

Dielectronic recombination of light Be-like and B-like ions

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Abstract. Dielectronic recombination cross sections from the ground and metastable states of the Be-like ions C^{2+} , O^{4+} and F^{5+} , and the B-like ions O^{3+} and F^{4+} , have been calculated and compared with experimental results obtained by a merged-beams technique. The comparison of theory and experiment is complicated by the presence of weak electric fields in the interaction region. However, we can qualitatively explain the main features of our experimental results. In particular, for Be-like ions we find evidence of a large contribution from the initial $2s2p\ ^3P$ metastable state recombining into an Auger metastable final state.

1. Introduction

With the advent of electron coolers, high energy-resolution dielectronic recombination (DR) cross sections have been measured, using a merged-beams technique, for a number of light H-like and He-like ions (see Andersen *et al* 1989, Kilgus *et al* 1990) and they are in good agreement with the results of theoretical calculations (see Badnell *et al* 1990, Pindzola *et al* 1990, Hahn and Bellantone 1989). The radiative stabilization for these ions is via a $\Delta n = 1$ transition and the effect of electric fields in the interaction region is negligible. A comparison of the recent experimental results of Andersen *et al* (1990) for Li-like ions with the theoretical results of Griffin *et al* (1989) shows that a significant field enhancement is still to be found when the radiative stabilization is via a $\Delta n = 0$ transition. Thus, the high resolution $\Delta n = 0$ DR measurements reported here for light Be-like and B-like ions can be expected to have been field enhanced. This was the case with the first (low resolution) DR measurements for Be-like and B-like ions which were carried out at Oak Ridge National Laboratory by Dittner *et al* (1987, 1988) and which were also studied theoretically by several workers (see Dittner *et al* 1988, LaGattuta *et al* 1987, Badnell and Pindzola 1989a, b).

The ion beams used in the present work were delivered from the EN-tandem accelerator at the University of Aarhus. Since the desired charge states of the ion beam were produced via collisions, some ions emerging from the accelerator were in metastable electronic states. For the Be-like ions (C^{2+} , O^{4+} , F^{5+}), which have a ground state configuration $2s^2\ ^1S$, the metastable $2s2p\ ^3P$ state was also present in the ion beam in a fraction of about 75%. For the B-like ions (O^{3+} , F^{4+}), which have a ground state configuration $2s^22p\ ^2P$, the metastable $2s2p\ ^2P$ state was estimated to be present in the ion beam in a fraction of 50%. Thus, the present results yield information on DR for two different initial configurations of the Be- and B-like ions.

In the light of the high experimental resolution now obtained, we have carried out a much larger structure calculation for those ions treated before (O^{3+} , O^{4+} and F^{5+} ,

see Badnell and Pindzola 1989a, b), to determine accurately the positions of the resonances and the radiative stabilization rates, as well as completely new calculations for the remaining ions (C^{2+} and F^{4+}). We will also consider a new DR pathway for the metastables, which has not been considered previously, and which entailed a new enlarged calculation for the autoionization rates. Thus, the present theoretical contribution is a major expansion of the earlier work by Badnell and Pindzola (1989a, b).

In section 2 of this paper we describe briefly the theory behind the calculations and its application to the DR of Be-like and B-like ions. In section 3 we describe our experimental arrangement. Our theoretical results are compared with our experimental results in section 4. We conclude with a short summary in section 5.

2. Theory

2.1. Formulation

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

$$\bar{\sigma}_d(i; j) = \frac{(2\pi a_0 I)^2}{E_c \Delta E_c} \frac{\omega(j)}{2\omega(i)} \frac{\tau_0 \sum_k A_r(j \rightarrow k) \sum_l A_a(j \rightarrow i, E_c l)}{\sum_h A_r(j \rightarrow h) + \sum_{m,l} A_a(j \rightarrow m, E_c l)} \quad (2.1)$$

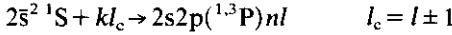
where E_c is the energy of the continuum electron, which is fixed by the position of the resonances, ΔE_c is an energy bin width and I is the ionization potential energy of hydrogen. $\omega(j)$ is the statistical weight of the $(N+1)$ -electron ion doubly excited state, $\omega(i)$ is the statistical weight of the N -electron ion initial target state and $(2\pi a_0)^2 \tau_0 = 2.6741 \times 10^{-32} \text{ cm}^2 \text{ s}$. With respect to the autoionization rates A_a , the sum over m in equation (2.1) is over all energetically accessible states of the N -electron ion. For the radiative rates A_r , the sum over h is over all possible states, while the sum over k is usually taken to be over all states which are stable against autoionization. However, this point needs to be re-examined for the case of metastable autoionizing states in an experimental environment. We illustrate this point by example in the following section 2.2. Equation (2.1) may be evaluated in a variety of approximations using a number of different computer codes. The bulk of the calculations were carried out using the AUTOSTRUCTURE package (see Badnell 1986, Badnell and Pindzola 1989a) which evaluates configuration-mixed rates in both LS coupling and intermediate coupling approximations but for zero external electric fields. For B-like ions (or any ion) maximum field-enhanced DR cross sections can be determined in the configuration-averaged approximation by a Clebsch-Gordan transformation of the autoionization rates from spherical to parabolic coordinates. Zero field and maximum field-enhanced configuration-averaged DR cross sections were evaluated for B-like ions using the DRACULA code (see Griffin *et al* 1985). For Be-like ions, a modified form of DRACULA was used which allows for configuration mixing and term dependence within the Be-like core but still averages over the coupling of the core to the Rydberg electron (see Dittner *et al* 1987).

2.2. Applications

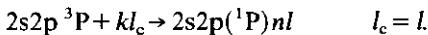
We describe below the transitions that we considered for Be-like and B-like ions; in each case the $1s^2$ core has been suppressed. The sum over the Rydberg states implicit in (2.1) and denoted below by nl , will be cut-off at the value of $n = n_c$, above which

the recombined ion is field ionized by the charge-state analyser used in the experiment, see section 3.

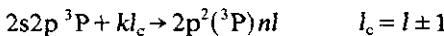
2.2.1. Be-like ions. For DR from the 2^1S ground state, we consider the dielectronic capture reaction



where $2\bar{s}^2$ denotes a configuration mixed target ($2s^2 + 2p^2$) and where capture to the 1P parent is dominant, being dipole allowed. For the $2s2p\ ^3P$ metastable, the contribution from the following capture is small, being spin-forbidden (see Badnell and Pindzola 1989b)

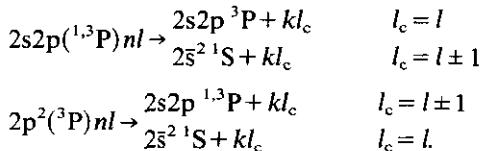


However, the capture transition

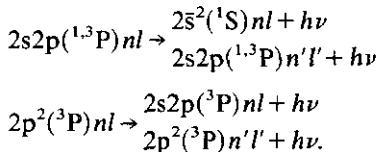


is strong, being dipole allowed, although it is normally assumed not to be able to radiatively stabilize. The $2p^2(^1D, ^1S)nl$ states are also included but have little effect.

The doubly excited states can decay by the autoionizing transitions

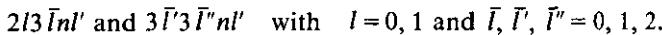


They can also decay by the following radiative transitions



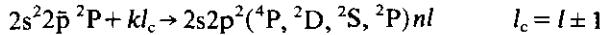
Usually, only those final states lying below the $2\bar{s}^2 1S$ continuum are assumed to have recombined, i.e. the associated radiative rates are included in the numerator of (2.1). However, the Auger lifetime of the $2s2p(^3P)nl$ states can be comparable with the time of flight to the experimental detector for high- l states and can thus be counted as recombined.

Given the high energy resolution of the experiment, the following correlation configurations have also been included in the calculations to improve the accuracy of the radiative rates and the position of the resonances,

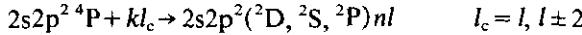


The spectroscopic orbitals were calculated using scaled Thomas-Fermi-Dirac-Amaldi (TFDA) model potentials, and the correlation orbitals ($3\bar{s}, 3\bar{p}, 3\bar{d}$) using screened hydrogenic potentials. The scaling/screening parameters were determined by minimizing a weighted sum of eigenenergies. The $2s2p\ ^1P \rightarrow 2\bar{s}^2\ ^1S$ and $2p^2\ ^3P \rightarrow 2s2p\ ^3P$ radiative rates were reduced by 10% to 20% for these ions through the inclusion of the correlation configurations. The Be-like core energy levels, calculated by including the correlation configurations, differed by 1% to 2% from those tabulated by Moore (1970), the remaining difference was eliminated by adjusting to those observed energies.

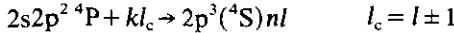
2.2.2. **B-like ions.** For DR from the ${}^2\text{P}$ ground state, we consider the dielectronic capture



where $2\text{s}^2 2\bar{\text{p}}$ again denotes a configuration-mixed target ($2\text{s}^2 2\text{p} + 2\text{p}^3$) and the doublet parents are dominant. For the $2\text{s}2\text{p}^2 {}^4\text{P}$ metastable, there is a small contribution from

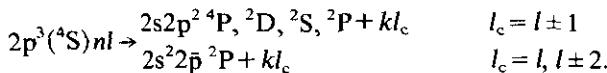
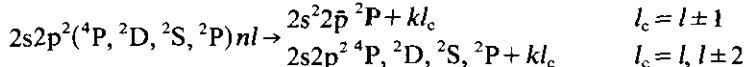


(see Badnell and Pindzola 1989a) while the capture

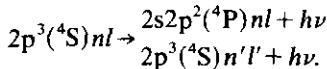
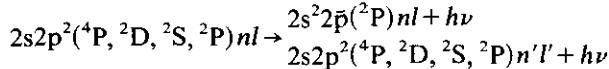


is again dipole-allowed. The $2\text{p}^3({}^2\text{D}, {}^2\text{P})nl$ states have little effect.

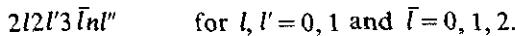
The doubly excited states can decay by the following autoionizing transitions



The possible radiative decays are



We also included the following correlation configurations in the calculation



In this case, the inclusion of the correlation configurations reduced the core radiative rates by about 25% while the resulting core energies differed by $\sim 1\%$ from Moore (1970) and were then adjusted to reproduce those observed values.

3. Experiment

The measurements which are reported here were performed at the Tandem accelerator at the Institute of Physics, University of Aarhus. $1.25 \text{ MeV amu}^{-1}$ ions were merged with an almost monoenergetic beam of electrons with essentially the same speed as the ion beam. Different relative energies were obtained by varying the electron-beam energy which was around 1 keV. The electron beam had a diameter of 1 cm and was guided by a magnetic field of about 150 G which was applied to compensate for the space charge field. Both the ion and electron beam could be modulated at a frequency of 2 MHz, so that the electrostatic pick-up plates could monitor the spatial position of the two beams in the interaction region. Thereby the two beams were brought into full overlap. Details of the experimental apparatus may be found in previous publications (Andersen *et al* 1990, Andersen and Bolko 1990).

The recombination process was identified by counting ions which had collected one electron after the passage through the interaction region. The number of recombined ions was then counted as a function of the relative energy to give the DR ‘rate coefficient’ as a function of energy. The background contribution due to electron capture in the rest gas (10^{-11} Torr) was found via a smooth fit to the yield of ions at energy regions outside the resonances.

Since very small relative energies were considered, the energy spread in the electron beam could not be neglected. Instead of the cross section, we determined the 'rate coefficient' which is defined as

$$\langle v\sigma \rangle = \frac{N^{(z-1)+} - N_0^{(z-1)+}}{N^{z+}} \frac{v_i}{L\rho\varepsilon} \quad (3.1)$$

where N^{z+} is the number of incoming ions with charge z , in any state, collected in the Faraday cup, $N^{(z-1)+}$ is the number of recombined ions detected by the position sensitive detector and $N_0^{(z-1)+}$ is the non-resonant background contribution; L is the length of the interaction section, ε is the ion detection efficiency, v is the electron velocity in the ion frame, v_i is the ion velocity and ρ is the electron density which was typically $5 \times 10^7 \text{ cm}^{-3}$.

In order to compare the experimental results with theory, a 'rate coefficient' may be obtained from the theoretical cross section via

$$\langle v\sigma \rangle = \int v\sigma(v)f(v) d^3v \quad (3.2)$$

where σ is the DR cross section obtained from the theory and $f(v)$ is the electron-velocity distribution associated with the longitudinal temperature T_{\parallel} and the perpendicular temperature T_{\perp} . It was found that the measured shape of the DR resonances contained information which could easily yield the two temperatures. The temperatures were given by $kT_{\perp} = 0.15 \text{ eV}$ and $kT_{\parallel} = 0.001 \text{ eV}$.

In the experiment a strong electric field ($\approx 10 \text{ kV cm}^{-1}$) was used to separate the direct beam from the ions which had collected an electron. This field caused Rydberg electrons to be field ionized. Thus, Rydberg levels with quantum numbers n greater than n_c were excluded from the evaluation of the 'rate coefficient', where n_c was calculated according to

$$n_c = (6.2 \times 10^8 z^3 / F)^{1/4} \quad (3.3)$$

where z is the ion core charge and F is the applied electric field in units of V cm^{-1} .

Due to the charge of the electrons, the ions experienced a small electric field transverse to the beam direction when they passed through the interaction region. From the geometry of the apparatus, the electron density and the size of the beams, we estimate the field to have been a few V cm^{-1} . Due to the presence of small transverse magnetic fields in the interaction region (typically 0.5 G) a motional electric field was also produced in the ion frame. This field may also have been of the order of a few V cm^{-1} . Thus, the total electric field in the interaction region is estimated to have been between 0 and 10 V cm^{-1} .

For the Be-like ions, the ions in the beam were found not only in the $1s^2 2s^2 1S$ ground state, but some fraction were found to be in the $1s^2 2s2p 3P$ metastable state. In order to determine the metastable fraction, we used the so called 'needle ionization' method (see Bruch *et al* 1987). In this method, the Be-like ion beam was passed through a thin He gas. Holes were then produced in the K-shell of the ions in the beam without much perturbation of the outer shells. The Auger electrons ejected from the excited states were then detected at zero degrees. In particular, we measured the Auger yield from the $1s2s^2 2S$ and $1s2s2p 4P$ states of C^{3+} and O^{5+} . By normalization to the earlier measurements of Bruch *et al* (1987) which were obtained with a higher energy resolution, we were able to obtain the metastable fractions from the ratio of the two Auger line intensities. We obtained $70\% \pm 10\%$ for O^{4+} and $75\% \pm 10\%$ for C^{2+} . This

is in close agreement with the results obtained at Oak Ridge National Laboratory by Dittner *et al* (1987). No measurements were performed for F^{5+} . Based on the results for the C and O beams, a metastable fraction of about 70% seems a reasonable estimate for F^{5+} .

No measurements of the metastable fraction were performed for the B-like ions. Instead, we assume that our metastable fractions were about the same as those that were obtained by Dittner *et al* (1988) at Oak Ridge National Laboratory, as was the case for Be-like ions. The same kind of accelerator and almost the same ion velocity were used in both sets of experiments. Thus, for B-like ions, we estimate that 50% of the ions in the beam were in the $1s^2 2s 2p^2 4P$ metastable state.

4. Results

Our earlier theoretical work has shown the effect of intermediate coupling to be negligible for light Be-like ions (Badnell and Pindzola 1989b) and to be small ($\leq 10\%$) for B-like ions (Badnell and Pindzola 1989a). In the light of the large uncertainties involved when making comparisons with experiment, the results presented below were calculated as described in section 2 using the *LS*-coupling approximation, unless otherwise stated.

4.1. C^{2+} , O^{4+} and F^{5+}

In figures 1-3(a)-(c) we present our zero-field results for DR from the ground (b) and metastable (c) states of the Be-like ions C^{2+} , O^{4+} and F^{5+} and compare them with our experimental results (a). The theoretical results are for 100% occupation of the initial ground and metastable states and with 100% survival of the final Auger metastable state. The cut-offs used were $n_c = 26, 43$ and 51 for C^{2+} , O^{4+} and F^{5+} , respectively. Thus, to make an absolute comparison between theory and experiment the theoretical results must be multiplied by the experimental population fractions and an enhancement factor due to the electric fields within the interaction region; additionally, the final Auger metastable results must be multiplied by a survival fraction. On statistical grounds, one would expect a $2s 2p\ 3P$ population fraction of about 75% and about 25% for the $2s^2\ 1S$ and this indeed was found to be the case (see section 3).

Using the modified form of DRACULA which averages over the coupling between the *LS*-coupled core and the Rydberg electron, we obtained a maximum field enhancement factor for the $2s^2\ 1S \rightarrow 2s 2p\ 1P$ Rydberg peak A of 3.1, 4.1, and 4.3 for C^{2+} , O^{4+} and F^{5+} , respectively. Assuming a $2s^2\ 1S$ population fraction of 25%, we would then require a field enhancement factor of about 1.5 for O^{4+} and 2.0 for F^{5+} . Allowing for decreased field enhancement (to an estimated factor of 1.2) with decreased residual charge (due to the decreasing cut-off), as illustrated by our maximum field enhanced results; then theory and experiment are consistent for C^{2+} if the $2s^2\ 1S$ population fraction is at the limit of the uncertainty of the measurement, i.e. 15% or so.

Next, for the $2s 2p\ 3P + e^- \rightarrow 2p^2(3P)nl \rightarrow 2s 2p(3P)nl$ reaction, we found that for all three ions, between 30% and 50% of the cross section ended up in the $2s 2p(3P)nl$ metastable states with Auger lifetimes in the milli- to microsecond range and hence could be counted as 'recombined' in the experiment. The resulting Rydberg peak (C) will also be field enhanced. Assuming a statistical population for the metastable initial

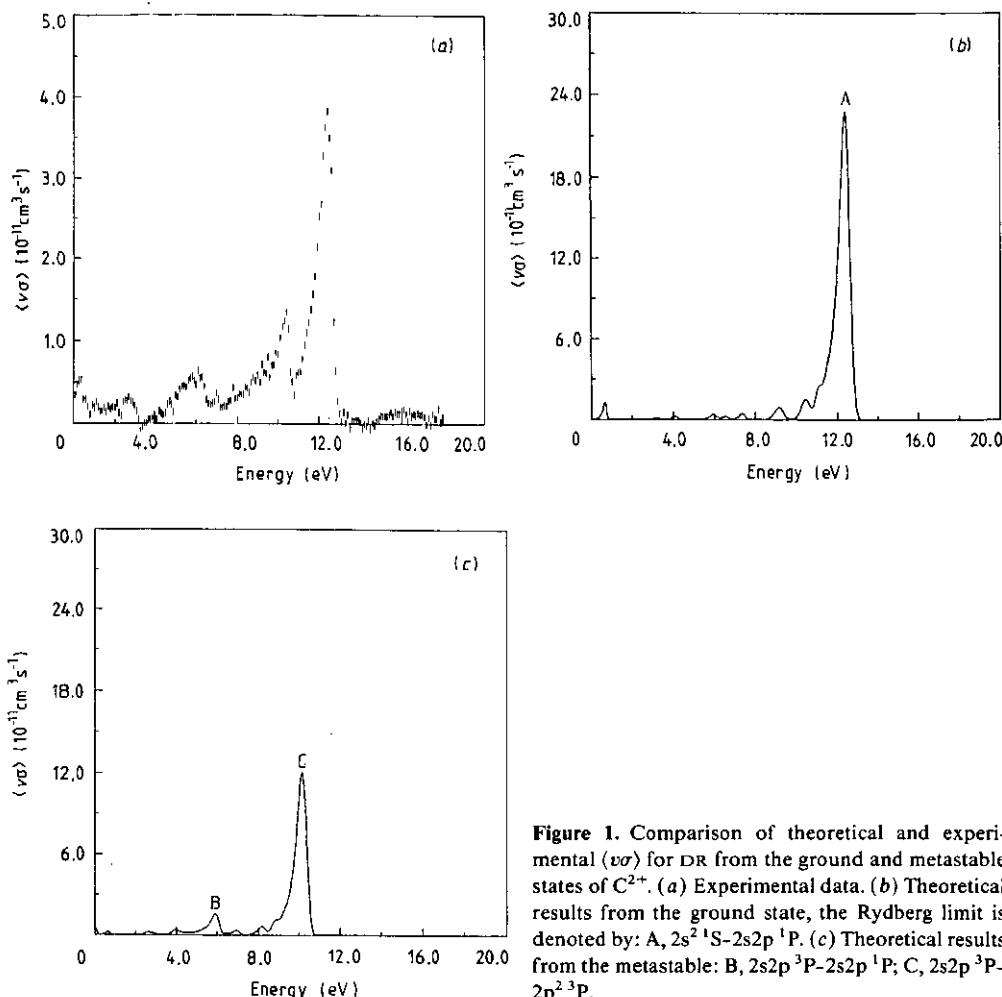
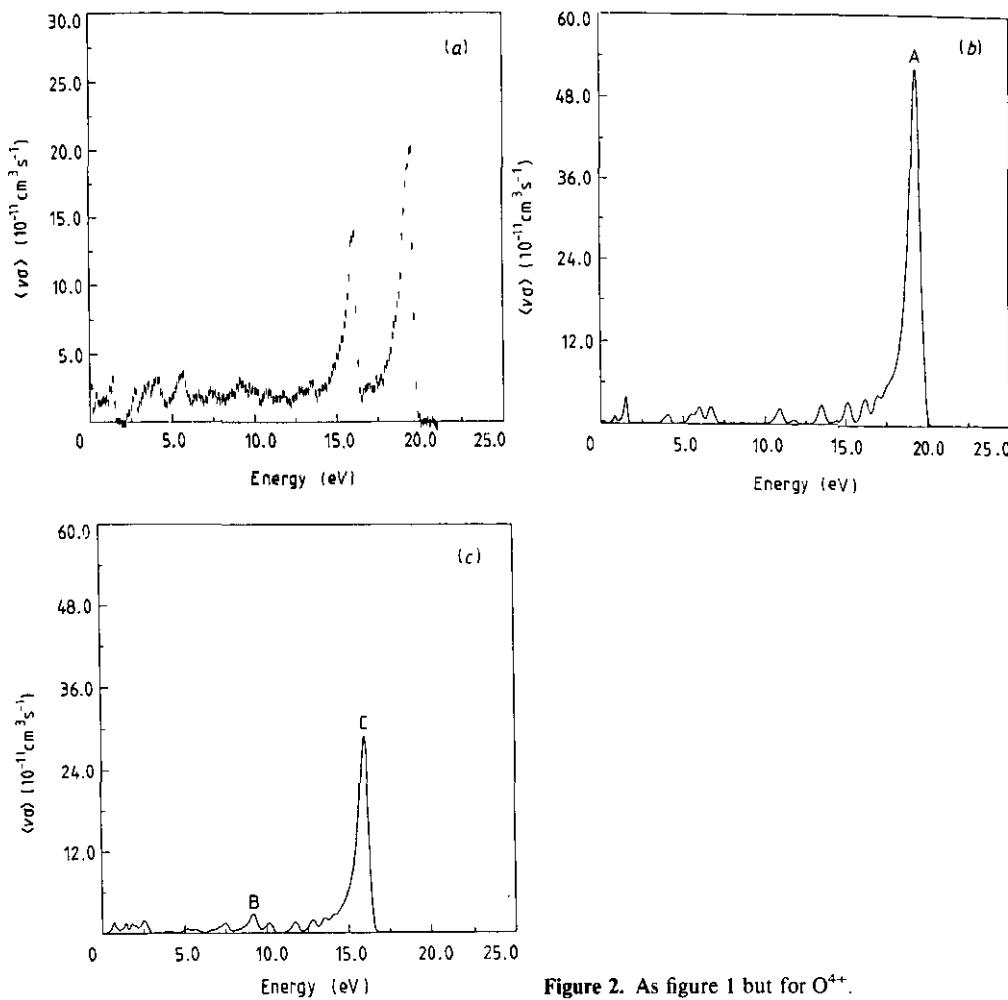


Figure 1. Comparison of theoretical and experimental $\langle\nu\sigma\rangle$ for DR from the ground and metastable states of C^{2+} . (a) Experimental data. (b) Theoretical results from the ground state, the Rydberg limit is denoted by: A, $2s^2 1S-2s2p\ 1P$. (c) Theoretical results from the metastable: B, $2s2p\ 3P-2s2p\ 1P$; C, $2s2p\ 3P-2p^2\ 3P$.

state of 75%, then the survival fraction of 50% to 30% is consistent with a field-enhancement factor of 1.5 to 2.0. Thus, we see that we can qualitatively explain the main experimental features, but all we can say quantitatively is that theory and experiment are consistent when using reasonable values for the unknown factors, as described above.

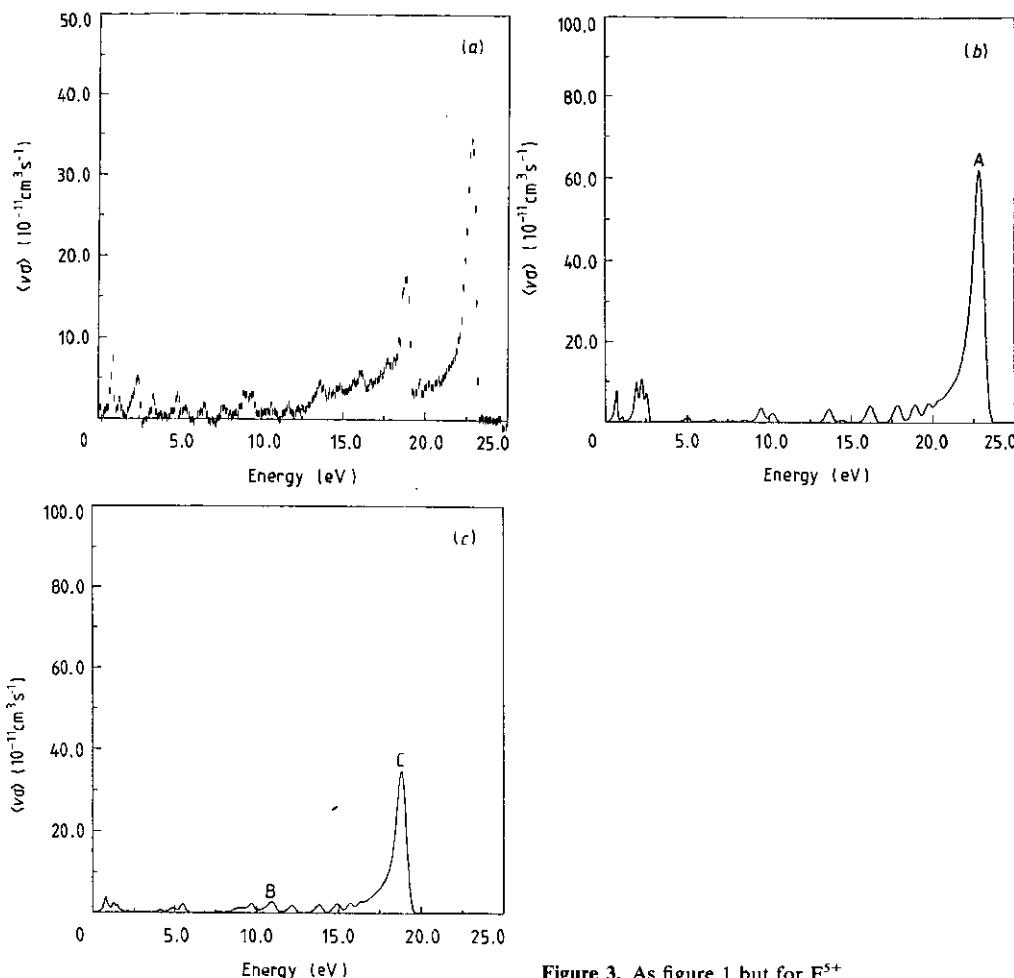
At this point, one might ask if a DR reaction ending up in an Auger metastable state, namely $2^3S + e^- \rightarrow 2^3P\ nl \rightarrow 2^3S\ nl$, might not explain certain anomalies found in the experiments on He-like ions (see Andersen *et al* 1990), rather than invoking some unknown mixing mechanism (see Badnell *et al* 1990). The answer is no, because this reaction relies on a $\Delta n = 0$ transition for radiative stabilization. Even with a 100% survival of the Auger metastable final state, we found the contribution from this reaction to be negligible compared with the $2^3S + e^- \rightarrow 2^1P\ nl \rightarrow 1^1S\ nl$ reaction, which relies on a $\Delta n = 1$ transition for radiative stabilization. Conversely, one might ask if some mixing mechanism, as invoked to explain anomalies in the experiments on He-like ions, might not explain the experiments on Be-like ions by mixing the accumulation of resonances $2p^2(^3P)nl$ ($n > 20$ say) with a low-lying $2s2p(^1P)n'l'$ resonance. Again, the answer is

Figure 2. As figure 1 but for O⁴⁺.

no because of the $\Delta n = 1$ and $\Delta n = 0$ transitions for the radiative stabilization. In the case of He-like ions, only a very weak mixing was required to generate a radiative rate for the 'forbidden' channel that was comparable with the Auger (and hence capture) rates for that resonance (because $A_r \gg A_a$ for the 'allowed' channel). In the case of Be-like ions ($A_r \ll A_a$) a weak redistribution of radiative rates from the 'allowed' to the 'forbidden' channel generates a negligible DR cross section (because $\sigma_d \sim A_r$).

4.2. O³⁺ and F⁴⁺

In figures 4 and 5(a)–(c) we present our zero-field results for DR from the ground (b) and metastable (c) states of the B-like ions O³⁺ and F⁴⁺ and compare them with our experimental results (a). The cut-offs used were $n_c = 34$ for O³⁺ and $n_c = 43$ for F⁴⁺. Again, the theoretical results are for 100% occupation of the initial states and 100% survival of the Auger metastable final states. We did not measure the population fractions for the B-like ions and, unlike the case of He-like ions (see Badnell *et al* 1990), we cannot determine theoretically what the experimental metastable fraction might be as the only real comparison that can be made between theory and experiment

Figure 3. As figure 1 but for F⁵⁺.

is for the field enhanced Rydberg peaks. However, as argued in section 3, it is reasonable to assume a statistical fraction, i.e. 50% ground and 50% metastable.

There are now three Rydberg peaks (A, B and C) to be seen for B-like ions corresponding to $2s^2 2p^2 P + e^- \rightarrow 2s 2p^2 (2D, 2S, 2P) nl \rightarrow 2s^2 2p^2 (2P) nl$. The experimental ratio for the 2P to 2D peaks is 1.8 for O³⁺ and 1.9 for F⁴⁺, compared to zero-field LS coupling ratios of 3.0 for O³⁺ and 2.7 for F⁴⁺. Our intermediate coupling results (still zero field) increase the 2P peak (C) by 10%, while there is little change in the 2D and 2S peaks (A and B), so this just increases the discrepancy. Previously (see Badnell and Pindzola 1989a) we obtained a maximum field enhancement factor of three but since this was obtained in the configuration-averaged approximation there is no term dependence. Thus, we would require different field enhancements of the 2D and 2P peaks to explain the experimental results; a similar finding was noted in the comparison between theory (Badnell and Pindzola 1989a) and the low-resolution experimental results of Dittner *et al* (1988). Assuming a 50%-50% population fraction for the ground and metastable states, we would then require field enhancement factors of 2.0 and 1.5 for the 2D peaks of O³⁺ and F⁴⁺, respectively, with little or no enhancement of the 2S and 2P peaks.

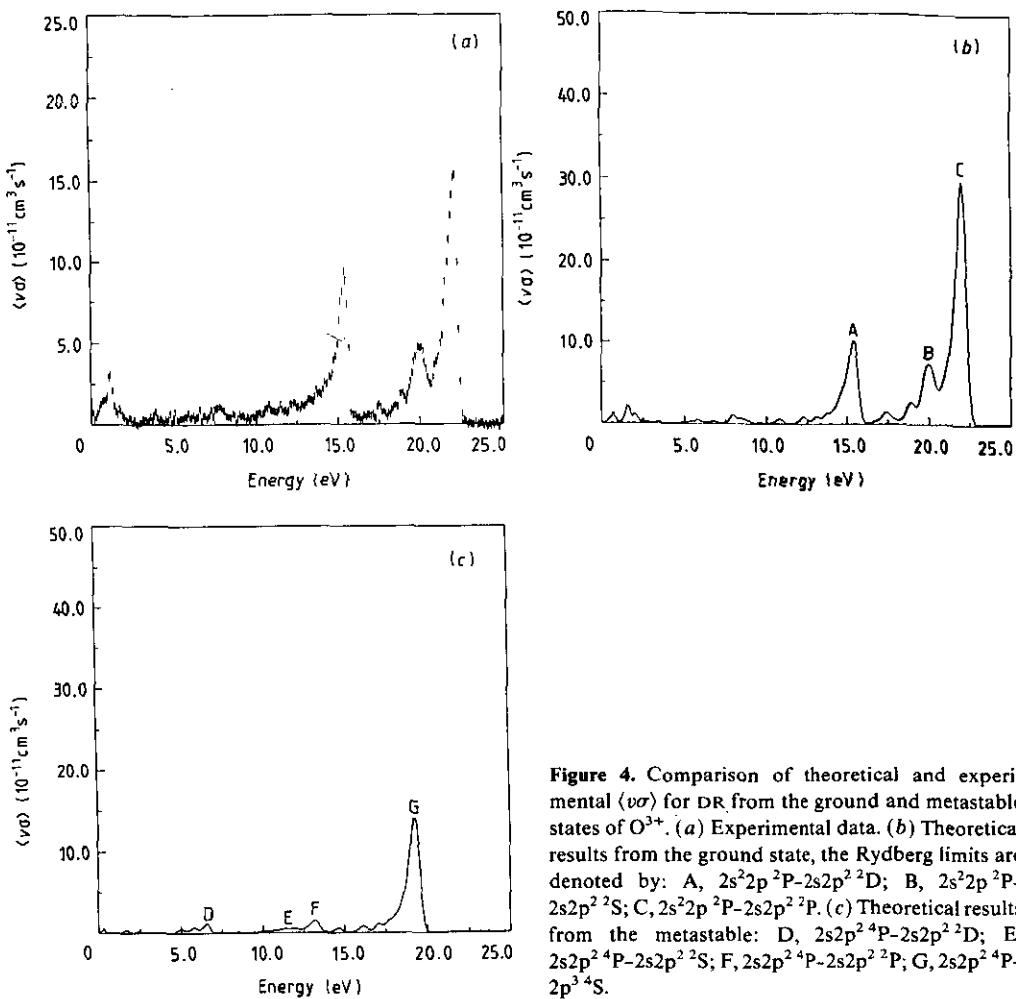
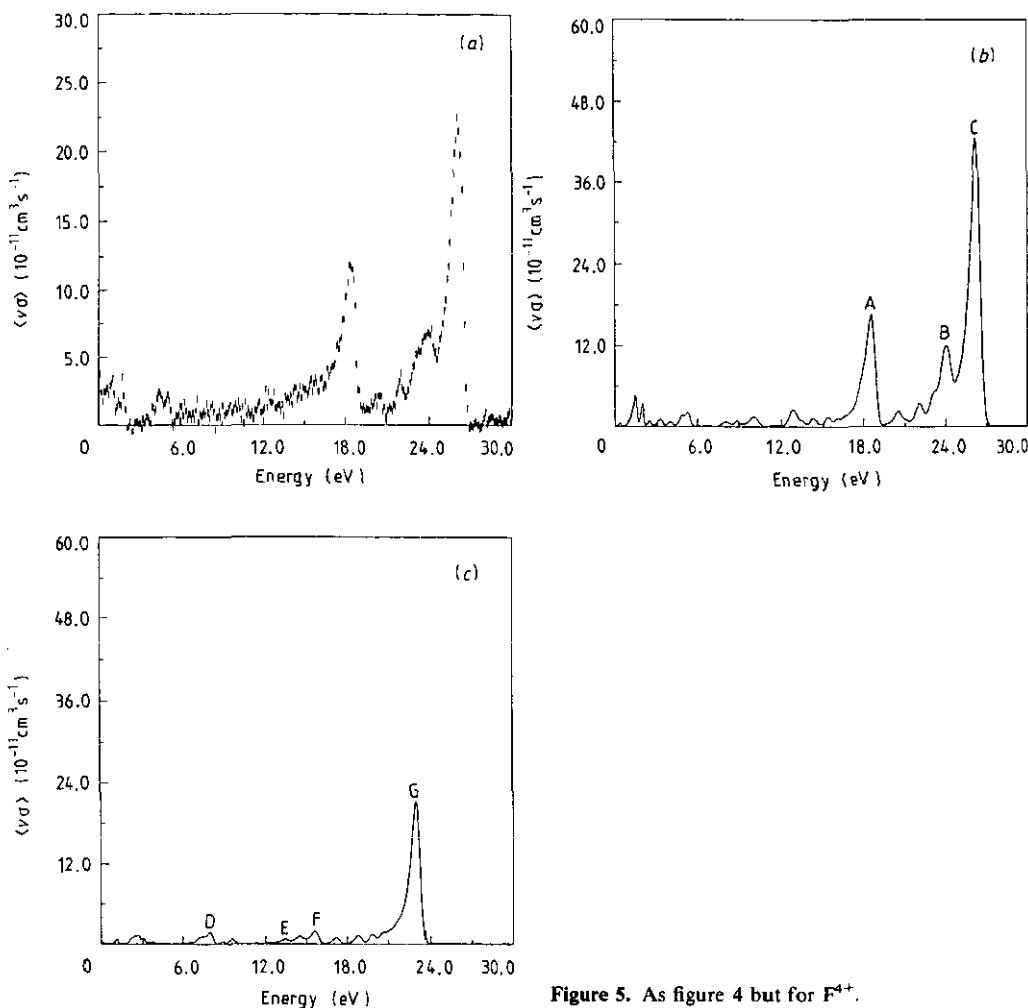


Figure 4. Comparison of theoretical and experimental $\langle v\sigma \rangle$ for DR from the ground and metastable states of O^{3+} . (a) Experimental data. (b) Theoretical results from the ground state, the Rydberg limits are denoted by: A, $2s^2 2p^2 P - 2s 2p^2 ^2D$; B, $2s^2 2p^2 P - 2s 2p^2 ^2S$; C, $2s^2 2p^2 P - 2s 2p^2 ^2P$. (c) Theoretical results from the metastable: D, $2s 2p^2 ^4P - 2s 2p^2 ^2D$; E, $2s 2p^2 ^4P - 2s 2p^2 ^2S$; F, $2s 2p^2 ^4P - 2s 2p^2 ^2P$; G, $2s 2p^2 ^4P - 2p^3 ^4S$.

For the $2s 2p^2 ^4P + e^- \rightarrow 2p^3 (^4S) nl \rightarrow 2s 2p^2 (^4P) nl$ reaction (peak G) we now find that only 10% to 20% of the DR cross section ends up in states with an Auger lifetime in the milli- to microsecond range. This, together with the smaller estimated metastable fraction than for Be-like ions, must explain why there is little evidence of DR from the metastable for B-like ions, unlike the case of Be-like ions. The Rydberg peak (G) for DR from the metastable would be buried just below the 2S peak (B). There may be some experimental evidence for this in the low-energy broadened 2S peak in F^{4+} , just below 24 eV, but not so for O^{3+} . Again, as for the Be-like ions, we can identify the main features of the experimental results and their magnitudes are consistent with theory, given the uncertainties described above.

5. Summary

We have continued our theoretical and experimental analysis of the DR of light ions. We have described the main features of the experiments on Be-like and B-like ions. We have shown how the metastable states could make a significant contribution

Figure 5. As figure 4 but for F^{4+} .

and have identified such a contribution in the experiments on Be-like ions, but not B-like ions. However, the main obstacle to a quantitative comparison between theory and experiment is still the presence of weak electric fields in the interaction region and they are likely to remain. Field dependent calculations have been carried out for several Li-like ions (Griffin *et al* 1989) but these used a constant field strength because the field in the interaction region is still largely unknown. A determination of the electric fields throughout the interaction region and of the beam-overlap profile would enable variable field dependent cross sections to be calculated. If satisfactory results were obtained for Li-like ions, then the same theoretical and computational approach could be extended to complex ions, in principle. If not, further effects would need to be investigated, e.g. *n*-mixing.

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