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Dielectronic recombination for metastable O VII and C V ions

Yukap Hahn and R. Bellantone
Department of Physics, University of Connecticut, Storrs, Connecticut 06269
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Dielectronic recombination cross sections for the metastable O VII ions are calculated and found to be extremely large, of the order of 10^{-15} cm^2 for the individual resonances. The rates are at the level of 10^{-9} cm^3/sec. With some field enhancement and assuming that the initial ion beam is a mixture of metastable $1s2s$ (^1S and ^3S) states, the overall feature of the recent experimental data of Andersen *et al.* [Phys. Rev. Lett. **62**, 2656 (1989)] is reproduced, including the broad peaks at the incident-electron kinetic energies of 4.7 and 12.5 eV, and partially also at 2.5 and 6.8 eV. With a slightly different mixture, the C V data are well reproduced.

I. INTRODUCTION

The dielectronic recombination process[1,2] (DR) has been the subject of much experimental[3,4] and theoretical[5–7] studies in recent years, because of its intrinsic interest as a dominant resonant phenomenon both in electron-ion and ion-atom collision processes. It also has important applications to the study of laboratory and astrophysical plasmas. In particular, the experimental data[3,4] on DR with electron capture to high Rydberg states (HRS) are strongly affected by external electric field, which may be present in the interaction region during the capture. The field enhancement and HRS cutoff of the DR cross sections by electric field, and often strong configuration mixing effect, are routinely included in the analysis of data.[2]

Very recently, a precise experimental measurement was reported[8] in which the initial ion beam of O^{6+} (and also C^{4+}) was prepared in the metastable states of $1s2s$. Precise state-selective measurements of the DR cross section were made with an energy resolution of nearly 0.1 eV. In addition to extremely sharp lines of width 0.1–0.3 eV, several large and wide peaks were observed at the incident-electron kinetic energy $e_c = 2.5$, 4.7, 6.8, and 12.5 eV, of widths 1–2 eV.

We present in this report a theoretical calculation of the DR cross sections for the metastable O^{6+} ions, and show that (a) the cross sections are extremely large, of the order of 10^{-15} cm^2, even for the individual resonance states involving low-lying Rydberg states, with $\Delta e_c = 0.1$ eV. This is translated into the DR rates of 10^{-9} cm^3/sec, and roughly an additional factor of 10 larger with field enhancement. These values are 1000 times larger than any previous DR cases studied. The electric field in the interaction region was estimated[8] to be of the order of 1–2 V/cm. (b) The recently measured cross-section profile[8] can be explained in terms of sizable mixture of metastable $1s2s$ singlet and triplet states in the ion beam. The effect of configuration interaction and intermediate coupling was tested and found to be small for the overall cross section, although the individual states are sometimes severely affected.[9]

The C V data are also analyzed by the same procedure, and, with a slightly different mixture of the metastable singlet and triplet states in the initial beam, an excellent agreement is obtained with experiment.

II. DIELECTRONIC RECOMBINATION

The process of interest here is described as

$$\begin{aligned} 1s2s(^{1,3}S)+e_c \to 1s2p(^{1,3}P)n &\to 1s^2nl+\gamma \\ &\to 1s^22p+\gamma' \\ &\to 1s2s(^1S)nl \to 1s^22s+\gamma'' . \end{aligned} \qquad (1)$$

We concentrate our discussion on O VII, where peculiar broad peaks were observed.

The energy splitting between the core states ($1s2s$, $1s2p$) are such that, as measured from the $1s2s\,^3S$, $E(1s2p\,^3P)=0.557$ Ry, $E(1s2s\,^1S)=0.571$ Ry, and $E(1s2p\,^1P)=0.948$ Ry. The energy difference between $1s2s\,^1S$ and $1s2p\,^1P$ is 0.368 Ry. These values determine the corresponding ionization thresholds of the three-electron intermediate states. Because of the small excitation energies involved, the captured electron will occupy HRS with large n. We define the different channels as

$$\begin{aligned} &\text{I. } 1s2s(^1S)+e_c \to 1s2p(^1P)nl,\ n \gtrsim 11 \text{ and } l \lesssim 11, \\ &\text{II. } 1s2s(^3S)+e_c \to 1s2p(^1P)nl,\ n \gtrsim 7 \text{ and } l \lesssim 4, \\ &\text{III. } 1s2s(^3S)+e_c \to 1s2p(^3P)nl,\ n \ge 9 \text{ and } l \lesssim 3, \\ &\text{IV. } 1s2s(^3S)+e_c \to 1s2s(^1S)nl,\ n \ge 8 \text{ and } l \lesssim 3. \end{aligned} \qquad (2)$$

For a short-lived $1s2p(^3P)$ state as the initial state, we can also define two additional channels:

$$\begin{aligned} &\text{V. } 1s2p(^3P)+e_c \to 1s2p(^1P)nl,\ n \gtrsim 10 \text{ and } l \lesssim 5, \\ &\text{VI. } 1s2p(^3P)+e_c \to 1s2s(^1S)nl,\ n \gtrsim 40 \text{ and } l \lesssim 4. \end{aligned} \qquad (2')$$

The DR theory was summarized in Ref. 1, where the DR cross section was defined in isolated resonance approximation and averaged over an energy bin of size Δe_c. The effect of electric field on the DR cross section and rate coefficient is reviewed in Ref. 2. The general approach adopted here closely follows the theory outlined in these two references.

The relevant energy levels are shown in Fig. 1, from which all possible radiative and Auger channels are deduced for each intermediate state. In order to analyze the experimental data,[8] we assume that (i) the intensity of the original beam is composed of mixtures of the following states:

$$I_{\rm beam} = F_0(1s^2\,{}^1S) + F_1(1s2s\,{}^1S) + F_3(1s2s\,{}^3S)\,. \qquad (3)$$

Since the experiment does not specify the beam composition, the beam-mixing constants F's could be determined here such that the relative intensity of each of the channels is consistent with the experimental data. (ii) The maximum field enhancement in the interaction region is given by the enhancement factor r_F which is defined for each principal quantum number n of the intermediate states as[6]

$$r_F = n/(l_{\rm max}+1)\,, \qquad (4)$$

where $l_{\rm max}$ is to be determined by explicit calculations of the DR cross sections involving high-l values. The field enhancement affects the cross sections most severely for those intermediate states which lie at energies just below the ionization thresholds for each channel.

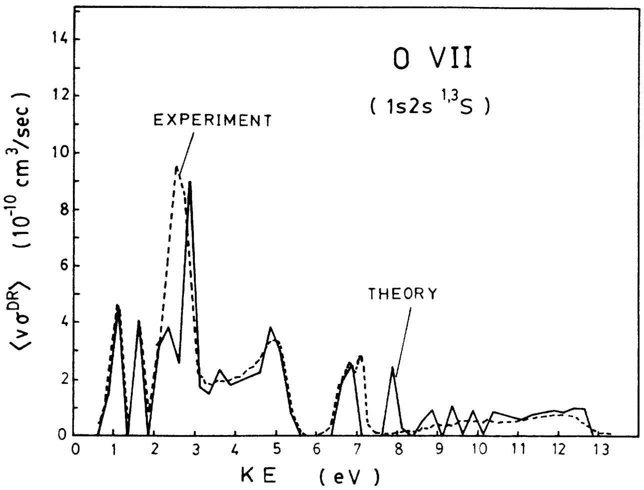

FIG. 2. The velocity-weighted DR cross sections $\langle v_c\sigma^{\rm DR}\rangle$ in units of 10^{-10} cm^3/sec are given for O VII, with the initial mixture of the beam as described by Eq. (2) and $F_0=0$, $F_1=0.011$, and $F_3=0.75$. The field enhancement factor $r=0.0$ was used, but $r\lesssim 0.1 r_F$ was also acceptable. The solid curve is the theoretical result and the dashed curve is the experimental data of Ref. 8.

III. RESULTS

The method of calculation employed in this paper was described earlier in Refs. 1 and 2; nonrelativistic Hartree-Fock wave functions were used in LS coupling. All the term energies and relevant Auger and radiative probabilities were calculated using Cowan's RCN/RCG code for the intermediate states with $l<6$. For both C^{4+} and O^{6+}, the energies obtained this way were not accurate enough, and the ionization threshold energies were adjusted using the more accurate values, as is stated earlier and shown in Fig. 1. For higher-l contributions, the MATRIX code was used and then matched to the values at lower l. It is important that all the open Auger channels are properly incorporated, including important Coster-Kronig channels.

The resulting velocity-weighted cross sections with field

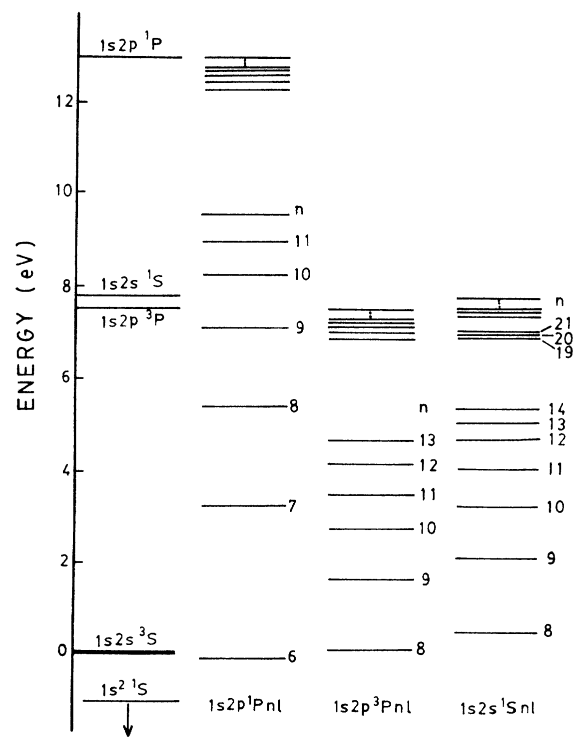

FIG. 1. The energy levels relevant to the DR process for the oxygen VII ions are presented, from which possible radiative and Auger transitions for the intermediate individual resonance states may be determined.

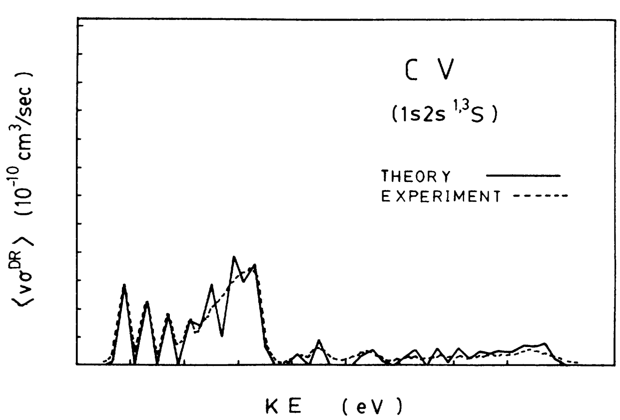

FIG. 3. The velocity-weighted DR cross sections $\langle v_c\sigma^{\rm DR}\rangle$ in units of 10^{-10} cm^3/sec are given for C V, with the initial mixture of the beam as described by Eq. (2) and $F_0=0$, $F_1=0.012$, and $F_3=0.30$. The field enhancement factor $r=0.0$ was used, but $r\lesssim 0.1 r_F$ was also acceptable. The solid curve is the theoretical result and the dashed curve is the experimental data of Ref. 8.

enhancement and field cutoff at $n=60$ are shown in Fig. 2 and compared with experimental data.[8] The incoming beam flux is taken to be $F_0=0$, $F_1=0.011$, and $F_3=0.75$. This is consistent with the experimental condition, with an uncertainty of ± 0.002 for F_1 and ± 0.25 for F_3. Approximate mixture of the metastable states in the experiment was estimated to be $F_1=0.01$–0.02 and $F_3=0.5$–0.8. The field enhancement factor $r \lesssim 0.2 r_F$ is also acceptable. The l_{max} used are $l_{max}=7.5$, 2.5, 1.5, 1.5, and 3, respectively, for the five channels in (2).

The gross features of the experimental data for O VII are reasonably well reproduced, including the peaks at 4.7 and 12.5 eV. The two peaks at 2.5 and 6.8 eV are only partially explained, with a secondary peak around 7 eV replaced by a new peak at 8 eV. By varying F_1, F_3, and r, we can alter the shape of the spectrum somewhat.[10]

Figure 3 contains the result of the calculation of C V, where $F_1=0.012$, $F_3=0.30$, and $r=0.0$ were used. We note that with $F_3 \gtrsim 0.6$, peaks similar to those in O VII at 2.5 eV show up around 3–4 eV. It is not clear why the mixture F_3 of the $1s2s\,^3S$ state was different in the two ions in the experiment.

IV. CONCLUSION

The extremely accurate DR data of Andersen *et al.*[8] have been explained in terms of the field enhancement, field cutoff, and a proper mixing of the initial beam in terms of the $1s2s\,^1S$ and ^3S metastable states. The calculated cross sections are extremely large, of the order of 10^{-16} cm^2 for the individual resonance peaks. The wide peaks in the regions of 4.7 and 12 eV, and 2.5 and 6.8 eV, are reasonably well explained. The carbon data are also in agreement with theory, where the peaks corresponding to those at 2.5 and 6.8 eV are absent. The details of these calculations, and the cross-section data will be reported elsewhere.[10] A result similar to ours was reported recently by Badnell.[11]

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