Relativistic calculations of dielectronic recombination coefficients for the Ne isoelectronic sequence

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Dielectronic recombination coefficients for ground-state ions of the Ne isoelectronic sequence have been calculated for seven ions, with atomic number $18 \leq Z \leq 54$, in the isolated resonance approximation, for temperatures in the range $0.2 \leq T \leq 6$ keV. The Auger and radiative rates of each doubly excited state were evaluated explicitly by using the multiconfiguration Dirac-Fock model. The calculations were performed with intermediate coupling. The effect of the configuration interaction was also included for the low-lying doubly excited states. The effect of Coster-Kronig-type transitions on the dielectronic rate coefficients has been found to be very significant for low-Z ions. However, it is quite small for medium and heavy ions. The effect of relativity on the total dielectronic coefficient and dielectronic satellite spectra is also discussed.

I. INTRODUCTION

Dielectronic recombination (DR) is an important recombination process for high-temperature laboratory and astrophysical plasmas.[1-3] Knowledge of DR coefficients is essential in the determination of the ionization balance of high-temperature plasmas. Furthermore, dielectronic satellite lines observed in the emission spectra can be used in plasma diagnostics. The DR process has been subjected to intense theoretical study.[2,3] The existing calculations are based on either the hydrogenic model or the distorted-wave method. A term-average approximation or LS coupling was employed in these previous calculations.[4-6] Recently, the relativistic configuration-interaction method has also been used to calculate dielectronic recombination rate coefficients.[7,8] DR coefficients have been calculated for a few selected Ne-like ions.[5,8-11] Several experiments have been carried out to measure dielectronic recombination coefficients or cross sections.[12-17]

In this paper we report on a systematic study of dielectronic recombination coefficients for ground-state ions of the Ne isoelectronic sequence. This is an extension of my previous work for the He-like ions.[7] The calculations cover seven ions with atomic number $18 < Z < 54$ and use the multiconfiguration Dirac-Fock (MCDF) model[18,19] to evaluate detailed transition energies and rates. The effects of relativity and autoionization to the excited states on the DR coefficients are also studied.

II. THEORETICAL METHOD

The dielectronic recombination coefficient, in the isolated resonance approximation, can be written as[2,3]

$$\alpha_{\mathrm{DR}}(i;\mathrm{total}) = \frac{1}{2g_i}\left[\frac{4\pi R}{kT}\right]^{3/2} a_0^3 \sum_{\kappa_2}\sum_{d}\sum_{f} \exp(-e_2/kT) g_d A_A(d\rightarrow i, e_2\kappa_2)\omega_d \tag{1}$$

with

$$\omega_d = A_r(d\rightarrow f)/[\Gamma_r(d)+\Gamma_A(d)] \,. \tag{2}$$

Here, g_d and g_i are the statistical weight factors for ionic states d and i, respectively; R is the Rydberg energy and a_0 is the Bohr radius; $A_A(d\rightarrow i, e_2\kappa_2)$ is the Auger rate from intermediate state d to initial state i of the recombining ion, with the free electron characterized by energy e_2 and relativistic quantum number $\kappa_2=(l_2-j_2)(2j_2+1)$; $A_r(d\rightarrow f)$ is the radiative rate from state d to f; Γ_r and Γ_A are the total radiative and Auger widths, respectively. The free electrons are assumed to have a Maxwellian distribution.

In the present work, the Auger and radiative rates and Auger energies required in the evaluation of Eq. (1) were calculated for each autoionizing state. No averaging procedure has been employed in the present study. The Auger transition probability is calculated from perturbation theory.[19,20] The transition rate in a frozen-orbital approximation is given by

$$A_A = \frac{2\pi}{\hbar}\left|\left\langle \psi_f \left| \sum_{\substack{a,b \\ (a<b)}} V_{ab} \right| \psi_i \right\rangle\right|^2 \rho(\varepsilon) \,. \tag{3}$$

Here, $\rho(\varepsilon)$ is the density of final states; V_{ab} is the two-electron interaction operator. In the present work, V_{ab} is taken to be the Coulomb operator.

The spontaneous radiative transition probability for a discrete transition $i\rightarrow f$ in a multipole expansion is given in perturbation theory by[21,22]

$$A_r(i\rightarrow f) = \frac{1}{2J_i+1}\sum_{L}\frac{2\pi}{2L+1}\,|\langle f||T_L||i\rangle|^2 \,. \tag{4}$$

TABLE I. Total dielectronic recombination coefficients (in 10^{-11} cm^3/sec) of Ne-like ions in ground state.

T (keV)	$_{18}Ar^{8+}$	$_{26}Fe^{16+}$	$_{34}Se^{24+}$	$_{36}Kr^{26+}$	$_{42}Mo^{32+}$	$_{47}Ag^{37+}$	$_{54}Xe^{44+}$
0.2	1.21	1.85	1.01	0.827	0.375	0.176	0.0484
0.5	0.647	2.68	3.01	2.83	2.06	1.57	0.951
0.8	0.386	2.12	3.17	3.17	2.70	2.30	1.66
1.0	0.295	1.78	2.95	3.05	2.79	2.49	1.91
1.5	0.174	1.20	2.33	2.49	2.55	2.47	2.11
2.0	0.118	0.872	1.83	1.99	2.17	2.22	2.02
3.0	0.0673	0.531	1.20	1.34	1.57	1.68	1.67
4.0	0.0448	0.363	0.861	0.973	1.18	1.30	1.36
5.0	0.0323	0.269	0.653	0.742	0.920	1.04	1.12
6.0	0.0248	0.208	0.517	0.591	0.743	0.851	0.933

Here, $\langle f||T_L||i\rangle$ is the relativistic Lth-multipole reduced matrix element.[21]

The transition matrix elements in Eqs. (3) and (4) can be written as the sums of terms involving the multiplication of the angular factor and radial integral by the use of Racah algebra. In the present work, the transition matrix elements were calculated in the framework of the MCDF model. For detailed information, the reader is referred to Refs. 7 and 19.

III. NUMERICAL PROCEDURE

Dielectronic recombination from a Ne-like ground state to a state of a Na-like ion can be represented by

$$A^{q+}(2s^22p^6)+e^-\rightleftarrows A^{(q-1)+}\times(2s\,2p^6nln'l'+2s^22p^5nln'l')\rightarrow A^{(q-1)+}(2s^22p^6n''l'')+h\nu\ .$$

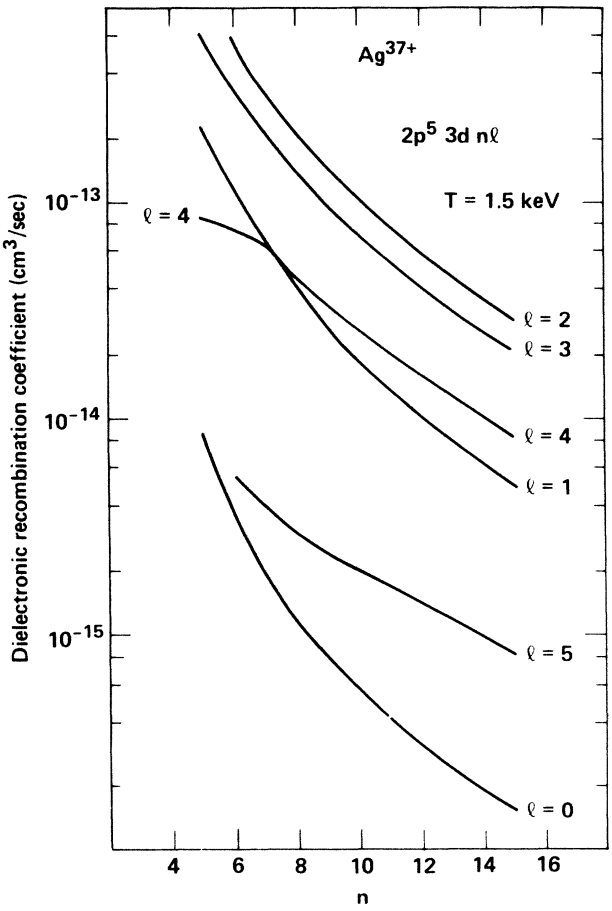

FIG. 1. Dielectronic recombination coefficients from the intermediate states $2p^53dnl$ for the Ag^{37+} ion at $T=1.5$ keV, with $l=1$ to 5, as functions of the principal quantum number n.

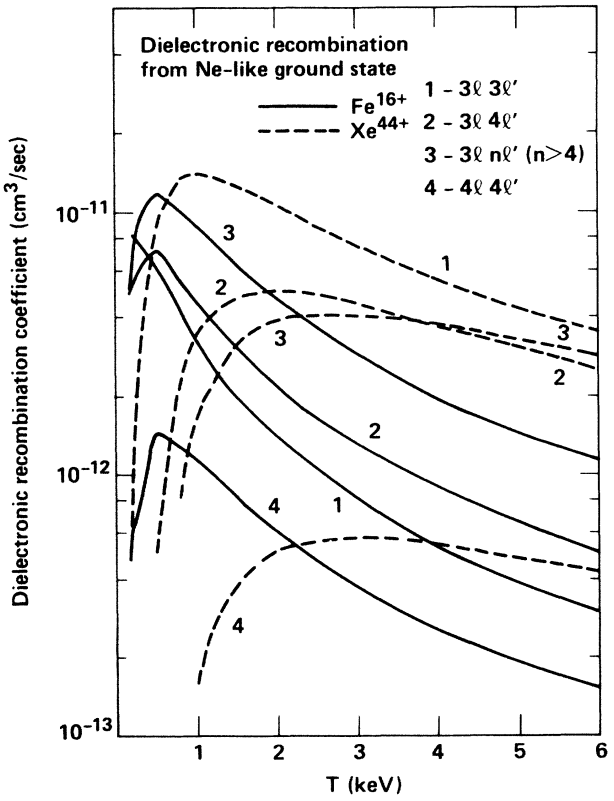

FIG. 2. Dielectronic recombination coefficients from the intermediate states $3l3l'$, $3l4l'$, $3lnl'$ ($n>4$), and $4l4l'$ for the Fe^{16+} and Xe^{44+} ions as functions of electron temperature. The solid curves indicate the results for the Fe^{16+} ion and the broken curves represent the values for the Xe^{44+} ion.

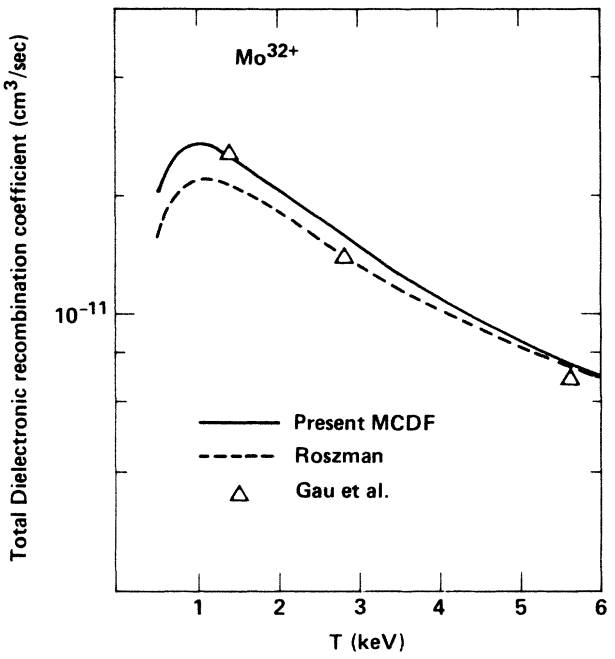

FIG. 3. Total dielectronic recombination coefficients for the Mo^{32+} ion as functions of electron temperature. The solid curve represents the present MCDF results. The dashed curve indicates the predictions from Roszman (Ref. 5), and the triangles are the values from Gau *et al.* (Ref. 11).

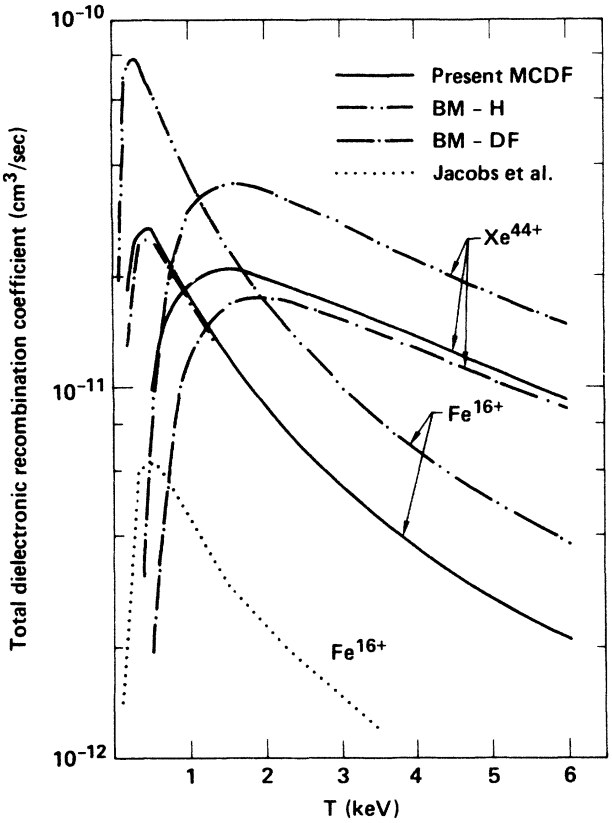

FIG. 4. Total dielectronic recombination coefficients for the Fe^{16+} and Xe^{44+} ions as functions of electron temperature. The solid curves represent the present MCDF results. The dotted curve indicates the predictions from Jacobs *et al.* (Ref. 9). The dashed-dotted and dashed-double-dotted curves display the results from the Burgers-Merts formula with the Dirac-Fock and hydrogenic oscillator strengths, respectively.

The doubly excited configurations included in the present work are $2s2p^6 3l3l'$, $2p^5 3l3l'$, $2s2p^6 3l4l'$, $2p^5 3l4l'$, $2p^5 3dnl$ ($n \geq 5$), $2p^5 3snl$ ($n \geq 5$), and $2p^5 4l4l'$.

The atomic energy levels and bound-state wave functions were calculated using the MCDF model in the averaged-level (AL) scheme.[18] The effects of quantum-electrodynamic (QED) corrections, finite nuclear size, and relaxation were included in calculations of transition energies for the low-lying $3l3l'$ states. However, the QED corrections were neglected for the other doubly excited states. The effects of intermediate coupling and the configuration interaction were included in the treatment of the low-lying $3l3l'$ and $3l4l'$ states. For the $3lnl'$ configurations with $5 \leq n \leq 15$ and $l' \leq 5$, the calculations were performed in intermediate coupling without the configuration interaction.

For the autoionizing states of the $2p^5 3dnl$ configurations, these intermediate states can also decay to the excited states of the recombining ion for certain large n values.[9,10] In the present work, these Auger transition rates were included in calculations of the stabilizing fluorescence yields.

For the $3lnl'$ configurations with $n > 15$, DR coefficients were estimated by using a n^{-3} extrapolation to the DR coefficient. The contributions from $4ln'l'$ with $n' > 5$ and $nln'l$ with $n,n' > 5$ were neglected.

The detailed Auger and electric dipole radiative rates for each autoionizing state were calculated according to Eqs. (3) and (4), respectively. The angular factors of the Auger and radiative matrix elements were computed by using the modified general angular momentum codes.[18,19]

The continuum wave functions required in calculations of the Auger matrix elements were obtained by solving the Dirac-Fock equations for the final state without including the exchange interaction between the bound and continuum electrons. For autoionization to the excited states which involves low-energy Coster-Kronig type transitions,[20] a local-exchange interaction[23] was used in calculations of the continuum wave functions.

The term-dependent transition energies and rates from the MCDF model were used to calculate the DR coefficients according to Eqs. (1) and (2). The radiative transitions leading to the other autoionizing states were neglected in the present work (e.g., $2p^5 3d4f \rightarrow 2p^5 3d^2$).

The effect of relativity on the DR coefficients and satellite structure is also investigated for the Xe^{44+} ion by comparing the results from the relativistic and nonrelativistic calculations. To obtain the nonrelativistic values, the DR coefficients were computed by using the nonrelativistic limit of the MCDF model which can be achieved by increasing the velocity of light a thousandfold.[18]

IV. RESULTS AND DISCUSSION

The total DR coefficients for ground-state Ne-like ions have been calculated for 7 ions with atomic number

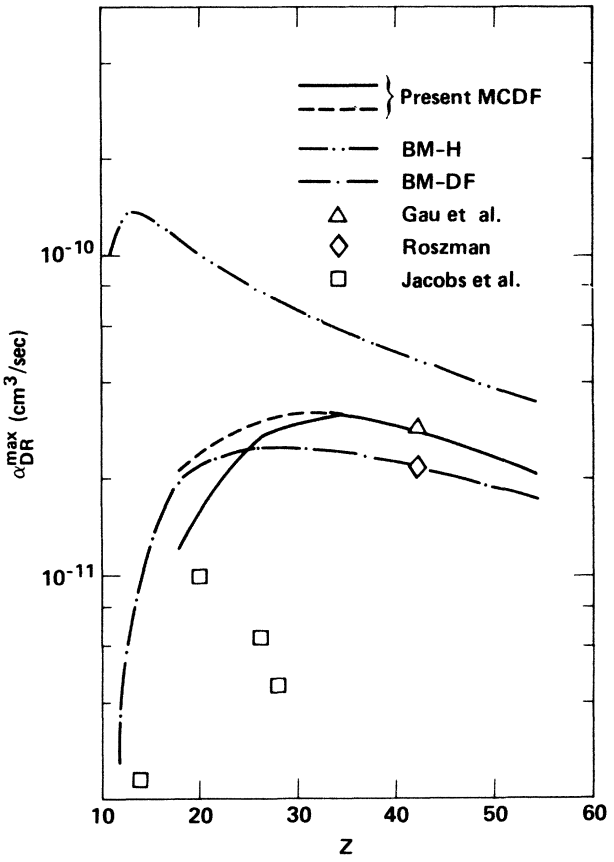

FIG. 5. Maximum total dielectronic recombination coefficients as functions of atomic number Z. The solid and dashed curves describe results from MCDF model with and without including autoionization to the excited states, respectively. The triangle is the value from Ref. 11. The diamond represents the result from Ref. 5 and the squares are the predictions from Refs. 9 and 10. The dashed-dotted and dashed-double-dotted curves illustrate the results from the Burgers-Merts formula with the Dirac-Fock and hydrogenic oscillator strengths, respectively.

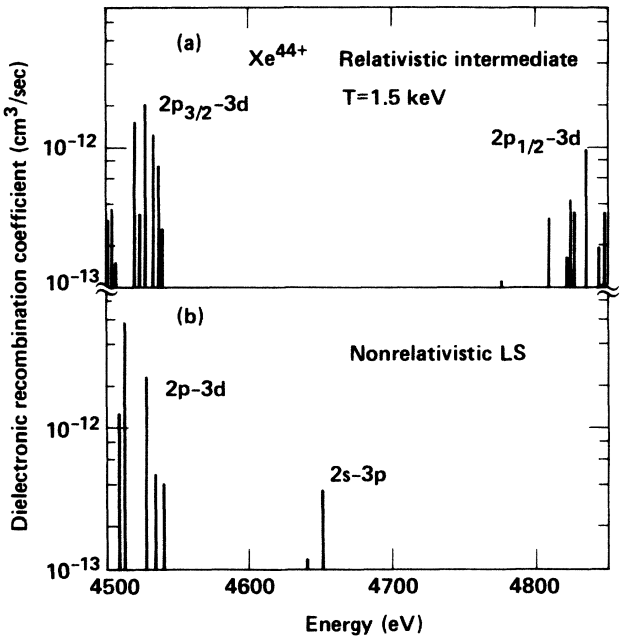

FIG. 6. Dielectronic satellite spectra for the intermediate states $3l3l'$ of the Xe^{44+} ion at $T=1.5$ keV. The upper half represents the results with the relativistic intermediate coupling and the lower half indicates the results with the nonrelativistic LS coupling.

$18 \leq Z \leq 54$ for electron temperatures $0.2 \leq T \leq 6$ keV. The results are listed in Table I.

In the present work, the effect due to autoionization to the excited states of the recombining ion on the dielectronic rate coefficients for $2p^5 3dnl$ Rydberg states was included. The Coster-Kronig-type[20] $2p^5 3dnl \rightarrow 2p^5 3p$ transitions have been found to be energetically possible for $n > 6$, 8, and 9 for the Ar^{8+}, Fe^{16+}, and Se^{24+} ions, respectively. In general, the Coster-Kronig transition rate is orders of magnitude larger than the Auger transition rate. They should be included in the determination of fluorescence yields whenever they are energetically possible. Since the DR coefficient for the low-Z ions is dominated by the high-n Rydberg states, the Coster-Kronig transitions have been found to play a major role in calculations of DR coefficients.[9,10] However, for Se^{24+} and the other heavier ions, the contribution from $2p^5 3dnl$ ($n \geq 9$) to the total DR coefficient is only $\sim 10\%$. Hence, the effect of autoionization to the excited states on the total DR coefficients for heavy ions is rather small.

In Fig. 1, the n and l dependence of the DR coefficients for the $2p^5 3dnl$ configurations of the Ag^{37+} ion is displayed. The DR coefficient peaks at $l=2$ and depends strongly on the orbital angular momentum l of the outer Rydberg electron. The contributions from $l > 5$ were neglected in the present work.

DR rate coefficients from the intermediate $3l3l'$, $3l4l'$, $3lnl'$ ($n > 4$), and $4l4l'$ states for the Fe^{16+} and Xe^{44+} ions are shown in Fig. 2. For the Xe^{44+} ion, the total DR coefficient is dominated by the low-lying excited states. However, for the Fe^{16+} ion, the contribution from the $3lnl$ ($n > 4$) configurations becomes dominant. For the low-Z ions such as Ar^{8+}, the contribution from the $2p^5 3dnl$ states to the total DR coefficient is drastically reduced because of the effect of autoionization to the excited states of the recombining ion.[9,10]

In Fig. 3, total DR coefficients for the Mo^{32+} ion from the present work are compared with the results of the previous nonrelativistic Hartree-Fock calculations.[5,11] The present results have been found to agree within 20% with the previous predictions.[5,11] DR coefficients for the low-lying $3l3l'$ states of the Ne isoelectronic sequence have also been studied independently by Dalhed *et al.*[8] by using the Dirac-Fock method. The DR rate coefficients for $3l3l'$ configurations from the present work agree better than 5% with the results fro Ref. 8.

The total DR rate coefficients for the Fe^{16+} and Xe^{44+} ions from the present MCDF model are compared with the results obtained by the Burgess-Merts (BM) formula[24,25] in Fig. 4. The theoretical predictions of Jacobs *et al.*[9] for the Fe^{16+} ion are also included for the purpose of comparisons. The results from the Burgess-Merts for-

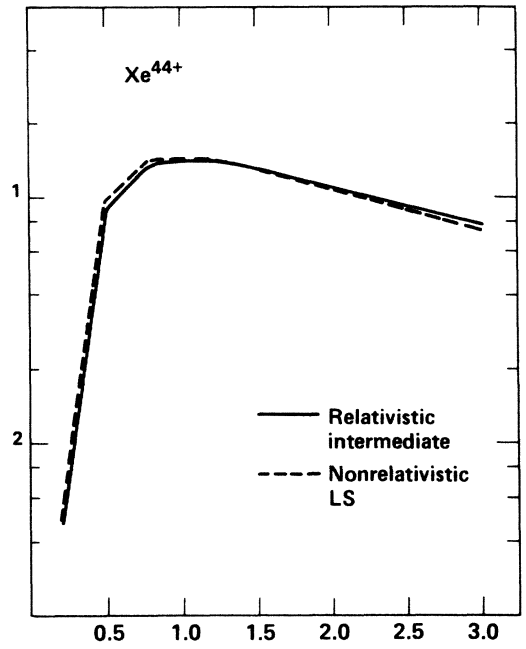

FIG. 7. Dielectronic recombination coefficients for the $3l3l'$ intermediate states of the Xe^{44+} ion as functions of temperature. The solid curve represents the results from MCDF calculations in intermediate coupling. The dashed curve describes the predictions from the nonrelativistic *LS* coupling calculations.

mula with the hydrogenic oscillator strengths and excitation energies (BM-H) are larger than the MCDF values by as much as a factor of 2 except at low temperature. The predictions from the Burgess-Merts formula with the Dirac-Fock (DF) oscillator strengths and energies (BM-DF) agree quite well with the results from the detailed calculations for high temperature. However, for low temperature, the BM-DF model underestimates the DR rate coefficient by as much as a factor of 4.

The DR rate coefficients of Jacobs *et al.*[9] for the Fe^{16+} ion are smaller than the results from the present MCDF model by a factor of 4 (Fig. 4). The dielectronic rate coefficients of Ref. 9 were obtained by using the autoionization rates derived from extrapolation of calculated electron-impact excitation cross sections. The extrapolation procedure and the use of dipole approximation have been found to introduce large errors in calculations of the Auger rates for the low-lying doubly excited states.[26] Furthermore, the reduction of the total DR coefficient due to the inclusion of autoionization to the excited states of the recombining ion is only $\sim 15\%$ in the present work in contrast to an order of magnitude reduction in Ref. 9. Large discrepancies have also been found for Li-like[27] and F-like[28] ions.

The dependence of the maximum total DR rate coefficient on atomic number is shown in Fig. 5. For comparison, the results from the previous works[5,9–11] and the Burgess-Merts formula are also displayed. The predictions from BM-H model are quite different from the results of *ab initio* calculations especially for the low-Z ions. The results from BM-DF model agree quite well with the present calculations for $Z > 20$. For the Ar^{8+} ions, the BM-DF model overestimates the DR coefficients by a factor of 2 because of the exclusion of autoionization to the excited states.[9,10] For the Mo^{32+} ion, fair agreement is attained between the present work and the previous Hartree-Fock predictions.[5,11] However, the maximum total DR coefficient as a function of atomic number from Refs. 9 and 10 exhibits quite different behavior from the present work. The results from Refs. 9 and 10 peak sharply around $Z=20$ while the values from the present MCDF model have much broader peak around $Z=34$. The discrepancies between the results from the present work and the predictions from Refs. 9 and 10 increase from $\sim 25\%$ to a factor of 6 as Z increases from 20 to 28.

The inclusion of Coster-Kronig rates in the determination of the stabilizing radiative branching ratios leads to a factor of 2 reduction in the total DR coefficients for the Ar^{8+} ion (solid versus dashed curve in Fig. 5). The corresponding reduction for the Fe^{16+} ion is only 15%, and is rather small for the other heavy ions.

The dielectronic satellite spectra for the $3l3l'$ states of the Xe^{44+} ion is shown in Fig. 6. In the nonrelativistic *LS* coupling approximation, the spectrum is dominated by the $2p$-$3d$ transitions. The addition of the relativistic effect splits them into two groups (i.e., $2p_{3/2}$-$3d$ and $2p_{1/2}$-$3d$) which are separated by $\sim$ 300 eV in energy. The lines of the $2s$-$3p$ transitions are shifted out of the region to higher energies and split into many weaker lines. However, the effect of relativity on the total DR coefficient is relatively small for the ions treated in the present work (Fig. 7). These observations are similar to the findings for the He isoelectronic sequence.[7]

The DR coefficients from the present MCDF calculations are suitable for the low-density plasmas. The effects of the plasma microfield, external electric field, and electron collisional mixing have been found to change the DR coefficients significantly for the $\Delta n = 0$ transitions involving the high Rydberg states.[29,30] However, for the Ne-like ions, the plasma density effect has been shown to have small impact on the DR coefficient for the low-lying $3l3l'$ states of the medium and heavy ions.[8] Since the DR coefficient for the medium and heavy Ne-like ions is dominated by the contribution from the low-lying autoionizing states, the density effect for these ions should be a minimum. For the high-density plasmas of the low-Z ions, the density effect should be included in calculation of the dielectronic recombination coefficient.

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