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

Intermediate-coupling effects in the dielectronic recombination of oxygen ions

N. R. Badnell* and M. S. Pindzola

Department of Physics, Auburn University, Auburn, Alabama 36849-5311

(Received 29 July 1988)

We have calculated $\Delta n=0$ dielectronic recombination (DR) cross sections and rate coefficients for O^{q+}, $q=1-5$, in configuration-mixing *LS*-coupling and intermediate-coupling approximations, using the program AUTOSTRUCTURE, as well as in a partitioned configuration-average (PCA) approximation. The intermediate-coupling cross sections (rate coefficients) are about 45% (25%) greater than the *LS*-coupling results in the case of O^+ and O^{5+}, due to the effect of core fine-structure interactions, while the increase is no more than 10% (5%) for O^{2+}, O^{3+}, and O^{4+}. There is good agreement between the zero-field PCA results and the intermediate-coupling results when DR takes place through a single core term, as in O^+, O^{4+}, and O^{5+}, but the PCA approximation gives poorer results when DR proceeds through more than one core term, as in O^{2+} and O^{3+}. The maximum-field-enhanced PCA results are about a factor of 3 greater than the zero-field results. 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 due to the neglect of autoionization into excited states or the averaging over incident angular momentum.

I. INTRODUCTION

The dielectronic recombination (DR) of oxygen ions is of current interest in fusion plasma research[1] and has been the subject of a number of recent experiments.[2-4] We have recently[5] carried out configuration-mixing *LS*-coupling and intermediate-coupling calculations for O^{3+} (and other B-like ions) in the zero-field limit using the program AUTOSTRUCTURE,[6] as well as partitioned configuration-average (PCA) calculations with zero-field and with maximum field enhancement. In this paper we apply the same calculational approach to $\Delta n=0$ core transitions in the oxygen isonuclear sequence; since few data exist for O^+ and O^{2+}, there exists a discrepancy between the results of two theoretical groups[3,7] for O^{4+}, and comparisons with previous *LS*-coupling and intermediate-coupling calculations[8,9] can be made for O^{5+}. Furthermore, high-resolution theoretical results will be required in support of future storage-ring experiments. Some discussion and results for O^{3+} will be included for completeness.

In Sec. II we give a brief description of the theory behind our calculations, in Sec. III we describe its application to oxygen ions, and in Sec. IV we present our results and compare them with experimental cross sections, where they exist, and with the Burgess[10] general formula for the rate coefficients. A brief conclusion is given in Sec. V.

II. THEORY

The energy-averaged dielectronic recombination cross section for a given initial state i through an intermediate state j is given by[11]

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

where E_c is the energy of the continuum electron, which is fixed by the position of the resonances, ΔE_c is the bin width, and I is the ionization potential of hydrogen; all in the same units of energy. $\omega(j)$ is the statistical weight of the $(N+1)$ electron doubly excited state, $\omega(i)$ is the statistical weight of the N-electron target ion, the rates are in units of inverse seconds, 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[11]

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

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 and in a partitioned configuration-average (PCA) approximation using a modified[5] form of DRACULA.[12] We can also use the PCA approximation to estimate the maximum field enhancement of the DR cross section by a Clebsch-Gordan transformation of the autoionization rates, for a fixed n, from spherical to parabolic coordinates. The calculational methods are the same as detailed in our earlier paper[5] on B-like ions and will not be repeated here.

III. APPLICATION TO OXYGEN IONS

We consider O^+, $1s^2$:

$$\begin{array}{ccccc} 2s^22p^3\,{}^4S^0,{}^2D^0,{}^2P^0+kl_c & \rightleftarrows & 2s2p^4({}^4P,{}^2D,{}^2S,{}^2P)nl & \rightarrow & 2s^22p^3({}^4S^0)nl+h\nu \\ & & \downarrow & & \\ & & 2s2p^4\,{}^4P,{}^2D,{}^2S,{}^2P+k'l'_c, & & \end{array}$$

where $l_c=l\pm1$ and $l'_c=l$. O^{2+}, $1s^2$:

$$\begin{array}{ccccc} \left.\begin{array}{l} 2s^22\bar{p}^{\,2}\,{}^3P,{}^1D,{}^1S+kl_c \\ 2s2p^3\,{}^5S^0+k'l'_c \end{array}\right\} & \rightleftarrows & 2s2p^3({}^5S^0,{}^3D^0,{}^3P^0,{}^1D^0,{}^3S^0,{}^1P^0)nl & \rightarrow & 2s^22\bar{p}^{\,2}({}^3P)nl+h\nu \\ & & \downarrow & & \\ & & 2s2p^3\,{}^3D^0,\ {}^3P^0,{}^3P^0,{}^1D^0,{}^3S^0,{}^1P^0+k'l'_c\ , & & \end{array}$$

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

$$|2s^22\bar{p}^{\,2}\,{}^3P,{}^1D\rangle=0.992|2s^22p^2\,{}^3P,{}^1D\rangle\pm0.125|2p^4\,{}^3P,{}^1D\rangle$$

and

$$|2s^22\bar{p}^{\,2}\,{}^1S\rangle=0.972|2s^22p^2\,{}^1S\rangle-0.235|2p^4\,{}^1S\rangle\ .$$

O^{3+}, $1s^2$:

$$\begin{array}{ccccc} \left.\begin{array}{l} 2s^22\bar{p}\,{}^2P^0+kl_c \\ 2s2p^2\,{}^4P+k'l'_c \end{array}\right\} & \rightleftarrows & 2s2p^2({}^4P,{}^2D,{}^2S,{}^2P)nl & \rightarrow & 2s^22\bar{p}({}^2P^0)nl+h\nu \\ & & \downarrow & & \\ & & 2s2p^2\,{}^2D,{}^2S,{}^2P+k'l'_c\ , & & \end{array}$$

where $l_c=l\pm1$, $l'_c=l,l\pm2$, and in LS coupling, $|2s^22\bar{p}\,{}^2P^0\rangle=0.981|2s^22p\,{}^2P^0\rangle-0.193|2p^3\,{}^2P^0\rangle$. O^{4+}, $1s^2$:

$$\begin{array}{ccccc} \left.\begin{array}{l} 2\bar{s}^{\,2}\,{}^1S+kl_c \\ 2s2p\,{}^3P^0+k'l'_c \end{array}\right\} & \rightleftarrows & 2s2p({}^3P^0,{}^1P^0)nl & \rightarrow & 2\bar{s}^{\,2}({}^1S)nl+h\nu \\ & & \downarrow & & \\ & & 2s2p\,{}^1P^0+k'l'_c & & \end{array}$$

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

$$|2\bar{s}^{\,2}\,{}^1S\rangle=0.966|2s^2\,{}^1S\rangle+0.257|2p^2\,{}^1S\rangle\ .$$

O^{5+}, $1s^2$:

$$\begin{array}{ccccc} 2s\,{}^2S+kl_c & \rightleftarrows & 2p({}^2P^0)nl & \rightarrow & 2s({}^2S)nl+h\nu \\ & & \downarrow & & \\ & & 2p\,{}^2P^0+k'l'_c, & & \end{array}$$

where $l_c=l\pm1$ and $l'_c=l$.

We sum the above processes over nl in the PCA, LS-coupling, and intermediate-coupling approximations, up to $n=1000$ for zero-field rate coefficients and up to $n=19$, 32, 44, 54, and 64 for O^{q+}, $q=1$ to 5, for the cross sections, to take account of field ionization by a 4.5 kV/cm analyzer as used in DR experiments[3] at Oak Ridge National Laboratory (ORNL). The radial functions are evaluated exactly as before,[5] and we estimate that errors in the structure could lead to errors in the $\bar{\sigma}_d$ and α_d of $\pm10\%$ at most.

IV. RESULTS

A. Convoluted cross sections

In Figs. 1–5 we compare our theoretical PCA, LS-coupling, and intermediate-coupling (IC) results for O^{q+}, $q=1$ to 5, having convoluted our energy-averaged cross sections with the Oak Ridge National Laboratory velocity distribution;[2] experimental results are also shown where they exist.[2,3] The results for O^+, O^{2+}, and O^{5+} are for a 100% occupied ground-state term, while for O^{3+} they are for 50% ground and 50% metastable and for O^{4+} they are for 30% ground and 70% metastable, as determined by experiment.[3,4] Except for O^{2+}, we find the peak DR cross section from the metastable levels to be no more than 5% of the peak DR cross section from levels of the ground-state term. For O^{2+}, this rises to 10% for the ^{1}D and 15% for the ^{1}S and ^{5}S metastable levels. Still, except at the lowest energies, DR from the metastables can be neglected as far as experiment is concerned. Thus to compare with future ORNL experiments the O^+ and O^{2+} results should be multiplied by the fraction of the ion beam in levels of the ground-state term.

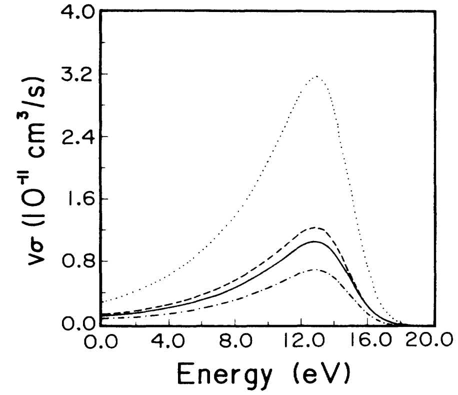

FIG. 1. DR cross sections for O^+ convoluted with ORNL velocity distribution. —·—·—, *LS* coupling; ——, intermediate coupling; — — —, zero-field PCA approximation · · · ·, maximum-field-enhanced PCA: all this work.

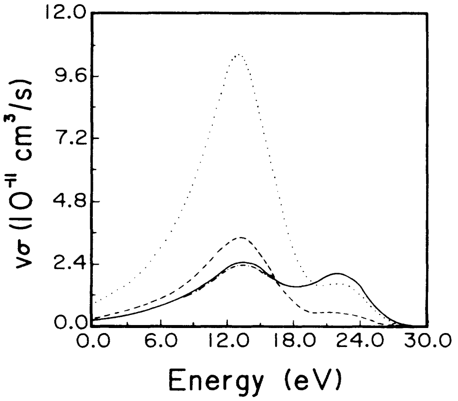

FIG. 2. DR of O^{2+}. Notation as in Fig. 1.

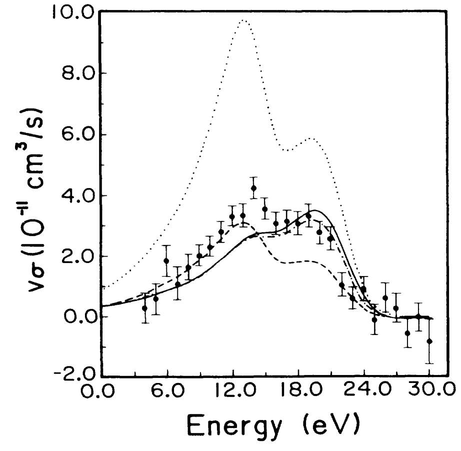

FIG. 3. DR of O^{3+}. Notation as in Fig. 1; Φ experimental points from Dittner *et al.* (Ref. 4).

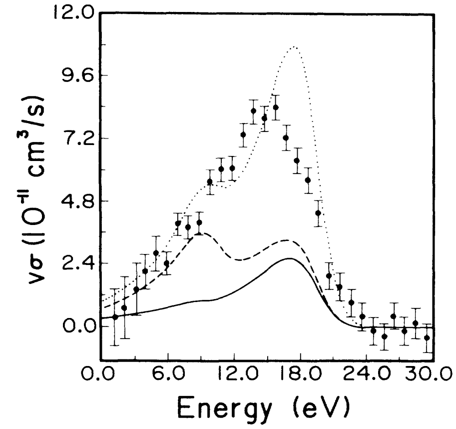

FIG. 4. DR of O^{4+}. Notation as in Fig. 1; Φ, experimental points from Dittner *et al.* (Ref. 3).

We now look at intermediate-coupling effects. Our IC results for O^{5+} are a factor of 1.4 larger than our *LS*-coupling results due to population, via core fine-structure interactions, of the $2p(^2P)nl\,^{1,3}L$ $(L=l)$ levels which are forbidden to autoionize in *LS* coupling; this increase is consistent with the factor of 1.5 expected from statistical weights. A similar argument applies to DR from levels of the ^4S ground-state term of O^+, the increase now being a factor of 1.5. The IC enhancement for levels of the ground-state terms of O^{2+} and O^{3+} is less than 5% and 10%, respectively, there being no *LS*-forbidden autoionizing terms that could contribute to DR. In the case of O^{4+} the IC and *LS*-coupling results differ by less than 1%. The reason for this is that the $2s2p(^1P)nl\,^2L$ $(L=l)$ levels, which are *LS*-forbidden to autoionize back to the $2s^2\,^1S$ ground-state level, can only autoionize in IC via

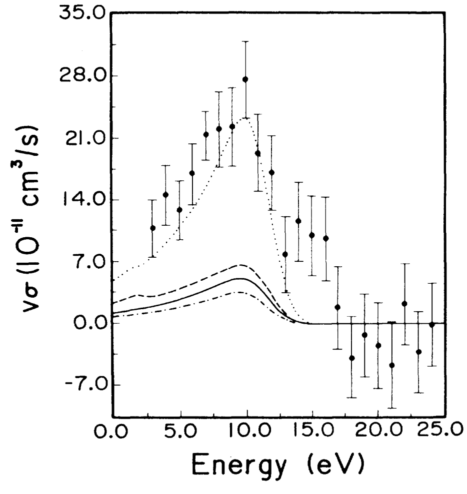

FIG. 5. DR of O^{5+}. Notation as in Fig. 1; Φ, experimental points from Dittner *et al.* (Ref. 2).

mixing due to the spin-orbit interaction of the *nl* valence electron, there being no core fine-structure interactions now. The resulting autoionization rates (and thus capture rates) are too small to significantly populate the ^2L ($L=l$) levels, particularly as they are depopulated by *LS*-allowed transitions into the continuum of the $2s2p\ ^3P$ levels which turn out to be several orders of magnitude larger. Finally, the IC enhancement for the metastable levels in all cases amounts to only a few percent, except for the ^5S levels of O^{2+}, where the increase is 11%.

We now compare our results with the theoretical results of other workers. The zero-field results of Griffin, Pindzola, and Bottcher[3] (not shown) for O^{4+} are a factor of 1.5 larger than our *LS*-coupling and IC results. This is consistent with their use of an *LS*-averaged approximation which allows the $2s2p(^1P)nl\ ^2L$ ($L=l$) levels to contribute to DR just as much as the $L=l\pm1$ levels when in fact they do not contribute as discussed above. The zero-field results of LaGattuta *et al.*[7] (not shown) differ by less than 10% from our *LS*-coupling and IC results for O^{4+}; this is not consistent with their use of an *LS*-averaged approximation. Our IC results for O^{5+} are in close agreement (10%) with the IC zero-field results of Griffin *et al.*[9] (not shown) while our *LS*-coupling results for O^{3+} lie 7–20% above the zero-field *LS*-coupling results of Hahn and Nasser[4] (not shown) as discussed before.[5]

The PCA approximation takes the configuration-average (CA) DR cross section for each *nl* and statistically partitions it over the intermediate levels of the core that can stabilize directly through electric dipole radiation and bins them according to the observed level energies. This approach leads to good agreement between the zero-field PCA and IC results for O^+, O^{4+}, and O^{5+}, where DR takes place through the Rydberg series attached to a single core term. However, it gives poorer results for O^{2+} and O^{3+}, where DR takes place through a Rydberg series attached to more than one core term. It turns out that the DR cross sections are not distributed statistically over the separate core terms. A further problem arises for O^{4+}; the low-energy peak is not due to DR from the metastable but is an artifact of the PCA approximation. In this case there exists a low-lying resonance in the CA approximation which is binned and convoluted at a higher energy in the PCA approximation causing this contribution to be inflated. We could have omitted the offending CA cross section, but we left it in as an illustration of a possible pitfall in using the PCA approximation. Turning to field effects, the maximum field enhancement in the PCA approximation is a factor of 2.5, 3.1, 3.1, 3.2, and 3.5 for O^{q+}, $q=1$ to 5, respectively. The experimental results for O^{3+} and O^{4+} lie between the zero-field and maximum-field-enhanced PCA results, while for O^{5+} they lie just above the maximum PCA results.

In Figs. 6–10 we present our zero-field IC energy-averaged DR cross sections for O^{q+}, $q=1$ to 5, convoluted with a 0.25 eV full width at half maximum (FWHM) Gaussian. These results are for a 100% occupied ground-state term with the *n* cut off as in Sec. III appropriate for a 4.5 kV/cm analyzer. With this resolution we can easily see the separate accumulation peaks due to DR via the Rydberg series attached to each core term: the ^4P for O^+; the $^3D^0$, $^3P^0$, and $^3S^0$ for O^{2+}; the ^2D, ^2S, and ^2P for O^{3+}; the $^1P^0$ for O^{4+}; and the $^2P^0$ for O^{5+}. These accumulation peaks are particularly sensitive to field effects. Furthermore, future experimentalists at this resolution should be able to choose between the results of calculations by different workers.

B. Maxwellian rate coefficients

In Table I we present our low-density zero-field IC DR rate coefficients for O^{q+}, $q=1$ to 5, statistically averaged over levels of the ground-state term. Except for the case of O^{5+}, $1\rightarrow n$ and $2\rightarrow n$ core transitions[11,13] can be neglected and therefore these can be regarded as total DR rate coefficients. Above $T=3\times10^6$ K the $1s\rightarrow2l$ core transitions in O^{5+} become important and eventually dominate the DR; results for this mode have been given by McLaughlin and Hahn.[8] DR via low-lying states becomes important at temperatures below those tabulated, and detailed *LS*-coupling calulations have been carried out by Nussbaumer and Storey[14] for these ions over $T=10^3-6\times10^4$ K; however, for the sensitive case of O^{4+}, the IC results of Badnell[15] are to be preferred. Results for temperatures higher than those tabulated may be obtained by scaling in $T^{-3/2}$.

Our IC results are no more than 5% greater than our *LS*-coupling results for O^{2+}, O^{3+}, and O^{4+}, while for O^+ and O^{5+} the IC results are about 25% greater. This IC enhancement is less than that for the cross sections because many higher *n* values contribute for which the DR rate coefficient is less sensitive to the new autoionization channels.

The *LS*-coupling rate coefficients of McLaughlin and Hahn[8] for O^{5+} and Ramadan and Hahn[15] for O^{3+} are about 20% and 5% higher, respectively, than our current *LS*-coupling results at the peak DR temperature, while those of McLaughlin *et al.*[17] and LaGatutta[18] for O^{4+} lie, respectively, 15% below and 20% above our earlier[13] *LS*-coupling results. The IC results for O^{4+} presented here include the low-temperature contribution evaluated previously,[15] while the *LS*-coupling results agree to a few percent with our earlier results,[13] which, apart from the mixing coefficients, were evaluated completely independently of the AUTOSTRUCTURE program. McLaughlin *et al.*[17] also obtained rate coefficients for $2\rightarrow3$ core transitions in O^{4+} and these are a factor of 3 larger than we obtained.[13] The reason for this is unclear; however, the $2\rightarrow3$ DR rate coefficient in low-*Z* ions[13] is particularly sensitive to the effect of $\Delta n=0$ secondary autoionization; see also the paper by Chen[19] on $2\rightarrow3$ core transitions in Ne-like ions. We note that rate coefficients for O^{6+} have been calculated by Chen[19] and by Nasser and Hahn,[21] and for O^{7+} by Burgess and Tworkowski.[22]

Our rate coefficients are valid in the zero-field low-density limit; however, both field effects and density effects have competing mechanisms for increasing and decreasing these limiting rates. High-*n* values are field or collisionally ionized, thereby reducing the DR rate, while field-mixing or *l*-changing collisions[23] enhance the DR rate for the remaining *n*. We have already seen[5] that

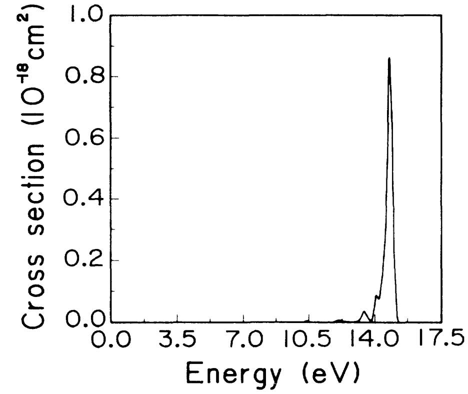

FIG.6 . Intermediate-coupling DR cross section for O^+ convoluted with a 0.25 eV FWHM Gaussian.

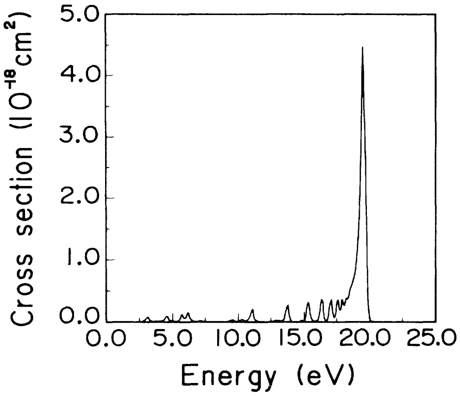

FIG. 9. DR of O^{4+}, details in Fig. 6.

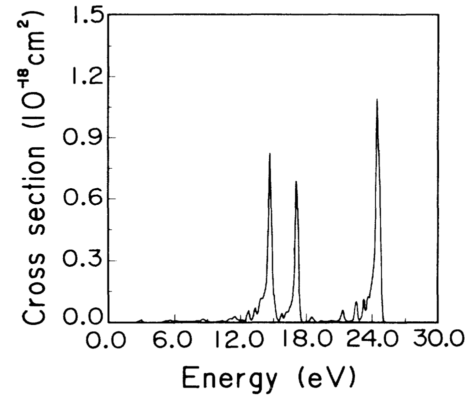

FIG. 7. DR of O^{2+}, details as in Fig. 6.

these two mechanisms can largely cancel each other out in the case of field effects.

The low-density zero-field DR rate coefficients can be compared directly with the Burgess[10] general formula (GF) which is commonly used in ionization balance calculations. The results of the Burgess GF lie 45% and 35% above our IC results for O^+ and O^{5+}, respectively, mainly due to the averaging over incident angular momenta in the calculations on which the GF is based, since our IC rate coefficients are only about 25% greater than our *LS*-coupling results rather than the factor of 1.5 expected due to statistical weights. Similarly, the GF overestimates the results for O^{4+} by a factor of 1.8, there being no intermediate coupling enhancement now. The GF results for O^{2+} and O^{3+} are 40% and 30%, respectively, greater than our IC results mainly due to autoionization into excited states[6] which reduces our results and which is not modeled by the GF. However, this is a small effect for O^{4+}; the GF overestimate only drops from a factor of 1.8 to 1.7 if we exclude autoionization into excited states from our calculations.

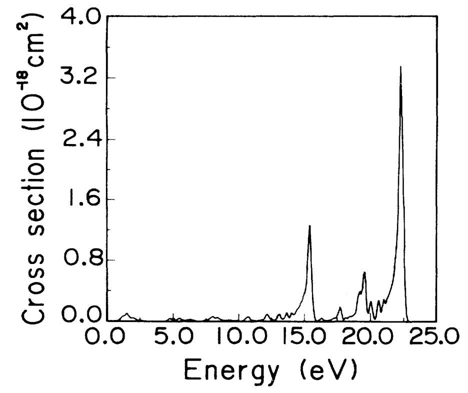

FIG. 8. DR of O^{3+}, details as in Fig. 6.

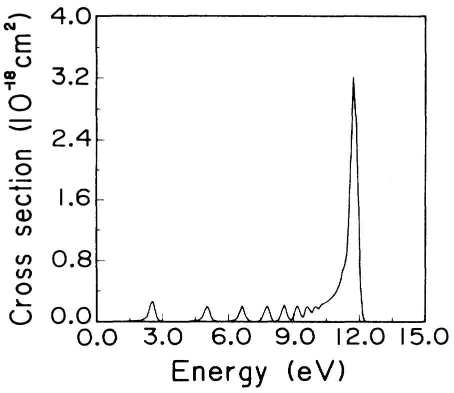

FIG. 10. DR of O^{5+}, details as in Fig. 6.

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

$\log_{10} T$ (K)	O^+	O^{2+}	O^{3+}	O^{4+}	O^{5+}
4.6	1.62[−12][a]	3.65[−12]	5.61[−12]	3.79[−11]	2.35[−11]
4.8	4.33[−12]	1.08[−11]	1.73[−11]	4.36[−11]	4.00(−11)
5.0	6.26[−12]	1.78[−11]	3.20[−11]	5.17[−11]	4.43(−11)
5.2	6.12[−12]	1.96[−11]	3.80[−11]	5.05[−11]	3.68[−11]
5.4	4.68[−12]	1.65[−11]	3.33[−11]	4.02[−11]	2.54[−11]
5.6	3.06[−12]	1.15[−11]	2.39[−11]	2.74[−11]	1.56[−11]
5.8	1.82[−12]	7.14[−12]	1.50[−11]	1.68[−11]	8.87[−12]
6.0	1.01[−12]	4.10[−12]	8.69[−12]	9.61[−12]	4.82[−12]
6.2	5.42[−13]	2.24[−12]	4.77[−12]	5.15[−12]	2.54[−12]
6.4	2.84[−13]	1.19[−12]	2.53[−12]	2.68[−12]	1.32[−12]
6.6	1.46[−13]	6.15[−13]	1.32[−12]	1.36[−12]	6.73[−13]
6.8	7.44[−14]	3.25[−13]	6.75[−13]	6.85[−13]	3.42[−13]

[a] 1.62[−12] = 1.62×10^{-12}.

V. CONCLUSION

We have calculated DR cross sections and rate coefficients for O^{q+}, $q=1$ to 5. Core fine-structure interactions cause an increase of about 45% (25%) in the IC cross sections (rate coefficients) over our *LS*-coupling results for O^+ and O^{5+}, but the increase is no more than 10% (5%) for O^{2+}, O^{3+}, and O^{4+}. DR from the metastables was found to be unimportant in all cases as far as experiment is concerned. The zero-field PCA results for O^+, O^{4+}, and O^{5+} are in good agreement with our intermediate-coupling results, while those for O^{2+} and O^{3+} are poorer since DR now takes place through a Rydberg series attached to more than one core term and the cross sections are not distributed statistically among them. The maximum field enhancement in the PCA approximations was found to be about a factor of 3. Finally, the Burgess GF overestimates the zero-field rate coefficients by a factor of between 1.3 and 1.8 due to the neglect of autoionization into excited states or to averaging over incident angular momenta.

ACKNOWLEDGMENTS

We would like to thank 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] N. R. Badnell, Phys. Scr. (to be published).
[2] P. F. Dittner, S. Datz, P. D. Miller, P. L. Pepmiller, and C. M. Fou, Phys. Rev. A **35**, 3668 (1987).
[3] P. F. Dittner, S. Datz, H. F. Krause, P. D. Miller, P. L. Pepmiller, C. Bottcher, C. M. Fou, D. C. Griffin, and M. S. Pindzola, Phys. Rev. A **36**, 33 (1987).
[4] 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).
[5] N. R. Badnell and M. S. Pindzola, Phys. Rev. A **39**, 1685 (1989).
[6] N. R. Badnell, J. Phys. B **19**, 3827 (1986).
[7] K. LaGattuta, I. Nasser, and Y. Hahn, J. Phys. B **20**, 1577 (1987).
[8] D. J. McLaughlin and Y. Hahn, Phys. Rev. A **29**, 712 (1984).
[9] D. C. Griffin, M. S. Pindzola, and C. Bottcher, Phys. Rev. A **33**, 3124 (1986).
[10] A. Burgess, Astrophys. J. **141**, 1588 (1965).
[11] Y. Hahn, Adv. At. Mol. Phys. **21**, 123 (1985).
[12] D. C. Griffin, M. S. Pindzola, and C. Bottcher, Phys. Rev. A **31**, 568 (1985).
[13] N. R. Badnell, J. Phys. B **20**, 2081 (1987).
[14] H. Nussbaumer and P. J. Storey, Astron. Astrophys. **126**, 75 (1983).
[15] N. R. Badnell, J. Phys. B **21**, 749 (1988).
[16] H. Ramadan and Y. Hahn (unpublished).
[17] D. J. McLaughlin, K. J. LaGattuta, and Y. Hahn, J. Quant. Spectrosc. Radiat. Transfer **37**, 47 (1987).
[18] K. J. LaGattuta, Phys. Rev. A **30**, 3072 (1984).
[19] M. H. Chen, Phys. Rev. A **34**, 1073 (1986).
[20] M. H. Chen, Phys. Rev. A **33**, 994 (1986).
[21] I. Nasser and Y. Hahn, J. Quant. Spectrosc. Radiat. Transfer **29**, 1 (1983).
[22] A. Burgess and A. S. Tworkowski, Astrophys. J. **205**, L105 (1976).
[23] A. Burgess and H. P. Summers, Astrophys. J. **157**, 1007 (1969).