Distorted-wave calculations of dielectronic recombination for C^{3+} and O^{5+} in small electric fields

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(Received 17 July 1989; revised manuscript received 16 August 1989)

The dielectronic recombination cross sections associated with the $2s \rightarrow 2p$ transition in Li-like carbon and oxygen ions in the presence of small electric fields have been calculated in the distorted-wave approximation. By convoluting the product of the electron velocity and the theoretical cross section with the experimental velocity distribution, we compare our calculations with recent measurements of high-resolution recombination rates $\langle v\sigma(v) \rangle$ by Andersen *et al.* With the exception of the magnitude of the low-energy peak due to the $2p4l$ resonances, the agreement between experiment and theory is excellent in C^{3+} for a field in the interaction region of just over 3 V/cm. In the case of O^{5+}, however, there is good agreement between experiment and theory for the low-Rydberg states, but there appear to be discrepancies between the measured rates and the theoretical rates for the high-Rydberg states, where the effects of fields are important.

In an earlier paper,[1] we reported on distorted-wave calculations of dielectronic recombination (DR) as a function of electric field strength for the $\Delta n = 0$ transitions in Li-like and Na-like ions. The results of these calculations have been compared to measurements of the DR rate $\langle v\sigma(v) \rangle$ as a function of electron energy made by Dittner *et al.* at Oak Ridge National Laboratory (ORNL).[2,3] In this set of experiments, the electric field in the interaction region was expected to have an average value of about 30 V/cm. Although the agreement between experiment and theory was quite good for the Na-like ions,[1,2] the measured rates were larger than the calculated rates for the Li-like ions, even for the maximum field enhancement of the theoretical cross sections.[3] Furthermore, the velocity distribution in these experiments was sufficiently wide that a comparison between experiment and theory for the low-Rydberg states, which are not affected by external electric fields, was impossible.

Andersen *et al.* have now completed measurements of DR for C^{3+} and O^{5+} using the Aarhus EN-tandem accelerator and a beamline equipped with an electron cooler.[4] The electric field in the interaction region is expected to be less than 5 V/cm and the velocity distribution is sufficiently narrow that the low-energy recombination resonances associated with a particular set of $2pnl$ configurations are resolved. For this reason, we have performed new calculations of the DR cross sections for these two ions for small electric fields between 0 and 7 V/cm. We then convoluted the electron velocity times our cross sections with the measured velocity distribution from the Aarhus group to determine the expected rate coefficients as a function of electron energy.

The theoretical methods used in these calculations have already been described in detail.[1] Here, it will suffice to say that the intermediate-coupled field-mixed eigenvectors for the $2pnl$ Rydberg states were determined by diagonalizing a Hamiltonian matrix which includes the internal electrostatic and spin-orbit terms, as well as the Stark matrix elements. The bound-state energies and the atomic orbitals were calculated using the Hartree-Fock program developed by Cowan,[5] and the continuum orbitals were calculated in a local distorting potential constructed in the semiclassical exchange approximation.[6]

These calculations were done in the isolated-resonance single-configuration approximation. In addition, the diagonalization of the Hamiltonian matrix includes only states with the same value of the principal quantum number n, so that n mixing by the external field is ignored. The effects of the configuration interaction on the total DR cross sections have been investigated and are expected to be small.[7] In addition, in the absence of external fields, the good agreement between calculations done using multichannel quantum-defect theory[8,9] with those that employ the isolated-resonance approximation indicate that the effects of overlapping resonances on the magnitude of the total DR cross section are small. However, in the presence of external fields, the effects of interference between resonances may be more pronounced since so many of the possible interfering resonances, after Stark splitting, will be less than the resonance widths. Sakimoto[10] and, independently, Harmin[11] have performed model calculations of DR in the presence of electric fields using an extension of multichannel quantum-defect theory.[8] Harmin's calculations indicate that the combined effects of field-induced n mixing and interference between resonances with different values of n will reduce the cross section. However, until this theory is applied to an atomic system such as Mg^+ where detailed experimental[12] and theoretical[13,14] results exist, the magnitude of such effects will not be clear.

In the isolated resonance approximation, the DR cross

section (in atomic units) through all states of a doubly excited autoionizing level j of the $(N+1)$-electron ion is given by

$$\sigma=\frac{2\pi^2}{\Delta\varepsilon k^2}\frac{g_j}{2G_i}\frac{\sum_i A_a(j\rightarrow i)\sum_f A_r(j\rightarrow f)}{\sum_m A_a(j\rightarrow m)+\sum_f A_r(j\rightarrow f)}, \quad (1)$$

where G_i is the statistical weight of the initial configuration i of the N-electron ion, g_j is the statistical weight of level j, $\Delta\varepsilon$ is an energy bin width larger than the largest resonance width but small compared to the experimental width, k is the linear momentum of the continuum electron, $A_a(j\rightarrow m)$ is the autoionizing rate from level j to a level m, and $A_r(j\rightarrow f)$ is the radiative rate from the level j to a lower level f. $\sum_i$ in Eq. (1) represents a sum over levels of the initial N-electron configuration only, while $\sum_m$ signifies a sum over all lower levels of the N-electron ion; however, for the Li-like ions considered here, the only possible autoionizing transitions are $2pnl\rightarrow 2s+e^-$, so that these two sums are identical. In these calculations, the bin width $\Delta\varepsilon$ was chosen to be 0.0005 hartree a.u. Two types of radiative transitions must be included: $2pnl\rightarrow 2snl+h\nu$ and $2pnl\rightarrow 2pn'l'+h\nu'$. For the first type of transition, the radiative rate is nearly independent of the Rydberg electron, and we employ the radiative rate obtained from the transition $2p\rightarrow 2s$ in the N-electron ion. The rates for the second type of transition are large for low values of n and they contribute in a significant way to the magnitude of the DR cross sections for the low-energy Rydberg states; however these rates decrease rapidly with n and become negligible for high values of n.

In addition to mixing effects due to fields in the interaction region, electric fields in the analyzing region of the experiment will field ionize recombined ions in high-Rydberg states. The amount of field ionization can be determined by employing hydrogenic field-ionization formulas such as the one developed by Damburg and Kolosov.[15] However, a much simpler method to estimate these effects is to assume that ions rapidly ionize for all values of $n>n_m$, where the cutoff is given by the semiclassical formula

$$n_m=\left[\frac{6.2\times 10^8}{E}q^3\right]^{1/4}, \quad (2)$$

and where E is the electric field in V/cm and q is the initial charge of the ion before recombination. It has been found that the cutoff determined from this formula agrees closely with the value of n for which the hydrogenic field-ionization formulas predict a very rapid increase in the rate of field ionization.[13] For the fields in the analyzing region of the Aarhus experiment, n_m is equal to 35 for C^{3+} and 53 for O^{5+}.

The electron-velocity distribution function in the rest frame of the ions for the Aarhus experiment is described in Ref. 4. It has the same general form as that obtained for the ORNL experiment[2] but is, of course, much narrower. As mentioned earlier, the electron velocity in the rest frame of the ion times the theoretical cross sections were convoluted with this distribution function to produce the rate $\langle v\sigma(v)\rangle$ as a function of energy.

Our results for C^{3+} for fields in the interaction region of 0, 1, 3, and 5 V/cm, in comparison with the experimental measurements, are shown in Fig. 1. The height of the measured rate due to the high-Rydberg states, in comparison with the calculated results, would seem to indicate that the field in the interaction region is just over 3 V/cm. This is very close to the estimated field in the experiment.[4] Furthermore, the calculated increase in the height of this peak in going from a field of 1 to 2 V/cm (not shown) is approximately 14%. In comparison, Andersen[16] has estimated that a reduction of 50% in the field causes a reduction of about 10% in this peak height.

The overall agreement between experiment and theory is also quite good, with the exception of the low-energy peak between 0 and about 0.6 eV. The peak is due to recombination through the $2p4d$ and $2p4f$ configurations of C^{2+}. The $^3F_{2,3,4}$ and $^1D_2$ levels of the $2p4d$ configuration are observed to be bound,[17] while the remaining levels of $2p4d$ and all the levels of $2p4f$ are just above the ionization limit for C^{3+}. The recombination cross section varies as the inverse of the electron energy [see Eq. (1)], and since these levels are just above the position of the $2s$ configuration of C^{3+}, the magnitude of the cross section is very sensitive to the calculated position of the levels. The levels from the terms ^1D, ^3F, ^3D, and ^1F of the $2p4d$ configuration, and the terms ^3G, ^3F, and ^3D of the $2p4f$ configuration, have been identified.[17] For this reason, we adjusted our Hartree-Fock-Slater parameters for these two configurations to give better agreement with the measured positions of these particular levels; such an adjustment will presumably provide better positions for those levels that have not been identified,

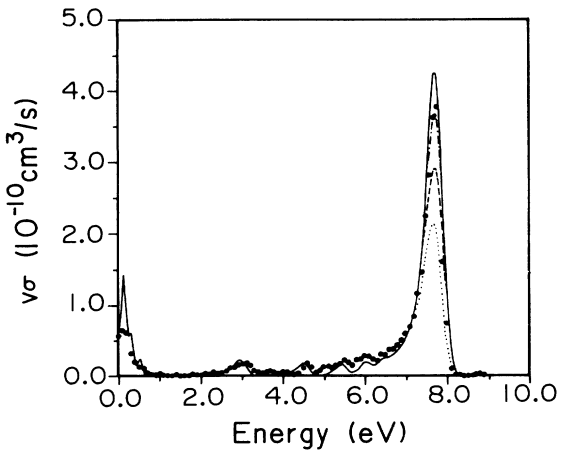

FIG. 1. Theoretical dielectronic-recombination-rate coefficients for C^{3+} (as measured in the Aarhus electron-ion merged-beam experiment) as a function of electron energy. . . . ., $E=0$ V/cm; — — —, $E=1$ V/cm; —·—·—·, $E=3$ V/cm; ——, $E=5$ V/cm. The calculations include all $2pnl$ resonances for C^{2+} up to $n=35$. The experimental points are from Ref. 4.

and thereby improve the magnitude of the predicted cross section. Nevertheless, the experimental rate is just a little over 50% of the calculated rate. In addition to its sensitivity to the exact energy of the $2p4d$ and $2p4f$ levels, the magnitude of the cross section for these low-energy resonances is primarily determined by the rates for radiative transitions of the second type mentioned above, in which the $4d$ and $4f$ electrons are the active electrons. Thus this discrepancy may be partially due to remaining errors in the energies of these levels as well as errors in these particular radiative rates.

The calculated rates for O^{5+} for fields of 0, 3, 5, and 7 V/cm are shown in Fig. 2 in comparison with the experimental measurements. The agreement between experiment and theory is good for the resonances due to low-Rydberg states, although the experimental rate for the lowest peak arising from recombination through the $2p6l$ levels of O^{4+} is about 30% lower than the rate determined from the theoretical cross sections. However, in contrast to the case of C^{3+}, the experimental peak due to the high-Rydberg states is larger than the calculated rate even for a field of 7 V/cm; for a field of 3 V/cm, where we obtained the best agreement for C^{3+}, the calculated peak height is only about 65% of the maximum rate from the experiment. In addition, the width obtained from convoluting the velocity times the theoretical cross sections with the velocity distribution is too narrow as compared to the experimental measurement.

The good overall agreement, which is revealed by this comparison of theory with the latest DR measurements, lends greater support to the relative accuracy of the isolated-resonance approximation for the calculation of total DR cross sections. However, since both the theoretical and experimental techniques used for C^{3+} and O^{5+} are the same, one would expect similar agreement for both ions. Therefore, the larger discrepancy in the case of O^{5+} is troubling, especially in light of the differences found between theory and the earlier DR measurements for the Li-like ions.[3] Additional comparisons of theory with high-resolution measurements of DR for other ionic species are needed if we are to gain a more complete understanding of the accuracy of the approximations inherent in the theoretical calculations.

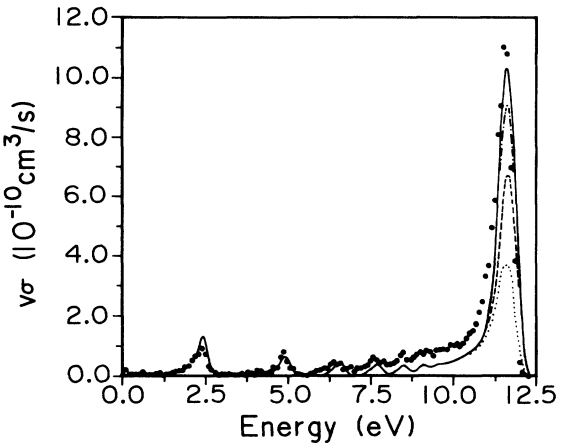

FIG. 2. Theoretical dielectronic-recombination-rate coefficients for O^{5+} (as measured in the Aarhus electron-ion merged-beam experiment) as a function of electron energy. . . . ., $E=0$ V/cm; − − −, $E=3$ V/cm; −·−·−·, $E=5$ V/cm; ——, $E=7$ V/cm. The calculations include all $2pnl$ resonances for O^{4+} up to $n=53$. The experimental points are from Ref. 4.

The authors would like to thank Lars Andersen and Jakob Bolko for providing us with their data prior to publication. We would also like to acknowledge helpful conversations with Pete Dittner. This work was supported by the Office of Fusion Energy, U.S. Department of Energy, under Contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc. and Contract No. DE-FG05-86ER53217 with Auburn University.

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