PHYSICAL REVIEW A VOLUME 39, NUMBER 4 FEBRUARY 15, 1989

Intermediate-coupling calculations for the dielectronic recombination of B-like ions

N. R. Badnell* and M. S. Pindzola
Department of Physics, Auburn University, Auburn, Alabama 36849-5311

(Received 24 June 1988)

We have calculated $\Delta n=0$ dielectronic recombination cross sections and rate coefficients for the B-like ions C^+, N^{2+}, O^{3+}, and F^{4+} in the *LS*-coupling and intermediate-coupling approximations, using the program AUTOSTRUCTURE, as well as in a partitioned configuration-average approximation (PCA). There is broad agreement between the zero-field PCA results and the *LS*-coupling and intermediate-coupling results, which differ by no more than 10%. The experimental cross sections obtained by Dittner *et al.* lie between the zero-field and the maximum-field-enhanced PCA results, the enhancement being a factor of 3. In the case of the rate coefficients the general formula of Burgess was found to overestimate the zero-field results by a factor of between 1.3 and 1.8, mainly due to the neglect of autoionization into excited states.

I. INTRODUCTION

In recent years there has been much theoretical and experimental interest in the dielectronic recombination (DR) of low-charge-state ions and the effect of external electric fields thereon, see the recent review by Belic and Pradhan.[1] In particular, there have been the experiments by Dittner *et al.*[2] on Li-like ions and theoretical calculations by Griffin *et al.*[3] and by LaGattuta,[4] while Be-like ions have been studied experimentally by Dittner *et al.*[5] and theoretically by Griffin, Pindzola, and Bottcher[3] and by LaGattuta *et al.*[6] There was an early experiment on the B-like ion C^+ by Mitchel *et al.*[7] over a very narrow energy range and a theoretical description by LaGattuta and Hahn.[8] Recently, Dittner *et al.*[9] have performed experiments on the B-like ions N^{2+}, O^{3+}, and F^{4+} and Hahn and Nasser[9] carried out theoretical calculations in *LS* coupling.

In the DR of complex ions structure effects become important and a number of core excitations (and deexcitations) are possible. In the case of B-like ions we have capture to and from levels of the ^4P metastable as well as transitions between levels of the $2p^2\,{}^2D$, ^2S, and ^2P terms. The term dependence of the core means that the usual configuration average[10] (CA) approximation is a poor one since the DR cross section is centered on the configuration-average energy and no account is taken of autoionization into excited states within the configuration. The first problem can be dealt with by redistributing the CA DR cross section over the individual core levels, but the second problem remains. Autoionization into excited states is also not allowed for in the semiempirical formulas[11,12] for DR rate coefficients used in non-local-thermodynamic-equilibrium plasma models. Thus we use the program AUTOSTRUCTURE (Refs. 13–15) to carry out *LS*-coupling and intermediate-coupling (IC) calculations in the zero-field limit and we use the program DRACULA (Ref. 10) modified to carry out a partitioned configuration-average (PCA) calculation with zero field and with maximum field enhancement.

In Sec. II we outline the theory behind our calculations, in Sec. III we describe its application to B-like ions, and in Sec. IV we present our results and compare them with experimental cross sections[9] and with the Burgess[11] general formula (GF) for the rate coefficients.

II. THEORY

The energy-averaged dielectronic recombination cross section for a given initial state i through an intermediate state j is given by[16]

$$\bar{\sigma}_d(i;j)=\frac{(2\pi a_0 I)^2}{E_c\Delta E_c}\,\frac{\omega(j)}{2\omega(i)}\times\frac{\tau_0\sum_k A_r(j\rightarrow k)\sum_l A_a(j\rightarrow i,E_c l)}{\sum_h\left[A_r(j\rightarrow h)+\sum_l A_a(j\rightarrow h,E_c l)\right]}\,, \tag{1}$$

where E_c is the energy of the continuum electron, which is fixed by the position of the resonances, and ΔE_c is the bin width. $\omega(j)$ is the statistical weight of the $(N+1)$ electron doubly excited state, $\omega(i)$ is the statistical weight of the N-electron target ion, and $(2\pi a_0)^2\tau_0=2.6741\times10^{-32}$ cm^2 sec. The total dielectronic recombination-rate coefficient may be written in terms of the energy-averaged cross section thus,[16]

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

where $(4\pi a_0^2)^{3/2}=6.6011\times10^{-24}$ cm^3.

Equations (1) and (2) may be evaluated in configuration-mixing *LS*-coupling and intermediate-coupling approximations using AUTOSTRUCTURE. In the past, AUTOSTRUCTURE has only been used to solve low-n problems.[13-15] To solve the high-n problem we make use of[17]

$$\lim_{n\to\infty}\left[\frac{\pi\nu_{nl}^3}{2z^2}\right]^{1/2} P_{nl}(r)=F_{kl}(r)|_{k=0} \quad (3)$$

at finite n. P_{nl} is a bound-state radial function and F_{kl}, a continuum radial function calculated in the same model potential. Here $k^2=E$, $\nu_{nl}=n-\mu_l$, and $\mu_l=\delta_l(0)/\pi$, where μ_l is the quantum defect and $\delta_l(0)$ is the non-Coulomb phase shift. This enables us to continue diagonalizing the Hamiltonian for each n so as to take account of the changing structure as n increases, in particular, the competition between the spin-orbit interaction and the electrostatic interaction. This detail is lost if one just extrapolates the rates as n^{-3}. We have incorporated asymptotic codes used in the scattering problem[18,19] to solve the long-range continuum-continuum integrals that arise from using Eq. (3). Furthermore, to cope with the wider range of continuum energies required for the DR of a complex ion, due to the number of different autoionizing channels, we have set up the program so that there is no restriction on the number of user-supplied interpolation energies; typically we used 10 to 15 energies. For each individual autoionizing energy the program selects the nearest N points to carry out the interpolation, currently $N=6$.

If we use DRACULA to evaluate Eq. (1) in the configuration-average approximation the presence of metastables severely distorts the results. We attempt to take account of the structure within a configuration by statistically partitioning the CA cross section over the nonmetastable intermediate levels of the core and binning them according to the observed level energies or those evaluated from Cowan's structure code.[17] We further partition the cross section over the target levels either by using a Boltzmann distribution for the initial-level population or by using the experimental population distribution. We denote this the partitioned configuration-average approximation; still, no account is taken of autoionization into excited states within a configuration. The motivation to improve the CA approximation comes from the knowledge that it becomes impractical to use IC or even LS coupling for ions with many open-shelled electrons that are of interest in fusion studies.

We estimate the maximum field enhancement of the DR cross section in the PCA approximation by a Clebsch-Gordan transformation of the autoionization rates, for a fixed n, from spherical to parabolic coordinates. This approach is probably accurate to within a factor of 2 and has previously been shown to be consistent with experiment.[2–6,20] In LS coupling or intermediate coupling a crude improvement would be to transform separately each set of autoionization rates attached to a core term or level. In fact, the general method to pursue would be the inclusion of the electric field term in the Hamiltonian and the diagonalization of individual M matrices as has been performed for each n by other workers[3] for the special case of a single core electron outside of a closed shell. Even this does not address the problem of n mixing which Harmin[21] and Sakimoto[22] have shown to be important in model calculations. If the findings of these model calculations are applicable to our case, then n-mixing would tend to reduce our maximum-field-enhanced results.

III. APPLICATION TO B-LIKE IONS

We consider $1s^2$:

$$\left.\begin{array}{l} 2s^2 2\bar{p}\;{}^2P^0+kl_c \\ 2s2p^2\;{}^4P+k'l_c' \end{array}\right\} \rightleftarrows \begin{array}{c} 2s2p^2({}^4P,{}^2D,{}^2S,{}^2P)nl \rightarrow 2s^2 2\bar{p}({}^2P^0)nl \\ \downarrow \\ 2s2p^2\;{}^2D,{}^2S,{}^2P+k'l_c', \end{array} \quad (4)$$

where $l_c=l\pm1$, $l_c'=l,l\pm2$, and in LS coupling,

$$|2s^2 2\bar{p}\;{}^2P^0\rangle=0.98|2s^2 2p\;{}^2P^0\rangle-0.19|2p^3\;{}^2P^0\rangle\ .$$

It has already been shown that the effect of $1\rightarrow2$[16] and $2\rightarrow3$[13] core transitions is negligible for low-Z Be-like ions, and the same can be expected to be true for B-like ions.

The core radial functions were determined using an N-electron Thomas-Fermi model potential with nl-dependent scaling parameters chosen so as to best represent the observed energy levels for the core. We also tried using scaling parameters obtained from minimizing a weighted sum of core energies. The resulting energy-level structure was not as good as before and it is interesting to note that the core radiative rates were 3–15 % lower, depending on the transition and the ion, indicating a level of uncertainty in our DR results of around 10% due to sensitivity to the core structure. Furthermore, if we neglect correlation the resulting core structure is again poor. Finally, the valence and continuum radial functions were evaluated using an $(N+1)$-electron Thomas-Fermi potential with the scaling parameters set to unity.

We sum process (4) over nl in the PCA, LS coupling, and intermediate-coupling approximations described in Sec. II. To compare with experiment[9] we impose a cutoff on n, to take account of field ionization by the analyzer, given by

$$n_c=\left[\frac{6.2\times10^8}{F}q^3\right]^{1/4}, \quad (5)$$

where F (V/cm) is the field strength and q is the initial change state of the ion. This simple formula (5) has been shown to be a very good approximation in comparison with hydrogenic field-ionization formulas.[23] For $F=4.5$ kV/cm we obtain $n_c=32$, 44, and 54 for N^{2+}, O^{3+}, and F^{4+}, respectively.

To evaluate the zero-field rate coefficient we sum up to $n=1000$; more precisely, we sum each n up to $n=20$ and then evaluate (1) at a series of n values up to $n=1000$ chosen such that $n_i^{-2}-n_{i+1}^{-2}\approx n_{i+1}^{-2}-n_{i+2}^{-2}$. The sum over n is converted into an integral which is evaluated by using Simpson's rule with the transformation $u=n^{-2}$. We can then compare this rate coefficient with that evaluated from the zero-field general formula of Burgess.[11] Although the presence of electric fields within a plasma will surely field ionize the high-n values, thus reducing the rate, they will also enhance the rate for those n that survive and the two effects tend to cancel. We return to this point in Sec. IV.

IV. RESULTS

A. Convoluted cross sections

In Figs. 1 to 3 we compare our theoretical PCA, *LS*-coupling, and intermediate coupling results for N^{2+}, O^{3+}, and F^{4+} with the experimental results of Dittner *et al.*[9] We have multiplied our energy-averaged cross sections by the relative velocity of the electron and ion beams and then convoluted this product with a relative velocity distribution function determined from earlier experiments.[2,20] Furthermore, since the experimental beam contains 50% of the ions in levels of the ground-state term and 50% in the metastable levels,[9] we then took half of the DR cross section from levels of the ground-state term plus half the DR cross section from the metastable levels. However, since DR from the metastables is negligible, Dittner *et al.*[9] multiplied their experimental results by a factor of 2 to get an approximate DR cross section for a 100% occupied ground term. This is why the results plotted in the paper by Dittner *et al.*[9] are a factor of 2 larger than those plotted here. The experimental results of Mitchel *et al.*[7] for C^+ cover only a very narrow energy range, and they do not know the fraction of the ion beam in the metastable states or the electron velocity distribution so little can be gained from a comparison with their results.

Our peak *LS* coupling and IC results for DR from the metastable levels are 5% of those for DR from levels of the ground-state term, so that DR from the metastable levels is negligible. Our IC results lie 5–10 % above our *LS*-coupling results for each ion. There are no *LS*-forbidden autoionizing terms that can contribute on switching to IC and this small enhancement is probably just due to the redistribution of the transition rates. The double-peak structure is due to DR via Rydberg series attached to the ^2D and ^2P cores; the contribution from the ^2S series is small and blends in with the other two. For all three ions the *LS* coupling and IC results predict a larger peak due to the ^2P core than the ^2D. Although the higher statistical weights are associated with the ^2D core, the ^2D-core radiative rate is a factor of 10 smaller than the ^2P, due in part to the smaller energy separation. While this appears true experimentally for N^{2+}, the position is reversed for O^{3+} and F^{4+}, although there is no reason to expect the field enhancement to be the same for both Rydberg series. The *LS*-coupling results of Hahn and Nasser[9] (not shown) lie 7–20 % below our *LS*-coupling results.

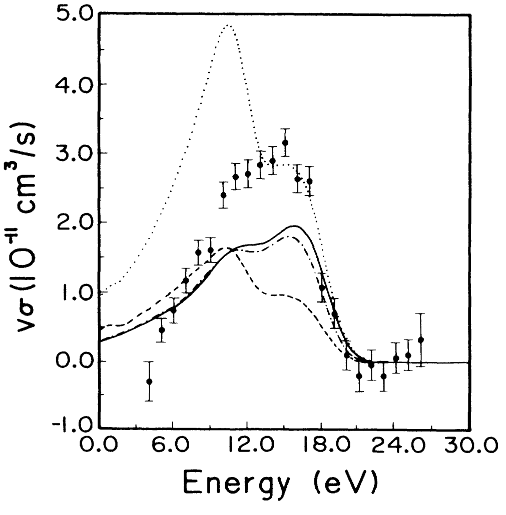

FIG. 1. DR cross sections for N^{2+} convoluted with Oak Ridge National Laboratory velocity distribution. —·—·—, *LS* coupling; ——, intermediate coupling; — — —, zero-field PCA approximation; · · · ·, maximum-field-enhanced PCA: all this work. Φ experimental points from Dittner *et al.* (Ref. 9).

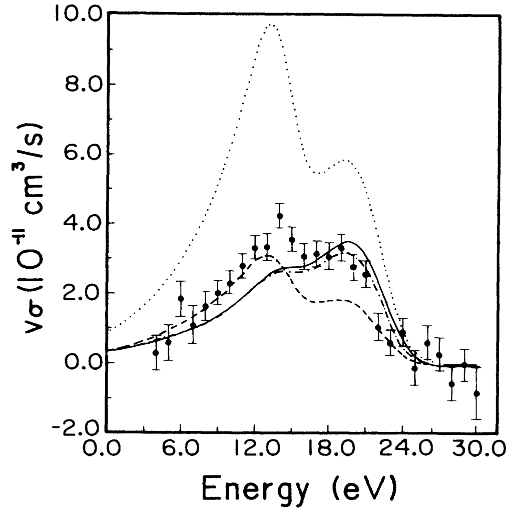

FIG. 2. DR of O^{3+}. Notation as in Fig. 1.

The zero-field PCA results are in fairly good agreement with the *LS*-coupling and IC results, although the ^2D peak is higher than the ^2P peak due to the statistical weighting within the PCA approximation. If we neglect autoionization into excited states, our *LS* coupling and *IC* results are increased by 20–30 %. The maximum field enhancement is a factor of 3, and the experimental results

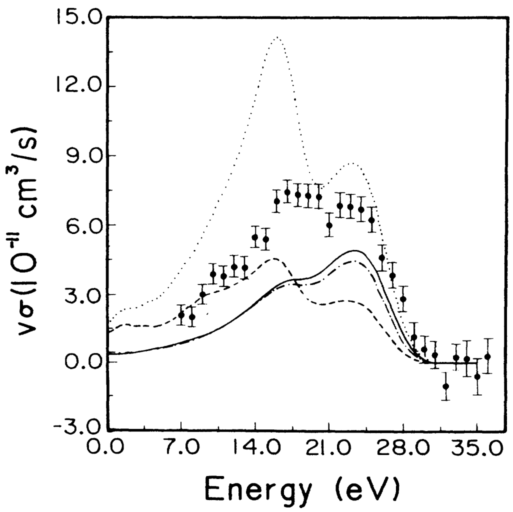

FIG. 3. DR of F^{4+}. Notation as in Fig. 1.

TABLE I. Dielectronic recombination rate coefficients (cm^3 s^{-1}).

$\log_{10}T$ (K)	C^+	N^{2+}	O^{3+}	F^{4+}
4.3	6.48[−13][a]			
4.4	1.72[−12]	1.28[−12]		
4.5	3.62[−12]	3.29[−12]	2.91[−12]	
4.6	6.25[−12]	6.95[−12]	5.61[−12]	4.87[−12]
4.8	1.17[−11]	1.82[−11]	1.73[−11]	1.46[−11]
5.0	1.38[−11]	2.74[−11]	3.20[−11]	3.17[−11]
5.2	1.20[−11]	2.80[−11]	3.80[−11]	4.32[−11]
5.4	8.54[−12]	2.21[−11]	3.33[−11]	4.16[−11]
5.6	5.35[−12]	1.68[−11]	2.39[−11]	3.16[−11]
5.8	3.09[−12]	8.93[−12]	1.50[−11]	2.07[−11]
6.0	1.70[−12]	5.03[−12]	8.69[−12]	1.23[−11]
6.2	8.99[−13]	2.71[−12]	4.77[−12]	6.85[−12]
6.4	4.67[−13]	1.42[−12]	2.53[−12]	3.67[−12]
6.6	2.39[−13]	7.35[−13]	1.32[−12]	1.92[−12]
6.8	1.22[−13]	3.75[−13]	6.75[−13]	9.89[−13]

[a] $6.48[-13]=6.48\times10^{-13}$.

lie between the zero-field and maximum-field-enhanced PCA results. Although Hahn and Nasser[9] obtain a maximum-field-enhancement factor of 6, this enhancement[9] is based on a simple counting argument[24] which is prone to overestimation. The field strength in the interaction region is difficult to assess.[2] However, earlier experimental results for Na-like[20] and Be-like[5] ions fell between the zero-field and maximum-field-enhanced results,[3,5] although the Li-like ions[2,3] did not. Finally, we note that allowing the outer electron to radiate increases our *LS* and IC results by only a few percent, while neglect of correlation increases them by 15%.

B. Maxwellian rate coefficients

In Table I we present our zero-field IC DR rate coefficients for C^+, N^{2+}, O^{3+}, and F^{4+} statistically averaged over levels of the ground-state term. Since $1\to n$ and other $2\to n$ core transitions[13,16] can be neglected, these can be regarded as total rate coefficients. Again, our IC results are no more than 5% greater than our *LS*-coupling results at the peak DR temperature. DR via low-lying state dominates at temperatures below those tabulated as the exponential factor in Eq. (2) cuts off the contribution from the full Rydberg series. Detailed calculations at low temperatures have been carried out by Nussbaumer and Storey[25] for C^+, N^{2+}, and O^{3+}. For $T<6\times10^4$ K their[25] low-temperature contribution should be added in as a correction. Rate coefficients at temperatures higher than those tabulated may be obtained by scaling in $T^{-3/2}$.

It is interesting to note that if we cut off the *n* contribution at $n_c=32$ for N^{2+}, for example, then the zero-field DR rate coefficient drops by a factor of 2.5. However, we have seen earlier that the maximum field enhancement for the remaining *n* is a factor of 3.0. The results of the zero-field Burgess general formula,[11] evaluated with the same energy levels and oscillator strengths, are a factor of 1.8, 1.4, 1.4, and 1.3 larger than our zero-field *LS*-coupling results for C^+, N^{2+}, O^{3+}, and F^{4+}, respectively. However, if we exclude autoionization into excited states from our calculations, which is not modeled by the GF, then the overestimate drops to a factor of 1.3, 1.2, 1.2, and 1.2 for the same ions.

V. CONCLUSION

We have calculated DR cross sections and rate coefficients for B-like C^+, N^{2+}, O^{3+}, and F^{4+}. We have modified the CA approximation and the zero-field results are in broad agreement with our *LS* coupling and IC results which themselves differ by no more than 10%. DR from the ^4P metastable levels was found to be negligible. The experimental results of Dittner *et al.*[9] lie between our zero-field and maximum-field-enhanced PCA results, the enhancement being a factor of 3. Finally, the Burgess GF (Ref. 11) overestimates the zero-field rate coefficients by between a factor of 1.3 and 1.8, mainly due to the neglect of autoionization into excited states.

ACKNOWLEDGMENTS

We would like to thank Dittner *et al.* for a copy of their paper (Ref. 9) prior to publication and Dr. D. C. Griffin for some helpful conversations. This work was supported by a grant from the Office of Fusion Energy of the U.S. Department of Energy under contract No. DE-FG05-86ER53217 with Auburn University.

---

*Present address: Atomic Weapons Establishment, Aldermaston, Reading, RG7 4PR, United Kingdom.

[1] D. Belic and A. K. Pradhan, Comments At. Mol. Phys. **20**, 317 (1987).

[2] P. F. Dittner, S. Datz, P. D. Miller, P. L. Pepmiller, and C. M. Fou, Phys. Rev. A **35**, 3668 (1987).

[3] D. C. Griffin, M. S. Pindzola, and C. Bottcher, Phys. Rev. A **33**, 3124 (1986).

[4] K. J. LaGattuta, J. Phys. B **18**, L467 (1985).

[5] P. F. Dittner, S. Datz, H. F. Krause, P. D. Miller, P. C. Pep-

miller, C. Bottcher, C. M. Fou, D. C. Griffin, and M. S. Pindozla, Phys. Rev. A **36**, 33 (1987).

[6] K. LaGattuta, I. Nasser, and Y. Hahn, J. Phys. B **20**, 1577 (1987).

[7] J. B. A. Mitchel, C. T. Ng, J. L. Forand, D. P. Levac, R. E. Mitchel, A. Sen, D. B. Miko, and J. W. McGowan, Phys. Rev. Lett. **50**, 335 (1983).

[8] K. LaGattuta and Y. Hahn, Phys. Rev. Lett. **50**, 668 (1983).

[9] P. F. Dittner, S. Datz, R. Hippler, H. F. Krause, P. D. Miller, P. L. Pepmiller, C. M. Fou, Y. Hahn, and I. Nasser, Phys. Rev. A **38**, 2762 (1988).

[10] D. C. Griffin, M. S. Pindzola, and C. Bottcher, Phys. Rev. A **31**, 568 (1985).

[11] A. Burgess, Astrophys. J. **141**, 1588 (1965).

[12] A. L. Merts, R D Cowan, and N. H. Magee, Los Alamos Scientific Laboratory Informal Report No. LA-6220-MS, 1976 (unpublished).

[13] N. R. Badnell, J. Phys. B **19**, 3827 (1986).

[14] N. R. Badnell, J. Phys. B **20**, 2081 (1987).

[15] N. R. Badnell, J. Phys. B **21**, 749 (1988).

[16] Y. Hahn, Adv. At. Mol. Phys. **21**, 123 (1985).

[17] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981).

[18] A. Burgess and V. B. Sheorey, J. Phys. B **7**, 2403 (1974).

[19] N. R. Badnell, J. Phys. B **16**, 3268 (1983).

[20] P. F. Dittner, S. Datz, P. D. Miller, P. L. Pepmiller, and C. M. Fou, Phys. Rev. A **33**, 124 (1986).

[21] D. Harmin, Phys. Rev. Lett. **57**, 1570 (1986).

[22] K. Sakimoto, J. Phys. B **20**, 807 (1987).

[23] C. Bottcher, D. C. Griffin, and M. S. Pindzola, Phys. Rev. A **34**, 860 (1986).

[24] I. Nasser and Y. Hahn, Phys. Rev. A **30**, 1558 (1984).

[25] H. Nussbaumer and P. J. Storey, Astron. Astrophys. **126**, 75 (1983).