# Dielectronic recombination from the ground and excited states of $C^{4+}$ and $O^{6+}$

# N. R. Badnell\*

Atomic Weapons Establishment, Aldermaston, Reading, RG74PR, United Kingdom

M. S. Pindzola

Department of Physics, Auburn University, Auburn, Alabama 36849

#### D. C. Griffin

Department of Physics, Rollins College, Winter Park, Florida 32789 (Received 21 August 1989)

We have calculated dielectronic recombination (DR) cross sections from the ground state  $(1 \, {}^{1}S)$  and excited states  $(2 \, {}^{3}S, 2 \, {}^{1}S, \text{ and } 2 \, {}^{3}P)$  of the He-like ions  $C^{4+}$  and  $O^{6+}$  in the *LS*-coupling and intermediate-coupling approximations, using the program AUTOSTRUCTURE. We find the effects of configuration interaction, intermediate coupling, and external electric fields to be small. We compare our results with the recent high-resolution measurements of DR from the excited states of these ions by Andersen *et al.* [Phys. Rev. Lett. **62**, 2656 (1989) and Phys. Rev. A **41**, 1293 (1990)] by convoluting our cross sections with their electron velocity distribution. For the case of  $C^{4+}$ , we obtain excellent agreement when we choose the  $2 \, {}^{3}S$  to  $2 \, {}^{1}S$  population ratio to be 18. For the case of  $O^{6+}$ , we obtain good agreement with experiment with a  $2 \, {}^{3}S$  to  $2 \, {}^{1}S$  population ratio of 70, except in the 6- to 8-eV energy region, where a model calculation indicates that coupling between resonances via the continuum may be important. By comparing experiment with theory, we have also estimated the metastable fraction of the  $2 \, {}^{3}S$  term to be 70% in  $C^{4+}$  and 20% in  $O^{6+}$ . The reason for this large difference is not understood.

## I. INTRODUCTION

The process of dielectronic recombination (DR) has long been recognized as the dominant electron-ion recombination mechanism for laboratory and astrophysical plasmas.<sup>1</sup> Dielectronic recombination has been studied in electron-ion merged-beam experiments,<sup>2</sup> by observation of satellites in tokamaks,<sup>3</sup> and via resonanttransfer excitation<sup>4</sup> in ion-atom collision experiments. All have suffered, to an extent, from poor energy resolution and little has been seen of the resonance structure, particularly in low charge states. High-resolution experimental results are required to differentiate between various theoretical approximations and indeed between the same approximations (in principle) incorporated into different computer codes.

Recently, an electron cooler at the University of Aarhus was utilized by Andersen *et al.*<sup>5,6</sup> to make high-resolution DR measurements in carbon and oxygen ions. Their results<sup>6</sup> for the Li-like ions  $C^{3+}$  and  $O^{5+}$  are in good agreement with the results of field-dependent calculations by Griffin, Pindzola, and Krylstedt.<sup>7</sup> In this paper, we present the results of calculations of DR cross sections from the 1<sup>1</sup>S, 2<sup>3</sup>S, 2<sup>3</sup>P, and 2<sup>1</sup>S states of the He-like ions  $C^{4+}$  and  $O^{6+}$  in the *LS*-coupling and intermediate-coupling (IC) approximations using the program AUTOSTRUCTURE.<sup>8,9</sup>

The experiments by Andersen *et al.*<sup>5,6</sup> do not measure cross sections directly but rather a quantity  $\langle v\sigma \rangle$ , which is the electron velocity times the cross section convoluted

with an electron velocity distribution function. Furthermore, their measurements were carried out at relative electron-ion energies such that the only initial states that could contribute to DR are the  $2^{3}S$  and  $2^{1}S$  metastables (the  $2^{3}P$  state must also be populated, but decays by radiative emission to  $2^{3}S$  before the ion beam reaches the interaction region). However, they did not determine the composition of their ion beams and so they reported relative values of  $\langle v\sigma \rangle$ .

Rate coefficients have been calculated in the past for DR from the 1 <sup>1</sup>S ground state of C<sup>4+</sup> and/or O<sup>6+</sup> by Bely-Dubau *et al.*,<sup>10</sup> Hahn,<sup>11</sup> Younger,<sup>12</sup> and by Chen.<sup>13</sup> The recent review article by Hahn and LaGattuta<sup>14</sup> provides a general guide to the current state of experiment and theory for DR and related processes.

The remainder of this paper is arranged as follows. In Sec. II, we outline the theory behind the calculations, and in Sec. III, we describe its application to the case of Helike ions. In Sec. IV, we present our rate coefficients from the ground state of  $C^{4+}$  and  $O^{6+}$ . We also present calculations of the quantity  $\langle v\sigma \rangle$  from both the ground and excited states of these ions and compare our results from the excited states with the measurements of Andersen *et al.*<sup>5,6</sup> A brief conclusion is given in Sec. V.

# **II. THEORY**

The energy-averaged dielectronic recombination cross section for a given initial state i through the intermediate state j is given by

41 2422

## DIELECTRONIC RECOMBINATION FROM THE GROUND AND ...

$$\overline{\sigma}_{d}(i;j) = \frac{(2\pi a_{0}I)^{2}}{E_{c}\Delta E_{c}} \frac{\omega(j)}{2\omega(i)} \times \frac{\tau_{0}\sum_{k}A_{r}(j\rightarrow k)\sum_{l}A_{a}(j\rightarrow i,E_{c}l)}{\sum_{h}A_{r}(j\rightarrow h) + \sum_{m,l}A_{a}(j\rightarrow m,E_{c}l)}, \quad (1)$$

where  $E_c$  is the energy of the continuum electron, which is fixed by the position of the resonances;  $\Delta E_c$  is an energy bin width, larger than the largest resonance width but small compared to the experimental width; and I is the ionization potential energy of hydrogen.  $\omega(j)$  is the statistical weight of the (N + 1)-electron ion doubly excited state,  $\omega(i)$  is the statistical weight of the N-electron ion initial target state, and  $(2\pi a_0)^2 \tau_0 = 2.6741 \times 10^{-32}$  cm<sup>2</sup> s. With respect to the radiative rates  $A_r$ , the sum over k in Eq. (1) is over all states which are stable against autoionization, while the sum over h is over all possible states. For the autoionizing rates  $A_a$ , the sum over m includes all possible states of the N-electron ion.

The total dielectronic recombination rate coefficient may be written in terms of the energy-averaged cross section as

$$\alpha_d(i; \text{tot}) = \left(\frac{4\pi a_0^2 I}{k_B T}\right)^{3/2} \frac{1}{(2\pi a_0 I)^2 \tau_0} \times \sum_j E_c \Delta E_c \overline{\sigma}_d(i; j) e^{-E_c / k_B T}, \qquad (2)$$

where  $(4\pi a_0^2)^{3/2} = 6.6011 \times 10^{-24} \text{ cm}^3$ .

Equations (1) and (2) may be evaluated in the LScoupling and IC approximations using AUTOSTRUC-TURE,<sup>8</sup> as detailed in the paper by Badnell and Pindzola.<sup>9</sup>

# III. APPLICATION TO THE He-LIKE IONS $C^{4+}$ AND $O^{6+}$

For DR from the  $1^{1}S$  ground state, we consider the dielectronic capture reactions

$$1s^{2} S + kl_i \rightarrow \begin{cases} 1s 2s (3, 1S)nl, & l = l_i \\ 1s 2p (3, 1P)nl, & l = l_i \pm 1 \end{cases}$$

TABLE I. Dielectronic recombination rate coefficients for the 1<sup>1</sup>S state of C<sup>4+</sup> and O<sup>6+</sup>, in units of cm<sup>3</sup>/s. Numbers in square brackets represent powers of 10; for example,  $6.14[-13]=6.14\times10^{-13}$ .

$\log_{10}[T(K)]$	C <sup>4+</sup>	O <sup>6+</sup>
6.0	6.14[-13]	1.24[-13]
6.2	1.08[-12]	5.88[-13]
6.4	1.19[-12]	1.25[-12]
6.6	9.88[-13]	1.56[-12]
6.8	6.80[-13]	1.40[-12]
7.0	4.16[-13]	1.01[-12]
7.2	2.37[-13]	6.40[-13]
7.4	1.29[-13]	3.71[-13]
7.6	6.78[-14]	2.04[-13]
7.8	3.51[-14]	1.09[-13]
8.0	1.79[-14]	5.64[-14]

while for the 2  ${}^{3}S$  metastable term, we have

$$1s2s \ {}^{3}S + kl_{i} \rightarrow \begin{cases} 1s2s \ ({}^{1}S)nl, & l = l_{i} \\ 1s2p \ ({}^{3,1}P)nl, & l = l_{i} \pm 1 \end{cases}$$

and for the  $2^{1}S$  metastable term, the possible transitions are

$$1s2s \, {}^{1}S + kl_{i} \rightarrow 1s2p({}^{1}P)nl, \ l = l_{i} \pm 1$$

**a** 1

The doubly excited states can decay by the autoionization transitions

$$1s2s ({}^{3}S)nl \rightarrow 1s^{2} {}^{1}S + kl_{c}, \quad l_{c} = l$$

$$1s2s ({}^{1}S)nl \rightarrow \begin{cases} 1s^{2} {}^{1}S + kl_{c}, \quad l_{c} = l \\ 1s2s {}^{3}S + kl_{c}, \quad l_{c} = l \\ n \geq 7 \text{ for } C^{4+}, \quad n \geq 8 \text{ for } O^{6+} \end{cases}$$

$$1s2p ({}^{3}P)nl \rightarrow \begin{cases} 1s^{2} {}^{1}S + kl_{c}, \quad l_{c} = l \pm 1 \\ 1s2s {}^{3}S + kl_{c}, \quad l_{c} = l \pm 1 \\ 1s2s {}^{3}S + kl_{c}, \quad l_{c} = l \pm 1 \end{cases}$$

$$1s2p ({}^{3}P)nl \rightarrow \begin{cases} 1s^{2} {}^{1}S + kl_{c}, \quad l_{c} = l \pm 1 \\ 1s2s {}^{3}S + kl_{c}, \quad l_{c} = l \pm 1 \\ 1s2s {}^{3}S + kl_{c}, \quad l_{c} = l \pm 1 \\ 1s2s {}^{3}S + kl_{c}, \quad l_{c} = l \pm 1 \\ 1s2s {}^{3}S + kl_{c}, \quad l_{c} = l \pm 1 \\ 1s2s {}^{1}S + kl_{c}, \quad l_{c} = l \pm 1 \\ 1s2s {}^{1}S + kl_{c}, \quad l_{c} = l \pm 1 \\ 1s2s {}^{1}S + kl_{c}, \quad l_{c} = l \pm 1 \\ 1s2p ({}^{1}P)nl \rightarrow \end{cases}$$

$$1s2p ({}^{1}P)nl \rightarrow \begin{cases} n \geq 8 \text{ for } C^{4+}, \quad n \geq 10 \text{ for } O^{6+} \\ 1s2p {}^{3}P + kl_{c}, \quad l_{c} = l, l \pm 2 \\ n \geq 9 \text{ for } C^{4+}, \quad n \geq 10 \text{ for } O^{6+} \end{cases}$$

If the doubly excited states radiatively decay to a bound state, the DR process is complete. The possible radiative transitions are

$$1s2s ({}^{3,1}S)nl \to 1s^{2}2s + h\nu, \quad l = 1$$
  

$$1s2p ({}^{3}P)nl \to 1s^{2}2p + h\nu, \quad l = 1$$
  

$$1s2p ({}^{1}P)nl \to \begin{cases} 1s^{2}2p + h\nu, \quad l = 1\\ 1s^{2}nl + h\nu, \quad all \ l. \end{cases}$$

Since the radiative rates from  $1s2s({}^{3}S)nl$ ,  $1s2s({}^{1}S)nl$ , and  $1s2p({}^{3}P)nl$  are quite small compared to the very large rates associated with the transitions  $1s2p({}^{1}P)nl$  $\rightarrow 1s^{2}nl$ , DR in these ions is dominated by dielectronic capture into the  $1s2p({}^{1}P)nl$  Rydberg states. However, for more highly ionized He-like ions where the spin-orbit interaction mixes the  $1s2p({}^{3}P)nl$  and  $1s2p({}^{1}P)nl$  states, dielectronic capture into  $1s2p({}^{3}P)nl$  is also important.

In addition, for dielectronic recombination from the  $1^{1}S$  ground state, dielectronic capture into the  $1s2s^{2}$ , 1s2s2p, and  $1s2p^{2}$  configurations must also be included. The radiative transitions from these states are

$$1s 2s 2p \rightarrow 1s^{2} 2s + hv ,$$
  

$$1s 2p^{2} \rightarrow 1s^{2} 2p + hv ,$$
  

$$1s 2s^{2} \rightarrow 1s^{2} 2p + hv ,$$



FIG. 1. Theoretical  $\langle v\sigma \rangle$  (relative electron velocity times the cross section convoluted with the Aarhus velocity distribution) for DR from the 1<sup>1</sup>S term of C<sup>4+</sup>.

where the last transition is possible through strong mixing of  $1s2s^2$  with  $1s2p^2$ .

We sum the above processes over nl in the LS-coupling and IC approximations up to n = 1000 for the zero-field, low-density rate coefficients; while for the calculations of  $\langle v\sigma \rangle$ , we sum only up to  $n_{max} = 45$  for C<sup>4+</sup> and  $n_{max} = 60$ for O<sup>6+</sup>, to take into account field ionization in the analyzing region of the Aarhus experiment (Andersen and co-workers<sup>5,6</sup>). The values of  $n_{max}$  were determined from the semiclassical field-ionization formula

$$n_{\max} = \left[ \frac{6.2 \times 10^8}{E} q^3 \right]^{1/4} , \qquad (3)$$

where E is the electric field in the analyzing region in V/cm and q is the charge of the ion before recombination. The radial wave functions were evaluated as before<sup>9</sup> using scaled Thomas-Fermi-Dirac-Amaldi model potentials, which have proved reliable in the past.<sup>15</sup>

#### **IV. RESULTS**

# A. Maxwellian rate coefficients

In Table I, we present our low-density, zero-field rate coefficients for DR from the 1 <sup>1</sup>S ground state of C<sup>4+</sup> and



FIG. 2. Theoretical  $\langle v\sigma \rangle$  for DR from the 2<sup>3</sup>S term of C<sup>4+</sup>. Solid curve, all autoionizing transitions retained; dashed curve, excluding transitions to the 2<sup>1</sup>S and 2<sup>3</sup>P continua.



FIG. 3. Theoretical  $\langle v\sigma \rangle$  for DR from the 2 <sup>1</sup>S term of C<sup>4+</sup>.

 $O^{6+}$ . Our *LS*-coupling and IC results differ by less than 1% and agree with those of Chen<sup>13</sup> to within 2% at the temperature of the peak value. The Burgess formula<sup>16</sup> overestimates the peak rate coefficient by a factor of 2.8 for C<sup>4+</sup> and 2.2 for O<sup>6+</sup>.

#### B. Convoluted cross sections

In Figs. 1-10, we present calculations of the relative electron velocities times our *LS*-coupling, energy-averaged DR cross sections convoluted with the Aarhus velocity distribution  $\langle v\sigma \rangle$ .<sup>6</sup> The results obtained using IC energy-averaged cross sections differ from these by less than 5%. The *n* values given in the figures indicate the various 2<sup>1</sup>*Pnl* resonances.

Figures 1-3 contain our results for DR from the 1  ${}^{1}S$ , 2  ${}^{3}S$ , and 2  ${}^{1}S$  terms of C<sup>4+</sup>. Although the 2  ${}^{3}P$  will not be populated within the interaction region of the Aarhus experiment, for completeness, we also show our calculation of DR from this term in Fig. 4. If we had not imposed an  $n_{\text{max}}$  of 45 to account for field ionization in the analyzing region, the difference would be negligible in the case of



FIG. 4. Theoretical  $\langle v\sigma \rangle$  for DR from the 2<sup>3</sup>P term of C<sup>4+</sup>.

 $1^{1}S$ , but there would be a small extension of the highenergy tail for  $2^{3}S$ ,  $2^{1}S$ , and  $2^{3}P$ .

In Fig. 2, we demonstrate the importance of autoionization from the  $2^{1}Pnl$  resonances to the  $2^{3}P$  continuum for  $n \ge 9$  and the  $2^{1}S$  continuum for  $n \ge 8$ . The solid curve is the calculation with all autoionizing transitions included, while the dashed curve is the result if we exclude autoionization to  $2^{3}P$  and  $2^{1}S$ .

Although the values of  $\langle v\sigma \rangle$  for DR from both 2<sup>3</sup>S and  $2^{1}S$  are large because of the relatively small excitation energies involved and the very large radiative rate associated with the  $2^{1}P \rightarrow 1^{1}S$  transition, those from  $2^{1}S$ shown in Fig. 3 are about a factor of 100 larger than those for  $2^{3}S$  shown in Fig. 2. This is due to the fact that the  $1s2s^{3}S + k_{i}l_{i} \rightarrow 1s2p(^{1}P)nl$  spin-changing dielectronic-capture transitions, which only go through exchange, have a negligible cross section for high values of l $(l \geq 4),$ while the dipole-allowed transitions  $1s 2s {}^{1}S + k_{i}l_{i} \rightarrow 1s 2p ({}^{1}P)nl$  have non-negligible contributions to the cross section up to about l = 12.

In the experiment of Andersen *et al.*,<sup>6</sup> the population fraction of the  $2^{3}S$  and  $2^{1}S$  metastable states is unknown, and they report their values of  $\langle v\sigma \rangle$  for some mixture of these states on a relative scale. In order to compare our calculated cross sections with experiment, we have varied the ratio of the  $2^{3}S$  to  $2^{1}S$  population fractions until we obtained the best agreement with their measurement. These results are plotted, along with the experimental points, on an arbitrary scale in Fig. 5. The ratio of 18 for the  $2^{3}S$  to  $2^{1}S$  populations, used to generate this figure, was found to give the best agreement with experiment.

The overlapping contributions from the two initial metastable states shown in Fig. 5 make the theoretical results exceedingly sensitive to errors in the relative energies of  $2^{3}S$  and  $2^{1}S$ . A relative error of 0.1 eV is enough



FIG. 5. Comparison of theoretical and experimental  $\langle v\sigma \rangle$  for DR from the metastable states of C<sup>4+</sup> on an arbitrary scale. To convert to the scale used in Ref. 6, multiply by 61.7. Solid curve, theory with the ratio of the population fractions of 2<sup>3</sup>S to 2<sup>1</sup>S equal to 18; closed circles, experimental points from Andersen, Bolko, and Kvistgaard, Ref. 6.



FIG. 6. Theoretical  $\langle v\sigma \rangle$  for DR from the 1<sup>1</sup>S term of O<sup>6+</sup>.

to produce qualitatively different results in the magnitude of the sum of the contributions from the various resonances as well as in contributions from individual resonances that lie close to the threshold of an additional autoionization channel. Therefore the  $2^{3}S - 2^{1}P$  and  $2^{1}S - 2^{1}P$  separations were set to the experimental values;<sup>17</sup> with these energy differences, excellent agreement between experiment and theory was obtained, but all the experimental resonances were low by 0.2 eV, with respect to the theoretical positions. To compensate for this apparent error in the experimental resonance energies and allow for an easier comparison of the size of the measured and experimental resonant contributions, we merely shifted the zeros of the energy axes for the theoretical curves by this amount. Such a shift, of course, has no effect on the calculated magnitude of  $\langle v\sigma \rangle$ .

2. O<sup>6+</sup>

Figures 6-9 contain our results for DR from the 1  ${}^{1}S$ , 2  ${}^{3}S$ , 2  ${}^{1}S$ , and 2  ${}^{3}P$  terms of O<sup>6+</sup>, while in Fig. 10, we compare our theoretical results with the experimental results of Andersen *et al.*<sup>5,6</sup> This time we found that a factor of 70 for the ratio of the 2  ${}^{3}S$  to 2  ${}^{1}S$  populations yield-



FIG. 7. Theoretical  $\langle v\sigma \rangle$  for DR from the 2<sup>3</sup>S term of O<sup>6+</sup>. Solid curve, all autoionizing transitions retained; dashed curve, excluding transitions to the 2<sup>1</sup>S and 2<sup>3</sup>P continua.



FIG. 8. Theoretical  $\langle v\sigma \rangle$  for DR from the 2<sup>1</sup>S term of O<sup>6+</sup>.

ed the best agreement between experiment and theory. This would imply that the  $2 {}^{1}S$  population drops by a factor of 4 relative to the  $2 {}^{3}S$  population in going from C<sup>4+</sup> to O<sup>6+</sup>. However, since theoretical predictions<sup>18</sup> for the lifetime of the  $2 {}^{1}S$  state drop by a factor of 5 in going from C<sup>4+</sup> to O<sup>6+</sup>, we do not find surprising this substantial decrease in the  $2 {}^{1}S$  population in O<sup>6+</sup> relative to C<sup>4+</sup>. Again we adjusted our core excitation energies to the observed values, <sup>19</sup> but this time, no adjustment of the zeros in the theoretical energy axes was required to obtain a match with experimental resonant positions.

The agreement between theory and experiment is not quite as good for  $O^{6+}$  as it was for  $C^{4+}$ ; there is a discrepancy around 2 eV, but again we find that the overlapping contributions from the 2  ${}^{3}S$  and 2  ${}^{1}S$  initial states to be very sensitive to the positions of the resonances. Nevertheless, except for the 6- to 8-eV energy region, all the main features of the experiment can be explained by the present calculation.

We now consider possible effects that might explain the remaining discrepancies. One possibility is that Stark mixing in the high-*n* states by the small field in the interaction region, which is believed to be less than 5 V/cm,<sup>6</sup> could enhance the cross section.<sup>20</sup> However, in order for such fields to have an appreciable effect on DR,



FIG. 9. Theoretical  $\langle v\sigma \rangle$  for DR from the 2<sup>3</sup>P term of O<sup>6+</sup>.

the autoionizing rates to the  $2^{3}S$  and  $2^{1}S$  continua must be larger than the radiative rates.<sup>21</sup> We find that this condition does not hold for the He-like ions. For example, for n = 20, the autoionizing rates from the  $1s2p({}^{1}P)nl$  resonances are smaller than the radiative rates to the  $1s^{2}nl$  bound states; thus field effects would be expected to be small, and definitely cannot be estimated by simple counting arguments.<sup>22</sup> We also calculated the maximum field enhancement for  $O^{6+}$  using the configuration-average approximation<sup>23</sup> and found it to be negligible.

The main discrepancy is between 6 and 8 eV where the contributions from the  $1s2s({}^{3}S) \rightarrow 1s2p({}^{1}P)9l$  dielectronic capture from the calculation described above are much smaller and narrower than experiment. For  $C^{4+}$ , and other features in  $O^{6+}$ , we have seen that the broadening due to the different positions of the various l states and the term splittings, together with the broadening due to the relative velocity distribution, is sufficient to match theory and experiment. In this energy region this is not true.

It has been suggested<sup>24</sup> that the resonances associated with 2<sup>1</sup>P term interact with those associated with 2<sup>1</sup>S and 2<sup>3</sup>P, either directly through configuration interaction of the doubly excited states, or via coupling with the adjacent continua. In cases where the radiative rates are much larger than the autoionizing rates, the DR cross section associated with a given excitation  $i \rightarrow j$  is proportional to  $\sum_{i} A_a(j \rightarrow i, E_c l)$  [see Eq. (1)]. For such a situation, interaction with an adjacent Rydberg series of resonances could transfer some radiative strength to that series without affecting the strength of DR associated with the original  $i \rightarrow j$  excitation. Thus we might expect



FIG. 10. Comparison of theoretical and experimental  $\langle v\sigma \rangle$  for DR from the metastable states of O<sup>6+</sup> on an arbitrary scale. To convert to the scale used in Ref. 6, multiply by 15.0. Solid curve, theory with the ratio of the population fraction of  $2^{3}S$  to  $2^{1}S$  equal to 70; dashed curve, theory with the effects of the interactions via the continua between the  $2^{1}P9l$  resonances and the resonances associated with  $2^{1}S$  and  $2^{3}P$ , from a model calculation; solid circles, experimental points from Andersen *et al.* (Refs. 5 and 6).

that, since the radiative rates are somewhat larger than the autoionizing rates for the  $2^{1}P9l$  resonances, the DR cross section could be enhanced in this region through interaction of  $2^{1}P9l$  with the resonances associated with  $2^{1}S$  and  $2^{3}P$ .

In order to investigate the effects of direct configuration interaction in this energy region, we performed a model calculation of the interaction of  $2^{1}P9l$  with  $2^{1}S25l$  and  $2^{3}P25l$ . We found, by varying the relative separation between the resonances, that the resonances associated with the  $2^{1}S$  and  $2^{3}P$  terms had to be within 0.02 eV of the  $2^{1}P9l$ , before the DR cross section was enhanced significantly. This implies that direct bound-bound configuration interaction could enhance, but not broaden, the DR cross section in this vicinity.

However, mixing of these resonances through interaction with the adjacent continua (i.e., coupling of the bound channels) is likely to be stronger, and resonances further away from  $2^{1}P9l$  might be affected; this could, in principle, broaden and enhance the DR cross section. Unfortunately, to include such mixing through the continua would require a rather involved calculation. Nevertheless, a simplified model calculation can be performed to simulate such interactions. We assumed that the  $2^{1}Snl$  and the  $2^{3}Pnl$  resonances with  $n \ge 20$  interact sufficiently, through the adjacent continua, with the  $2^{1}P9l$  resonances to acquire radiative strength from the  $2^{1}P \rightarrow 1^{1}S$  channel. The  $2^{1}P9l$  DR cross section remained largely unaffected, but the enhancement and broadening due to the interaction with the resonances associated with  $2^{1}S$  and  $2^{3}P$  can be seen in Fig. 10 (dashed curves). It gives rise to the double peak structure seen by experiment. The amount of radiative strength transferred was fixed by matching to peak experimental value in the 6- to 8-eV range. However, multiconfiguration, close-coupling calculations would be required to prove that this experimental feature in  $O^{6+}$  can be explained in this way, and to show why such features apparently are not seen in the case of  $C^{4+}$ .

It was also suggested<sup>24</sup> that autoionization of the  $2^{1}Pnl$  resonances to the  $2^{1}S$  and  $2^{3}P$  continua would largely reduce the DR cross section above 8 eV. We see from Fig. 7 that autoionization to these excited states has some effect in O<sup>6+</sup>, although it is weaker than in the case of C<sup>4+</sup> (see Fig. 2); however, the calculated peak value at 12 eV is largely unaffected and is consistent with that observed by experiment (Fig. 10).

#### C. Ion-beam populations

As indicated earlier, we have adjusted the ratio of the  $2^{3}S$  to  $2^{1}S$  population fractions in  $C^{4+}$  and  $O^{6+}$  to obtain the best agreement with the experimental measurements of Andersen *et al.*,<sup>5,6</sup> and we have plotted our final results for  $\langle v\sigma \rangle$  on an arbitrary scale. Again, the sensitivity of the theoretical results to the overlapping contributions from the two initial metastable states means that we cannot change the ratio of the populations by more than 10% without producing significantly different results. However, Andersen, Bolko, and Kvistgaard present their results on a scale in which  $\langle v\sigma \rangle$  was calculated in terms of  $N^{q+}$ , the total number of ions in the in-

coming beam [Ref. 6, Eq. (11)]. By converting to their scale, and focusing on resonances that are due to either dielectronic capture from the  $2^{3}S$  term or the  $2^{1}S$  term, but not some mixture of the two, we can estimate the metastable fractions from our theoretical values of  $\langle v\sigma \rangle$ .

For  $O^{6+}$ , we obtain a value of 20% for the 2 <sup>3</sup>S population fraction and 0.3% for  $2^{1}S$ , with the remaining 80% of the ions in the  $1^{1}S$  ground state. Andersen, Bolko, and Kvistgaard<sup>6</sup> state that approximately 30% of the initial  $C^{4+}$  and  $O^{6+}$  ions should be in the 2<sup>3</sup>S metastable term. This estimate originates from measurements of Kx-ray emission for He-like  $F^{7+}$  produced by a thin poststripping foil from F ions emerging out of the EN tandem Van de Graff at Kansas State University.<sup>25</sup> However, examination of the data from Ref. 25, as well as data of K-Auger-electron production from He-like  $C^{4+}$ ,  $N^{5+}$ ,  $O^{6+}$ , and  $F^{7+}$ ,  $^{26}$  would indicate that 20% for the  $2^{3}S$  term in  $O^{6+}$  is quite reasonable. Furthermore, on the basis of the relative statistical weight and lifetime of the  $2^{1}S$  term, as well as the time of flight of the ion beam. Andersen, Bolko, and Kvistgaard<sup>6</sup> estimate that the fraction of initial ions in the  $2^{1}S$  term should be less than 1%. In light of the uncertainties in this estimate, a fraction of 0.3% also seems quite reasonable.

Using the same method for  $C^{4+}$ , we obtain a population fraction of 70% for  $2^{3}S$  and 4% for  $2^{1}S$ . The reason for these large differences in the predicted metastable fractions between  $C^{4+}$  and  $O^{6+}$  is that theory predicts a small increase in the cross section from the metastable states in going from  $C^{4+}$  to  $O^{6+}$  (compare Figs. 2 and 3 with Figs. 7 and 8) while the measured values of  $\langle v\sigma \rangle$ decrease substantially. One might expect about the same fraction of  $2^{3}S$  metastables in both ions, so this difference in the predicted values remains a mystery. However, we do not believe that this could be due to errors in the calculated cross sections for  $C^{4+}$ , since the theoretical methods used for both ions are identical.

# **V. CONCLUSIONS**

The high-resolution experiments by Andersen *et al.*<sup>5,6</sup> on DR from excited states of C<sup>4+</sup> and O<sup>6+</sup> are very well described by calculations using single-configuration *LS*-coupling zero-field approximations, except for the structure between 6 and 8 eV in O<sup>6+</sup>, where a model calculation indicates that coupling between resonances via the continuum may be important. The population fractions of metastable states determined by comparing the calculated and measured values  $\langle v\sigma \rangle$  appear quite reasonable in the case of O<sup>6+</sup>, but unexpectedly large in the case of C<sup>4+</sup>.

#### **ACKNOWLEDGMENTS**

We wish to thank P. F. Dittner and P. Hvelplund for a number of useful conversations. We would also like to thank L. H. Andersen for providing us with the  $C^{4+}$  data prior to publication. This work was supported in part by the Office of Fusion Energy, U.S. Department of Energy, under Contract No. DE-FG05-86ER53217 with Auburn University and Contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

\*Present address: Department of Physics, Auburn University, Auburn, Alabama 36849.

- <sup>2</sup>P. F. Dittner, S. Datz, H. F. Krause, P. D. Miller, P. L. Pepmiller, C. M. Fou, Y. Hahn, and I. Nasser, Phys. Rev. A 38, 2762 (1988).
- <sup>3</sup>F. Bombarda, R. Giannella, E. Kalne, G. J. Tallents, F. Bely-Dubau, P. Faucher, M. Cornille, J. Dubau, and A. H. Gabriel, Phys. Rev. A 37, 504 (1988).
- <sup>4</sup>J. A. Tanis, E. M. Bernstein, M. W. Clark, W. G. Graham, R. H. McFarland, T. J. Morgan, J. R. Mowat, D. W. Mueller, A. Müller, M. P. Stockli, K. H. Berkner, P. Gohil, R. J. McDonald, A. S. Schlachter, and J. W. Sterns, Phys. Rev. A 34, 2543 (1986).
- <sup>5</sup>L. H. Andersen, P. Hvelplund, H. Knudsen, and P. Kvistgaard, Phys. Rev. Lett. **62**, 2656 (1989).
- <sup>6</sup>L. H. Andersen, J. Bolko, and P. Kvistgaard, Phys. Rev. A **41**, 1293 (1990).
- <sup>7</sup>D. C. Griffin, M. S. Pindzola, and P. Krylstedt, Phys. Rev. A **40**, 6699 (1989).
- <sup>8</sup>N. R. Badnell, J. Phys. B 19, 3827 (1986).
- <sup>9</sup>N. R. Badnell and M. S. Pindzola, Phys. Rev. A **39**, 1685 (1989).
- <sup>10</sup>F. Bely-Dubau, J. Dubau, P. Faucher, and L. Steenman-Clark, J. Phys. B 14, 3313 (1981).
- <sup>11</sup>Y. Hahn, Phys. Scr. **T28**, 25 (1989).
- <sup>12</sup>S. M. Younger, J. Quant. Spectrosc. Radiat. Transfer 29, 67 (1983).

- <sup>13</sup>M. H. Chen, Phys. Rev. A 38, 6430 (1988).
- <sup>14</sup>Y. Hahn and K. J. LaGattutta, Phys. Rep. 166, 195 (1988).
- <sup>15</sup>N. R. Badnell and M. S. Pindzola, Phys. Rev. A **39**, 6165 (1989).
- <sup>16</sup>A. Burgess, Astrophys. J. 141, 1588 (1965).
- <sup>17</sup>C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) Circ. No. 3 (U.S. GPO Washington, D.C., 1970), Vol. 3.
- <sup>18</sup>R. K. Janev, L. P. Presnyakov, and V. P. Shevelko, *Physics of Highly Charged Ions* (Springer-Verlag, Berlin, 1985), p. 27.
- <sup>19</sup>C. E. Moore, Atomic Energy Levels (Ref. 17), circ. No. 3, Vol. 11.
- <sup>20</sup>D. C. Griffin, M. S. Pindzola, and C. Bottcher, Phys. Rev. A 33, 3124 (1986).
- <sup>21</sup>D. C. Griffin, M. S. Pindzola, and C. Bottcher, Atomic Excitation and Recombination in External Fields, edited by M. H. Nayfeh and C. W. Clark (Harwood Academic, New York, 1985).
- <sup>22</sup>I. Nasser and Y. Hahn, Phys. Rev. A 30, 1558 (1984).
- <sup>23</sup>D. C. Griffin, M. S. Pindzola, and C. Bottcher, Phys. Rev. A 31, 568 (1985).
- <sup>24</sup>K. Taulbjerg and J. Macek, Phys. Rev. Lett. 62, 2766 (1989).
- <sup>25</sup>M. Terasawa, T. J. Gray, S. Hagmann, J. Hall, J. Newcomb, P. L. Pepmiller, and P. Richard, Phys. Rev. A 27, 2868 (1983).
- <sup>26</sup>T. R. Dillingham, J. Newcomb, J. Hall, P. L. Pepmiller, and P. Richard, Phys. Rev. A **29**, 3029 (1984).

<sup>&</sup>lt;sup>1</sup>A. Burgess, Astrophys. J. **139**, 776 (1964).