Dielectronic recombination of P^{5+} and Cl^{7+} in configuration-average, *LS*-coupling, and intermediate-coupling approximations

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We have calculated dielectronic recombination cross sections and rate coefficients for the Ne-like ions P^{5+} and Cl^{7+} in configuration-average, *LS*-coupling, and intermediate-coupling approximations. Autoionization into excited states reduces the cross sections and rate coefficients by substantial amounts in all three methods. There is only rough agreement between the configuration-average cross-section results and the corresponding intermediate-coupling results. There is good agreement, however, between the *LS*-coupling cross-section results and the corresponding intermediate-coupling results. The *LS*-coupling and intermediate-coupling rate coefficients agree to better than 5%, while the configuration-average rate coefficients are about 30% higher than the other two coupling methods. External electric field effects, as calculated in the configuration-average approximation, are found to be relatively small for the cross sections and completely negligible for the rate coefficients. Finally, the general formula of Burgess was found to overestimate the rate coefficients by roughly a factor of 5, mainly due to the neglect of autoionization into excited states.

I. INTRODUCTION

The comparison between theoretical and experimental dielectronic recombination (DR) cross sections has been complicated by the presence of external electric fields which greatly enhance the DR cross section for $\Delta n = 0$ core transitions in low-charge-state ions.[1] However, field enhancement can be expected to be small for $\Delta n = 1$ core transitions since, except for low-n values for which the Stark mixing is weak, the autoionization rates are smaller than the radiative rates and so the DR cross sections are insensitive to the redistribution of the autoionization rates by Stark mixing. Experiments are currently under way at the Oak Ridge National Laboratory[2] (ORNL) on the DR of the Ne-like ions P^{5+} and Cl^{7+} and so we make use of the program AUTOSTRUCTURE (Ref. 3) to carry out *LS*-coupling and intermediate-coupling calculations in the zero-field limit. We also make use of the program DRACULA (Ref. 4) to carry out configuration-average calculations with zero field and with maximum field mixing. The same calculational methods have recently been applied to B-like ions[5] and to oxygen ions.[6]

The Ne isoelectronic sequence has been treated in recent years by Jacobs *et al.*,[7] who evaluated DR rate coefficients for Mg^{2+}, Si^{4+}, S^{6+}, and Fe^{16+}; Hahn *et al.*,[8] who evaluated DR rate coefficients for Ar^{8+}, Fe^{16+}, and Mo^{32+}; Dalhed *et al.*,[9] who evaluated DR rate coefficients for 17 ions from Ar^{8+} to W^{64+}; Chen,[10] who evaluated DR rate coefficients for 7 ions from Ar^{8+} to Xe^{44+}; and Romanik,[11] who evaluated DR rate coefficients for 7 ions from Mg^{2+} to Ni^{18+}. Quite recently Moussa *et al.*[12] have evaluated both DR cross sections and rate coefficients for Mg^{2+}, P^{5+}, and Cl^{7+} in a nonrelativistic *LS*-coupled calculational method.

In Sec. II we briefly outline the theory behind our calculations, in Sec. III we describe its application to Ne-like ions, and in Sec. IV we present and discuss our results. A short summary is found 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[13]

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

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 $(2\pi a_0)^2 \tau_0 = 2.6741 \times 10^{-32}$ cm^2 sec. The total dielectronic recombination rate coefficient may be written in terms of the energy-averaged cross section thus,[13]

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

where $(4\pi a_0^2)^{3/2} = 6.6011 \times 10^{-24}$ cm^3.

Equations (1) and (2) may be evaluated in configuration-mixing *LS*-coupling and intermediate-coupling approximations using AUTOSTRUCTURE (Ref. 3)

and in a configuration-average approximation using DRACULA.[4] We can also use the configuration-average approximation to estimate the maximum field mixing 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 papers[5,6] and will not be repeated here.

III. APPLICATION TO Ne-LIKE IONS

We consider

$1s^2$:

$$2s^22p^6+kl_c \leftrightarrows 2s^22p^53l_dnl \begin{array}{l} \nearrow\ 2s^22p^6nl+h\nu_1 \\ \searrow\ 2s^22p^63l_d+h\nu_2 \end{array}$$
$$\downarrow$$
$$2s^22p^53l_d'+k'l_c'$$

where l_d, $l_d'=0,1,2$ and $l_c,l_c'=l,l\pm1,l\pm2$. We could also consider $2s\rightarrow 3l_d$ excitations but we find that their contribution is only a few percent of that from $2p\rightarrow 3l_d$ excitations and so we have neglected them.

We sum the above process over nl in the configuration-average, LS-coupling, and intermediate-coupling approximations, up to $n=1000$ for zero-field rate coefficients and up to $n=64$ and 82 for P^{5+} and Cl^{7+} for the cross sections, to take account of field ionization by a 4.5 kV/cm analyzer as used in DR experiments[14] at Oak Ridge. However, the total DR cross section is relatively insensitive to the analyzer field strength in the case of $\Delta n=1$ core transitions. A 10.0-kV/cm analyzing field reduces the cutoff to $n=52$ for P^{5+} but the DR cross section for the Rydberg series attached to the $3s$ core falls by only 1% while that for the $3d$ core falls by 7%, the effect on Cl^{7+} is even smaller.

The radial wave functions are evaluated with the same model potentials as used previously.[5,6] As a check on the model potentials we calculated the DR cross sections for Cl^{7+} using Hartree-Fock core orbitals in the AUTOSTRUCTURE program. The change in the total DR cross sections did not exceed 10%, while the DR rate coefficients were virtually unaffected.

IV. RESULTS

All the results presented here are for a 100% occupied ground-state term. The energy-averaged DR cross sections in Figs. 1–6 have been convoluted with the experimentally determined ORNL velocity distribution,[14] while the cross sections in Figs. 7 and 8 are convoluted with a Gaussian energy distribution.

A. Convoluted cross sections

In Figs. 1 and 2 we show the effect of omitting autoionization into excited states from our LS-coupling calculations for P^{5+} and Cl^{7+}. The low-energy peaks, 50 to 120 eV in P^{5+} and 100 to 180 eV in Cl^{7+} are mainly due to excitation and capture to $n=3$, i.e., the $3l3l'$ autoionizing configurations. The peak centered on 130 eV in P^{5+} is due in the main ($\sim$75%) to DR via the $3snl$ ($n>3$) Rydberg series and in part ($\sim$25%) to the $3d4l$ configurations. The peak centered on 165 eV in P^{5+} is due almost solely to DR via the $3dnl$ ($n>5$) Rydberg series. Since the $3dnl$ configurations can autoionize to $3s+kl_c$ for all $n>3$ and to $3p+kl_c$ for higher n, the contributions at 130 eV are reduced substantially, while the peak at 165 eV is reduced by a factor of 4.0. The $3pnl$ Rydberg series only contributes a few percent to the results as stabilization can only take place via outer electron transitions (for $n>3$). The peak centered at 210 eV in Cl^{7+} is due in the main ($\sim$75%) to the $3d4l$ configurations and in part ($\sim$25%) to the $3snl$ Rydberg series; just the opposite from P^{5+}. In the case of Cl^{7+} the $3dnl$ configurations can only autoionize to $3s+kl_c$ for $n>4$. Together with transitions into the $3p$ continuum, the contributions at 210 eV are reduced slightly, while the peak at 265 eV due to the $3dnl$ Rydberg series is reduced by a factor of 2.5.

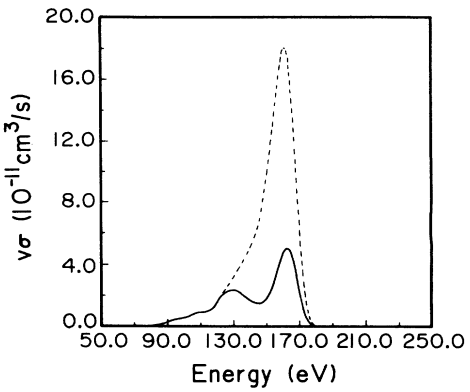

FIG. 1. Dielectronic recombination cross section for P^{5+}, in LS coupling, convoluted with ORNL velocity distribution. Solid curve, all autoionizing transitions retained; dashed curve, excluding autoionization into excited states.

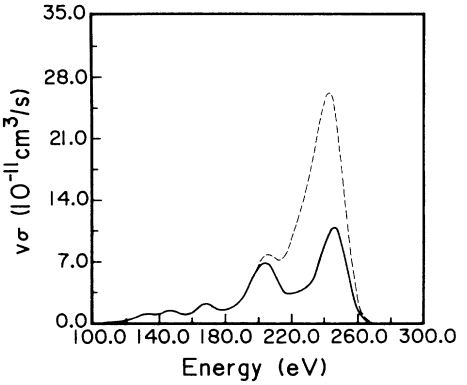

FIG. 2. Dielectronic recombination cross section for Cl^{7+}, in LS coupling, convoluted with ORNL velocity distribution. Solid curve, all autoionizing transitions retained; dashed curve, excluding autoionization into excited states.

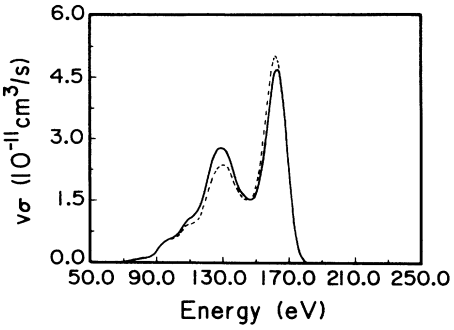

FIG. 3. Dielectronic recombination cross section for P^{5+} with ORNL velocity distribution. Solid curve, intermediate coupling; dashed curve, *LS* coupling.

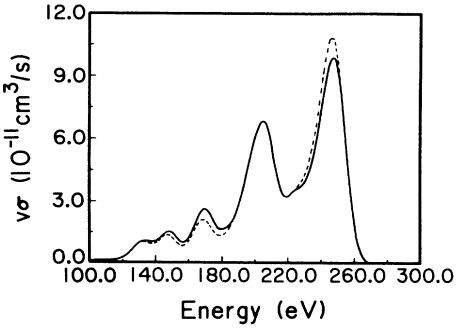

FIG. 4. Dielectronic recombination cross section for Cl^{7+} convoluted with ORNL velocity distribution. Solid curve, intermediate coupling; dashed curve, *LS* coupling.

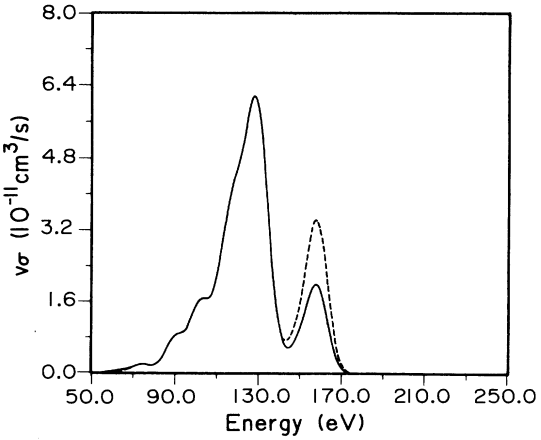

FIG. 5. Dielectronic recombination cross section for P^{5+}, including field mixing effects, convoluted with ORNL velocity distribution. Solid curve, zero-field configuration average; dashed curve, maximum-field configuration average.

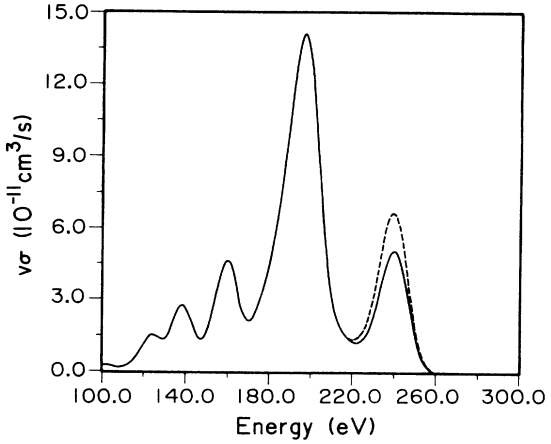

FIG. 6. Dielectronic recombination cross section for Cl^{7+}, including field-mixing effects, convoluted with ORNL velocity distribution. Solid curve, zero-field configuration average; dashed curve, maximum-field configuration average.

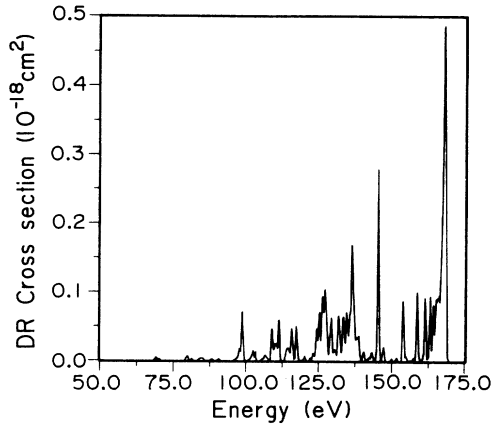

FIG. 7. Dielectronic recombination cross section for P^{5+}, in intermediate coupling, convoluted with a 0.5-eV FWHM Gaussian.

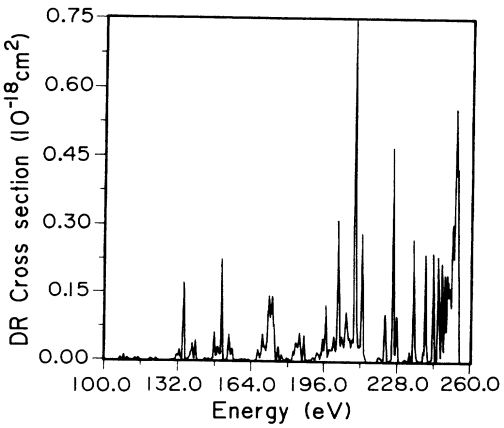

FIG. 8. Dielectronic recombination cross section for Cl^{7+}, in intermediate coupling, convoluted with a 0.5-eV FWHM Gaussian.

In Figs. 3 and 4 we present *LS*-coupling and intermediate-coupling (IC) calculations for P^{5+} and Cl^{7+}. There are several competing effects of IC. Firstly, since $A_a \leq A_r$ new radiative channels can increase the cross section, for example, $^3L_1$ parental mixing with the $^1P_1$ level allows the *LS*-forbidden triplet $J=1$ parents to stabilize. Secondly, transitions between fine-structure levels within a term lead to additional autoionization into excited states which can decrease the cross section. Also, we now have level-to-level branching ratios which may differ from term to term (or configuration-average) ratios when A_a and A_r are comparable. The net result is to decrease the high-energy peak by 7% and 10%, for P^{5+} and Cl^{7+}, respectively, and to increase the lower-energy peak by 14% and 20%, respectively.

In Figs. 5 and 6 we show configuration-average calculations at zero field and maximum field mixing for P^{5+} and Cl^{7+}. The zero-field results for both ions differ substantially from the *LS*-coupling and intermediate-coupling results of Figs. 3 and 4. Although autoionization into excited configurations is included in the configuration-average calculations, the averaging procedure is obviously only good to a factor of 2 or 3 for these ions. As pointed out previously,[4] the configuration-average method is especially suspect when $A_a \approx A_r$, as is the case for $\Delta n = 1$ DR cross sections. What can be learned from the configuration-average calculations is that field mixing has only a small effect on the overall cross section. For low n, the effects of fields are negligible, while at the $3dnl$ Rydberg series limit at 165 eV for P^{5+} and 265 eV for Cl^{7+} the cross section is enhanced by a factor of 75% and 33%, respectively.

In Figs. 7 and 8 we present our zero-field IC energy-averaged DR cross sections for P^{5+} and Cl^{7+}, convoluted with a 0.5-eV full width at half maximum (FWHM) Gaussian to show more detail than the ORNL convoluted cross sections. These should provide suitable stimulation for the next generation of DR experiments.

B. Maxwellian rate coefficients

In Table I we present low-density zero-field intermediate-coupling DR rate coefficients for P^{5+} and Cl^{7+} and these differ by only a few percent ($\leq 5\%$) from our *LS*-coupling results. Autoionization into excited states reduces the rate coefficients by up to a factor of 2.7 for P^{5+} and 1.8 for Cl^{7+}. The contribution from $2 \rightarrow n$ ($n > 3$) transitions can be expected to be small due to the additional autoionization channels available (e.g., $4 \rightarrow 3$) and so these may be regarded as total rate coefficients. Results for temperatures higher than those tabulated may be obtained by scaling in $T^{-3/2}$.

TABLE I. Dielectronic recombination rate coefficients ($cm^3 s^{-1}$) for P^{5+} and Cl^{7+}. The numbers in square brackets represent powers of 10.

$\log_{10}T$ (K)	P^{5+}	Cl^{7+}
5.6	1.79[−12]	1.09[−12]
5.8	4.03[−12]	4.29[−12]
6.0	5.39[−12]	8.70[−12]
6.2	5.07[−12]	1.09[−11]
6.4	3.80[−12]	9.88[−12]
6.6	2.45[−12]	7.25[−12]
6.8	1.44[−12]	4.62[−12]
7.0	8.04[−13]	2.69[−12]
7.2	4.29[−13]	1.49[−12]
7.4	2.24[−13]	7.81[−13]
7.6	1.15[−13]	4.14[−13]

TABLE II. Peak values of the dielectronic recombination rate coefficient ($cm^3 s^{-1}$) for P^{5+} and Cl^{7+}. The numbers in square brackets represent powers of 10.

Method	P^{5+}	Cl^{7+}
Intermediate coupling (AUTOSTRUCTURE)	5.4[−12]	1.1[−11]
Configuration average (DRACULA)	7.0[−12]	1.4[−11]
Nonrelativistic *LS* coupling (Moussa *et al.*, Ref. 12)	4.4[−12]	7.0[−12]
Relativistic intermediate coupling (Chen, Ref. 15)	7.5[−12]	1.3[−11]

In Table II we compare the peak values of the DR rate coefficients for P^{5+} and Cl^{7+} calculated in intermediate coupling using AUTOSTRUCTURE,[3] in the configuration-average approximation using DRACULA,[4] in nonrelativistic *LS* coupling by Moussa *et al.*,[12] and in relativistic intermediate coupling by Chen.[15] The two surprising results from Table II are (1) that the intermediate-coupling calculations differ by 30% and (2) the configuration-average calculation is reasonably accurate. Further atomic-structure sensitivity studies are needed to investigate (1), while extension of the present calculations to other atomic ions are needed to test (2).

The Burgess general formula[16] (GF) overestimates the rate coefficient by a factor of 6.6 for P^{5+} and 4.3 for Cl^{7+}. If we again exclude autoionization into excited states from our calculations, which is not modeled by the GF, then the overestimate drops to a factor of 2.5 for P^{5+} and 2.4 for Cl^{7+}. Similar reductions for low-Z Ne-like ions have been found by Chen.[10]

V. CONCLUSIONS

The results of our present series of papers[5,6] on dielectronic recombination show that, in the low-density zero-field limit, the most important factor is to include all energetically allowed autoionizing transitions; next, to choose a suitable coupling scheme, usually *LS* coupling; and finally to use a reasonably accurate structure that allows for configuration mixing with the core. In the case of field effects, it is only possible in general to estimate the maximum field mixing; field-dependent calculations are only available for simple systems.[17,18] Nevertheless, the present series of papers show that field effects on dielectronic recombination greatly diminish when going from $\Delta n = 0$ to $\Delta n = 1$ transitions in low-Z atomic ions. In the case of density effects, only at a high enough density is a simple cutoff appropriate,[19] otherwise collisional mixing should also be included.

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