[10] carried out by a crossed-beam technique. Using the cutoff $n_c=80$ and $\Delta e_c = 0.3$ eV we obtain the cross-section peak value of

$$\begin{aligned} &\sum_{nl}\overline{\sigma}^{\rm DR}\approx 2.3\times 10^{-18}\ \text{cm}^2\quad (n\leq n_c=80)\ ,\\ &\sum_{nl}\overline{\sigma}^{\rm DR}\approx 1.8\times 10^{-17}\ \text{cm}^2\quad (\text{all } n)\ . \end{aligned} \qquad (9)$$

Note the drastic reduction in the cross section by nearly a factor of 8 when n is cut off at $n=n_c=80$. This is in sharp contrast with the $e^- + Mg^{1+}$ system where the reduction was only a factor of ~ 4 even for $n_c = 64$.

To compare the theory with experiment more meaningfully, we have to fold the above cross section over a typical beam profile; we simulate this by reducing the cross section by a factor 0.7 and obtain

$$\begin{aligned} \sum_{nl}\overline{\sigma}^{\rm DR}(n\leq n_c) &\approx 1.6\times 10^{-18}\ \text{cm}^2,\quad \Delta e_c=0.3\ \text{eV}\\ &\approx 1.0\times 10^{-18}\ \text{cm}^2,\quad \Delta e_c=0.5\ \text{eV}\ . \end{aligned} \qquad (10)$$

The experimental peak has a width of roughly $0.3 \sim 0.5$ eV, and a peak value of 1.8×10^{-17} cm^2. A discrepancy of a fac-

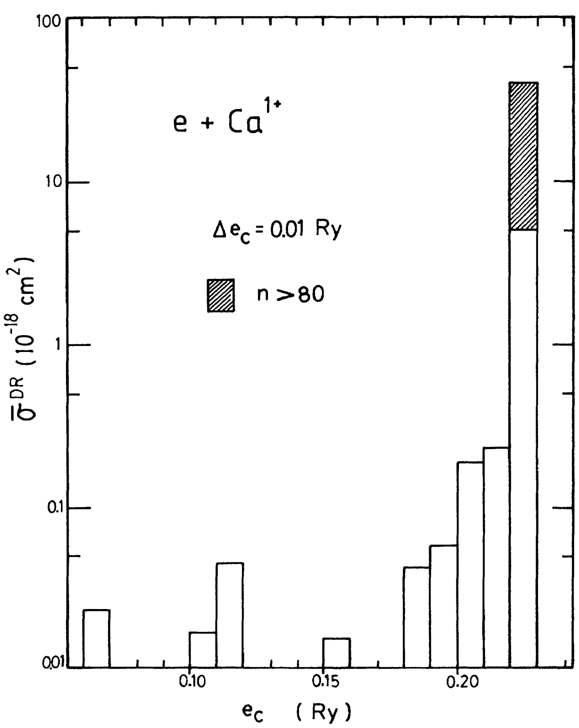

FIG. 1. The DR cross sections, averaged over a bin size of $\Delta e_c = 0.01$ Ry, are presented as a function of the incident electron energy e_c.

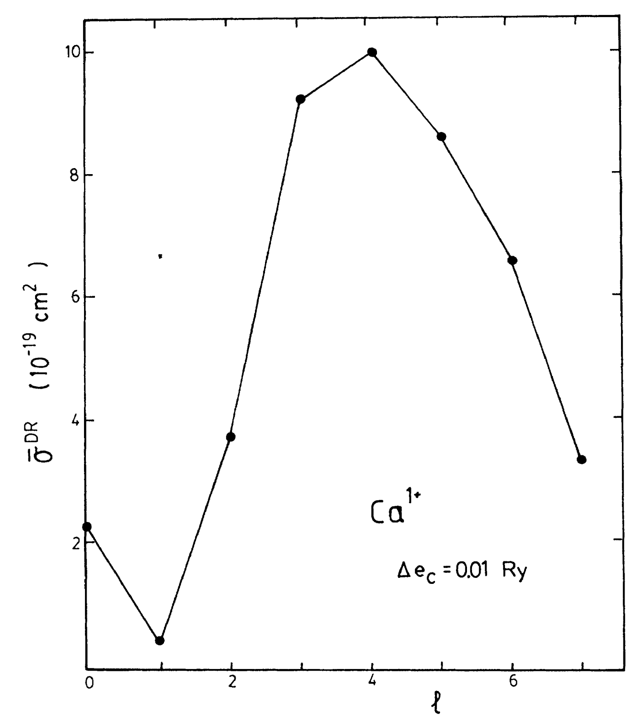

FIG. 2. The l dependence of $\sum_n\overline{\sigma}^{\rm DR}$ for $n\leq n_c=80$ is presented. The large dip in the $l=1$ contribution is due to an accidental cancellation in the matrix elements of A_a.

tor of $7 \sim 18$ exists between the experiment and (10), which is yet to be resolved. The fact that $\bar{\sigma}^{DR}_{exp}$ is twice as large[10] as Burgess[12]-Merts[13] formula (which include all n and all excitations) implies that, aside from the $\Delta n_t \neq 0$ contribution to σ^{DR} included in the Burgess-Merts formula, the experimental values seem to be too high again by as much as a factor of $10 \sim 20$, while the present calculation is consistent with the empirical formula[12-14] to within a factor of 2.

We speculate that the above discrepancy could be either due to theoretical uncertainties caused by the approximations introduced, such as the LS coupling and the isolated resonance approximation, or, more likely, caused by as yet unknown stray field,[9] of the order of $3 \sim 10$ V/cm. The argument in favor of the field effect is made more plausible by comparing the present result with that of Mg in Table I. Using the various scaling properties discussed above, a rough consistency check can be made. Note that, within $\pm 30\%$, the two cases are compatible with each other.

A crude estimate of the field effect can be made by noting that the cross section for $n < n_m$, given by (4) and (8), is constant independent of n. Therefore, the l mixing by an external field requires essentially a different state counting, and the final result is rather insensitive to the actual strength of the field so long as it is strong enough. We may set

$$S_0 \equiv \sum_n^{n_c} \sum_l^{l_m} \sigma(\text{without field}) \propto n_c l_m (l_m+1) \;,$$

$$S_F \equiv \sum_n^{n_c} \sum_m^{l_m} \sum_\kappa \sigma(\text{with field}) \propto n_c^2 l_m \;.$$

With $l_m \approx 7$ and $n_c = 80$, we then have the enhancement factor

$$S_F/S_0 \cong n_c/(l_m+1) \approx 10 \;,$$

TABLE I. Comparison of the scattering parameters for the Ca^{1+} and Mg^{1+} cases. A rough consistency check is made between the two calculations, demonstrating the various factors in Eq. (8) that determine the total DR cross sections. The numbers in parentheses denote powers of 10.

Parameters	Ca	Mg
A_r (sec^{-1})	1.60(+8)	2.80(+8)
e_c (max)	3.1 eV	4.4 eV
n_c	80	64
Δe_c	0.3 eV	0.3 eV
$\sum_\sigma^{\text{total}}$	1.8(−17) cm^2	8.0(−18) cm^2
$\sum_\sigma^{\text{cutoff}}$	2.31(−18) cm^2	
$\sum_{\sigma^{\text{cutoff}}_{\text{folded}}}$	1.6(−18) cm^2 1.0(−18) cm$^{2\,a}$	2.0(−18) cm^2
$\sum_\sigma^{\text{Expt.}}$	1.8(−17) cm^2	1.2(−17) cm^2
Discrepancy (without field)	$7 \sim 18^a$	6

[a]For $\Delta e_c = 0.5$ eV.

which roughly accounts for the discrepancy, to within a factor of 2. A more careful study of the field effect is in progress.

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