Dielectronic recombination of the Be-like ions: C^{2+}, N^{3+}, O^{4+}, and F^{5+}

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The first measurements of dielectronic recombination rate coefficients associated with the $2s \rightarrow 2p$ excitation in the Be-like ions C^{2+}, N^{3+}, O^{4+}, and F^{5+} are reported. We observed the amount of electron capture attending the passage of MeV/nucleon ion beams through a collinear, magnetically confined, space-charged-limited electron beam as a function of relative energy. The initial beams contained large numbers of ions for which the metastable states of the term $2s2p\ ^3P$ were populated, and the fraction of ions in the metastable states to those in the ground-state configuration $2s^2$ were measured. The experimental rate coefficients are consistent in magnitude and shape with rates determined from distorted-wave calculations of the dielectronic recombination cross sections. The large fraction of metastable states in the initial ion beams had a pronounced effect on the shape and magnitude of the rate coefficients.

I. INTRODUCTION

In earlier papers,[1-3] we have reported on measurements and theory[4-6] of dielectronic recombination (DR) associated with $\Delta n = 0$ excitations for the Li-like ions B^{2+}, C^{3+}, N^{4+}, and O^{5+}, and for the Na-like ions P^{4+}, S^{5+}, and Cl^{6+}. This paper presents the results of our measurements for DR associated with the $2s \rightarrow 2p$ excitation in the Be-like ions C^{2+}, N^{3+}, O^{4+}, and F^{5+}. In addition to being the first DR measurements of Be-like ions, these measurements are the first for which the fraction of the ions initially in a metastable state are well characterized by direct measurement. This fraction was indeed large and critically affected the interpretation of the experiment. The DR processes we measured in the merged-beam experiments were

$$\left.\begin{matrix} A^{q+}(2s^2\ ^1S) \\ [A^{q+}(2s2p\ ^3P)]^* \end{matrix}\right\} + e^- \rightarrow [A^{(q-1)+}(2s2p\ ^1P, nl)]^{**} \rightarrow [A^{(q-1)+}(2s^2\ ^1S, nl)]^* + h\nu\ , \quad (1)$$

where q is the initial charge state of the ion, n and l are the principal and orbital-angular-momentum quantum numbers of the Rydberg electron, respectively, and ν is the frequency of the emitted radiation for the core relaxation $2s2p\ ^1P \rightarrow 2s^2\ ^1S$.

In the past theoretical calculations of dielectronic recombination rate coefficients for the Be-like ions in the absence of any external fields have been reported.[7] In addition, theoretical calculations as a function of electric field strength of the DR cross section associated with the $2s \rightarrow 2p$ excitation for O^{4+} have recently been completed.[8] In this paper we report on the results of theoretical calculations of DR for the Be-like ions C^{2+} through F^{5+} in the absence of an electric field and with complete field mixing. The calculations were performed using a modified version of the configuration-average, distorted-wave method described elsewhere.[4,5] The maximum enhancement of the DR cross section due to the external electric field in the interaction region was approximated in the linear Stark approximation by transforming the calculated autoionizing rates from a spherical to a parabolic basis.

The remainder of this paper is arranged as follows. In Sec. II we give a brief description of the experimental procedure. In Sec. III we briefly describe the theoretical methods employed in the calculations, and in Sec. IV we compare the measurements and calculations. In Sec. V we consider the implications of these results.

II. EXPERIMENTAL PROCEDURE

We have described our experimental apparatus, experimental procedure, and data reduction procedure in previ-

ous papers on the DR measurements for the Li-like ions,[2] and the Na-like ions;[3] thus, only a brief summary shall be given here. We observe the amount of electron capture attending the passage of MeV/nucleon ion beams through a collinear, magnetically confined, space-charge-limited electron beam. The separation of charge states of the ion beam following the interaction region is accomplished via electrostatic deflection. The relative energy E_r of the ions and electrons is varied from 0 to several electron volts above the energy of the $2s^2\,{}^1S \rightarrow 2s2p\,{}^1P$ transition energy. Approximately 1-eV steps in E_r are taken by changing the ion energy E_i with the electron energy fixed. Background subtraction is accomplished by a modulation of the electron energy at fixed E_i, at each E_r. For each run we determine the electron density ρ_e from the cathode voltage, previous measurements of the electron beam profile, and the perveance of the electron gun. The length of the interaction region L is fixed by geometry and is known. At each E_i, and hence at each E_r, the ion velocity v_i is known, and the ratio of the number of ions with charge state $(q-1)+$ to the number of ions in the incoming beam of charge state $q+$ is measured. This ratio, which we refer to as R_s, is corrected for background after each run. We then calculate a quantity, having the dimensions of a rate coefficient (cm^3/s), at every E_i or E_r, which is the product of the relative velocity v_r, and the cross section σ convoluted with the relative velocity distribution of the two intersecting beams. This quantity, $\langle v_r\sigma\rangle$, is given in terms of the measured values by the expression

$$\langle v_r\sigma\rangle = \frac{R_s v_i}{\rho_e L} \ . \tag{2}$$

This rate coefficient can be compared with that calculated from theoretical predictions for the DR cross section.

We used K-shell ionization by He, "needle ionization," followed by zero-degree Auger spectroscopy[9] to determine the metastable fraction Φ_m of the Be-like ions issuing from the Oak Ridge National Laboratory EN tandem Van de Graaff accelerator. The ion beam is allowed to pass through a He target where ionization of the $1s$ electron may occur. The relative yields of Auger electrons from states of the $1s2s^2\,{}^2S$ and the $1s2s2p\,{}^4P$ terms relate to the original population of ground and metastable states. Measurements on O^{4+} and C^{2+} beams gave values of Φ_m of ≈ 0.63 and ≈ 0.75, respectively, in agreement with a value of ≈ 0.7 determined from simple statistical arguments. For comparison with the theoretical calculations, Φ_m was set equal to 0.70 for all the Be-like ions.

III. THEORETICAL METHODS

In the isolated-resonance, configuration-average (CA) approximation,[4,5] the energy-averaged dielectronic recombination cross section, for cases in which the only possible autoionizing transitions are to the initial configuration, is given by the expression

$$\sigma = \frac{2\pi^2}{\Delta\varepsilon k_i^2}\frac{G_J}{2G_I}\frac{A_a(n,l)A_r(n,l)}{\overline{A}_a(n,l)+\overline{A}_r(n,l)} \ , \tag{3}$$

where G_J is the total statistical weight of the doubly excited autoionizing configuration; G_I is the total statistical weight of the initial configuration; $\overline{A}_a(n,l)$ and $\overline{A}_r(n,l)$ are the average autoionizing rates and radiative rates, respectively, of the doubly excited configuration with principal quantum number n and orbital-angular-momentum quantum number l; k_i is the linear momentum of the continuum electron; and $\Delta\varepsilon$ is an energy bin width chosen to be larger than the largest resonance width and yet much smaller than the experimental width. In the case of $\Delta n = 0$ transitions in Li-like ions, this expression has been shown to yield DR cross sections in good agreement with those calculated in intermediate coupling.[10]

In order to employ this approximation of the calculation of the DR cross sections associated with the $2s \rightarrow 2p$ excitation in Be-like ions, we must make a number of modifications. This is most easily understood by referring to the energy-level diagram for the case of O^{4+} shown in Fig. 1. Dielectronic recombination from the ground state and metastable states of $2s2p\,{}^3P$ is dominated by the transitions:

$$\left.\begin{matrix} O^{4+}(2s^2\,{}^1S) \\ [O^{4+}(2s2p\,{}^3P)]^* \end{matrix}\right\} + e^- \rightarrow [O^{3+}(2s2p\,{}^1P,nl)]^{**} \rightarrow \begin{cases} [O^{3+}(2s^2,nl)]^* + h\nu \\ [O^{3+}(2s2p\,{}^1P,n'l')]^{**} + h\nu \ , \end{cases} \tag{4}$$

where, by far, the dominant radiative transition is the $2s2p\,{}^1P \rightarrow 2s^2$ core relaxation. The competing autoionizing transitions are

$$[O^{3+}(2s2p\,{}^1P,nl)]^{**} \rightarrow O^{4+}(2s^2) + e^- \tag{5}$$

and

$$[O^{3+}(2s2p\,{}^1P,nl)]^{**} \rightarrow [O^{4+}(2s2p\,{}^3P)]^* + e^- \ . \tag{6}$$

In addition, we can have resonant recombination from the ground state to the autoionizing states of $2s2p\,{}^3P,nl$; however, since there is no mixing between $2s2p\,{}^3P,nl$ and $2s2p\,{}^1P,nl$ in these light systems, the only possible radiative transitions are to the bound states of $2s2p\,{}^3P,n'l'$, for which the rates are quite small. Finally, the $2s^2$ ground state mixes strongly with $2p^2$, and this will affect both autoionizing rates of $O^{4+}(2s^2)$ and radiative rates to $O^{3+}(2s^2,nl)$.

To apply the CA approximation to these transitions, we modify the configuration-averaged expressions for $\overline{A}_a(nl)$ and $\overline{A}_r(nl)$ and the values of G_I and G_J so that they apply to transitions to and from the individual ^1P and ^3P terms of $2s2p$. In addition, the autoionizing rates to $O^{4+}(2s^2)$ and the radiative rates to $O^{3+}(2s^2,nl)$ are modified to include the effects of configuration interaction between $2s^2$ and $2p^2$. Finally, we replace the autoionizing rate to the ground state in the denominator of Eq. (3) by the total autoionizing rate to $2s^2$ and $2s2p\,{}^3P$.

In the presence of an electric field, the orbital angular momentum of the Rydberg electron is no longer a good quantum number, and the spherical basis $2s2p\ ^1P,nl$ is no longer a valid representation of the doubly excited Rydberg states. Such a redistribution of orbital angular momentum among the Rydberg states opens up more recombination channels and thereby enhances the rate of dielectronic recombination.[4-6] As we have shown in earlier work, by comparison with our more detailed calculations of DR as a function of electric field strength,[6] one can estimate the maximum-field enhancement of the DR cross section by employing the linear Stark approximation,[4,5] in which one assumes that the doubly excited Rydberg states with the same values of n but different values of l are all degenerate. With this assumption, the field mixed rates can be determined by employing a parabolic basis set of the Rydberg states obtained from a simple Clebsch-Gordon transformation from the spherical basis.[4] This field mixing will, of course, have a negligible effect on the radiative rates involving relaxation of the core electron, and it will have a small effect on radiative rates for which the Rydberg electron is the active electron. However, it will have a very large effect on the autoionizing rates.

The calculations of dielectronic recombination in the absence of a field and with complete field mixing were performed using our configuration-averaged distorted-wave DR code DRACULA,[4] modified to take into account the individual terms of the $2s2p$ configuration, as described above. A detailed description of the calculational procedures used in this program is given in Ref. 4, and will not be repeated here.

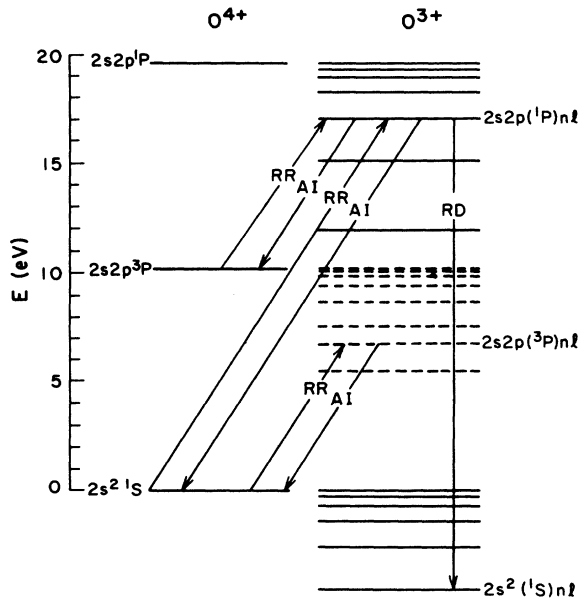

FIG. 1. Schematic energy-level diagram showing the possible resonant recombination (RR), autoionizing (AI), and radiative (RD) transitions associated with dielectronic recombination in O^{4+}.

IV. EXPERIMENTAL AND THEORETICAL RESULTS

In order to make meaningful comparisons of the experimental results with calculations, we must first consider the effect of the electric field in the analyzing region on the measured dielectronic recombination rate. This field will ionize states of $A^{(q-1)+}(2s^2,nl)$ with high values of n. The amount of field ionization can be determined by employing hydrogenic field-ionization formulas such as the one developed by Damburg and Kolosov.[11] However, a much simpler method to estimate the effects of field ionization is to assume that ions rapidly ionize for all values of $n > n_m$ where the cutoff is given by the semiclassical formula

$$n_m = \left[\frac{6.2\times 10^8}{E} q^3 \right]^{1/4}, \tag{7}$$

where E is the electric field strength in volts per centimeter, and q is the initial charge on 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.[12] In this experiment the deflection field used was 4.5 kV/cm for all four ions. From Eq. (7) we then obtain values of $n_m = 32$, 44, 54, and 64 for C^{2+}, N^{3+}, O^{4+}, and F^{5+}, respectively. Thus we see that the DR rate coefficient extracted from the data will represent only a fraction of the total dielectronic recombination which occurs in the interaction region.

The theoretical energy-averaged DR cross section for C^{2+} in the absence of a field and with complete field mixing, calculated using the methods described in Sec. III, is shown in Fig. 2. The energy bin width is 0.136 eV which is quite small compared to the experimental width. As can be seen, the low-energy peak due to DR transitions from the metastable states of $2s2p\ ^3P$ is quite small in magnitude as compared to the high-energy peak due to transitions from the ground state. This is true even though it is assumed in this calculation that only 30% of the ions are in the ground state, and the remaining 70% are in the metastable states of $2s2p\ ^3P$. Furthermore, we see that the maximum-field enhancement is quite large for both sets of DR transitions. As already discussed in Sec. II, in order to compare the calculated results with experiment, we must first determine a rate coefficient for the measured quantity by multiplying the energy-averaged cross section $\bar{\sigma}$ with the relative velocity of the electron and ion beams, v_r, and then convoluting this product with a relative velocity distribution function determined from previous experiments.[2,3] The theoretical rate coefficients for C^{2+} calculated in this way are shown in comparison with our experimental results in Fig. 3. The error bars indicate the relative uncertainties, which include counting statistics and background subtraction. The absolute uncertainty is dominated by imprecise knowledge of the electron density ρ_e. We estimate the uncertainty in ρ_e to be $\pm 30\%$, and thus, the absolute uncertainty in the data is $\approx \pm 35\%$.

The experimental rate coefficients are seen to be about halfway between the theoretical no-field and maximum-

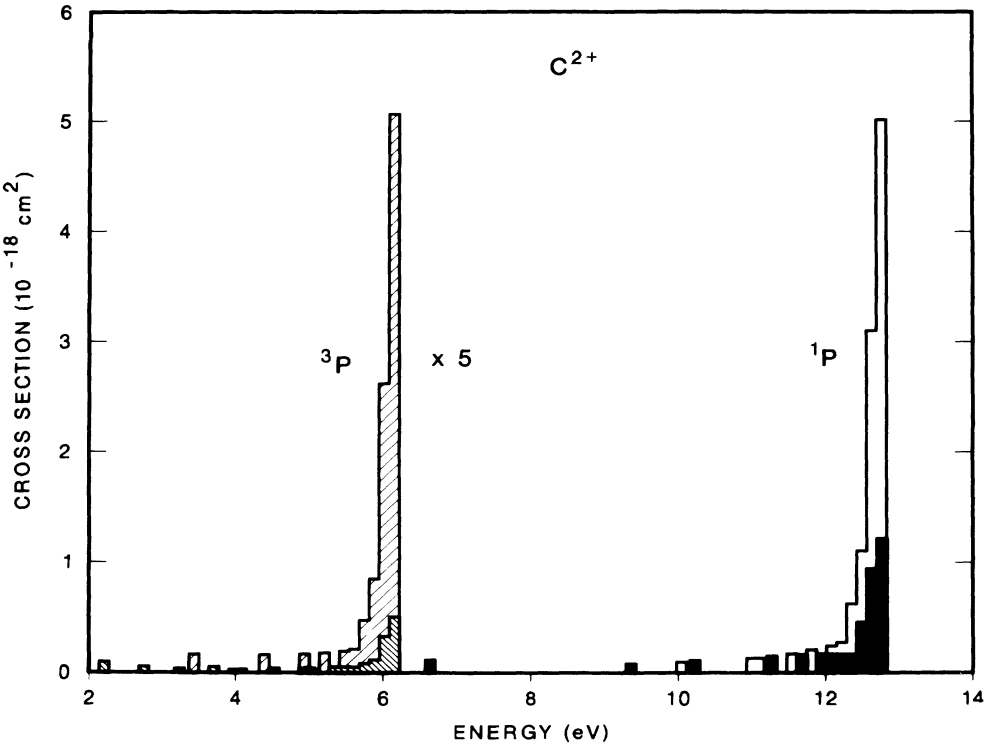

FIG. 2. Bar graph of the calculated energy-averaged DR cross section for C^{2+} as a function of electron energy. Energy bin widths equal 0.136 eV. The solid bars represent the cross section from the ^1S state in the absence of a field and the open bars represent the cross section from the ^1S state for complete field mixing. The heavily hatched bars represent the cross section ($\times 5$) from the ^3P state in the absence of a field and the lightly hatched bars represent the cross section ($\times 5$) from the ^3P state for complete-field mixing. This calculation includes all resonances up to $n_m = 32$.

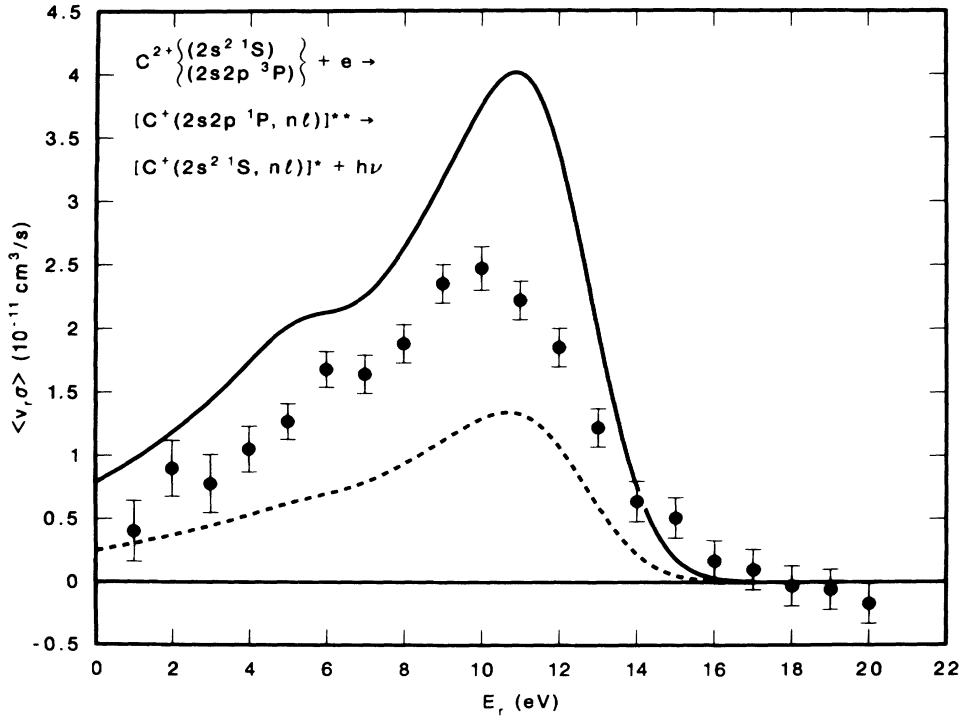

FIG. 3. The DR rate coefficient $\langle v_r \sigma \rangle$ vs the relative energy E_r for C^{2+}. Points are the experimental data. The dashed curve is the calculated rate coefficient for no-field mixing and the solid curve is the rate for complete-field mixing. The calculations include all resonances up to $n_m = 32$.

field results, and the relative positions of the low- and high-energy peaks appear to be consistent with the calculations. Similar plots are shown in N^{3+}, O^{4+}, and F^{5+} in Figs. 4, 5, and 6, respectively. The agreement between experiment and theory is similar in all four cases. Also shown in Fig. 5 for O^{4+} are the DR rate coefficients from the calculations of LaGattuta, Nasser, and Hahn[8] as a function of field strength. They employ a modified version of the configuration-average approximation, quite similar to the one employed here. Their calculations were done for field strengths of 0, 8, 24, 120, 1200, and 6400 V/cm. Since the effect of the field is amply demonstrated by the curves for fields of 0, 120, and 6400 V/cm and for reasons of clarity, the curves for the other fields are not shown in Fig. 5. The two calculations (Ref. 8 and this paper) should produce the same result for the no-field case. Since a field of 6400 V/cm results in complete mixing of all but the lowest n values, the 6400-V/cm case of Ref. 8 and the maximum-field results of this paper should agree. As can be seen in Fig. 5, the two calculations do not agree. We have compared our autoionizing rate as a function of l with those of Ref. 8 and they appear to be quite similar. The discrepancy between the two calculations is not clear at this time. A comparison of experimental rate coefficients[3] with those calculated as a function of electric field strength[6] for Na-like ions also indicate that, for the fields in the interaction region in these experiments, the measured rate coefficients are about halfway between the no-field and maximum-field calculated rate coefficients. However, in the case of the Li-like ions, a similar comparison between experiment[2] and theory[6] shows that the experimental results are as large, or even larger, than the calculated results for maximum-field mixing. The reason for this difference for dielectronic recombination associated with the $2s \rightarrow 2p$ excitation in Li-like ions is not yet understood.

V. CONCLUSIONS

We have measured dielectronic recombination rate coefficients for the Be-like ions C^{2+}, N^{3+}, O^{4+}, and F^{5+}. This is the first observation of dielectronic recombination in a case for which a known and substantial fraction of the initial ions are in metastable states. The experimental results are in reasonably good agreement with rate coefficients calculated using a modified version of the isolated-resonance, configuration-averaged approximation. These measurements again indicate that external fields in the interaction region have a significant effect on the magnitude of the dielectronic recombination process. The next challenge to experimental research on DR is the measurement of cross sections for highly ionized systems, where the field effects are expected to be substantially reduced.[13]

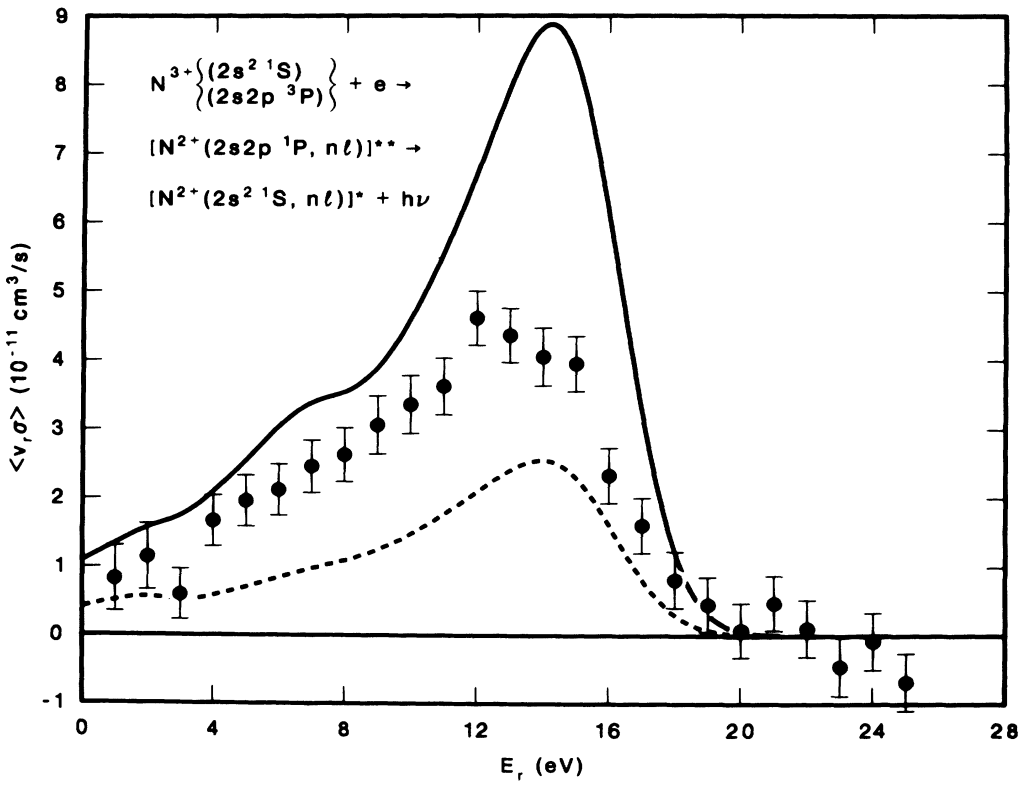

FIG. 4. The DR rate coefficient vs E_r for N^{3+}. All notation is the same as in Fig. 3. The calculated values include all resonances up to $n_m = 44$.

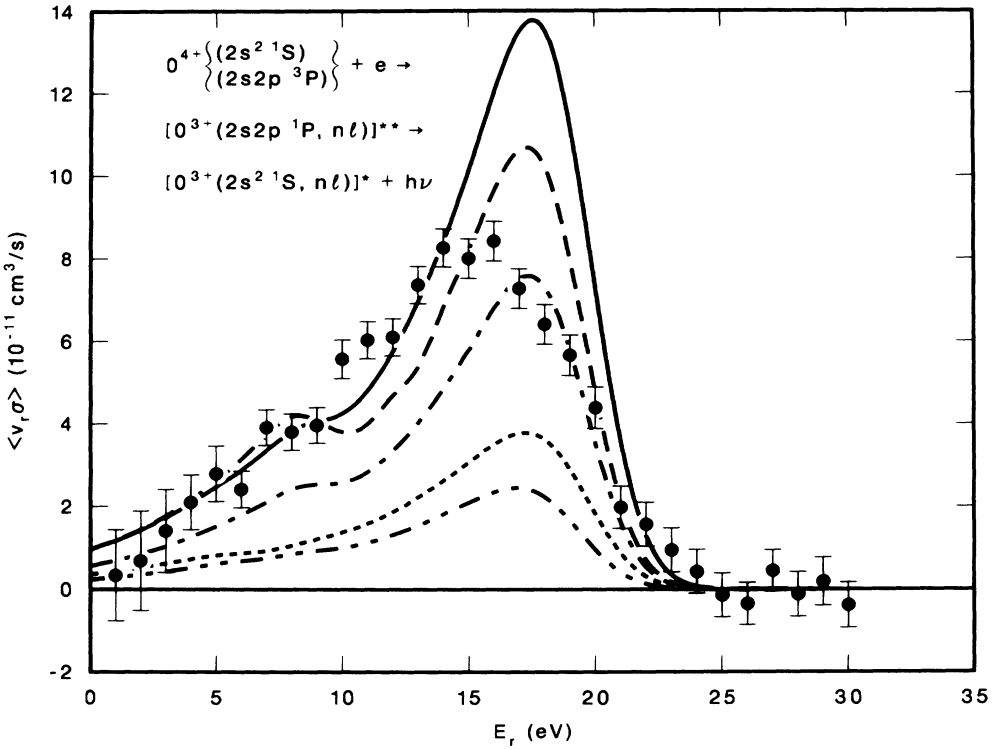

FIG. 5. The DR rate coefficient vs E_r for O^{4+}. The dashed curve (----) is our calculated rate coefficient for no-field mixing and the solid curve is that for complete-field mixing. The other curves are rate coefficients calculated from Ref. 8 for a field of 0 V/cm (--———--), 120 V/cm (-—-—-), and 6400 V/cm (– – –). The calculated values include all resonances up to $n_m = 54$.

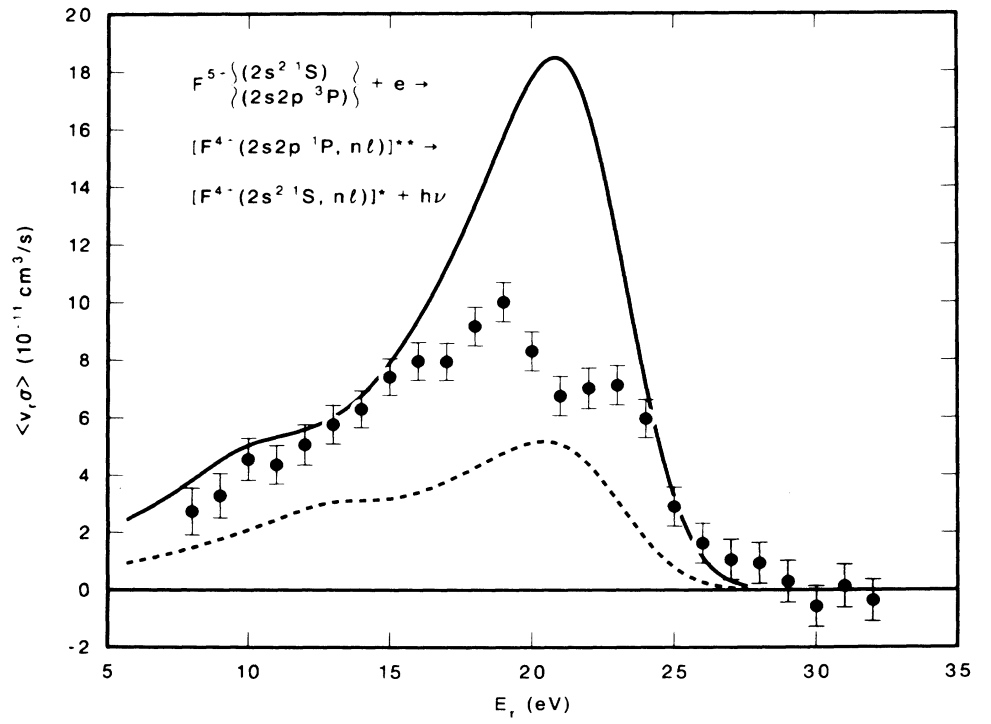

FIG. 6. The DR rate coefficient vs E_r for F^{5+}. All notation is the same as in Fig. 3. The calculated values include all resonances up to $n_m = 64$.

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