

Effect of Coster-Kronig transition on dielectronic recombination of the He-like ions

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Dielectronic recombination rate coefficients have been calculated for He-like ions with atomic numbers $Z = 5, 6, 7, 8$, and 9 . The calculations include the influence of the Coster-Kronig channels to the excited states of the recombining ion on the rate coefficients. The detailed Auger and radiative rates were calculated using the multiconfiguration Dirac-Fock model in intermediate coupling with configuration interaction. The total dielectronic recombination coefficients for B^{3+} , N^{5+} , and F^{7+} ions have been found to reduce by 60%, 13%, and 4%, respectively, due to the inclusion of Coster-Kronig channels. For the B^{3+} ion, the dielectronic recombination coefficient from the present work is smaller than the value derived from the Burgess-Merts formula by a factor of 3 at electronic temperature $T = 100$ eV.

I. INTRODUCTION

Dielectronic recombination (DR) rate coefficients are basic atomic data required for the modeling of high-temperature plasmas. Since experimental data on the dielectronic rate coefficients for highly charged ions are very scarce or nonexistent in most cases, there is heavy reliance on the semiempirical formula or theoretical values for practical applications. For He-like ions there have been several nonrelativistic distorted-wave calculations in the last few years¹⁻³ of DR rate coefficients for a few selected ions. Recently, we have carried out multiconfiguration Dirac-Fock (MCDF) calculations of DR rate coefficients for the He isoelectronic sequence.⁴ In these previous theoretical studies, Coster-Kronig transitions from autoionizing Rydberg states were not taken into account in calculations of radiative branching ratios. In this paper, we report on the calculations of dielectronic recombination rate coefficients for He-like ions with atomic numbers $5 \leq Z \leq 9$ using the MCDF model. The calculations include Coster-Kronig transitions from the doubly excited Rydberg states to the singly excited states of recombining ions whenever they become energetically possible. The influence of autoionization to excited states of the recombining ion on dielectronic recombination was first discussed by Jacobs *et al.*⁵ This effect has become rather well known and has been routinely included in many recent calculations when it is important.

II. THEORETICAL METHOD

The detailed information on theoretical calculations of dielectronic recombination coefficients for He-like ions using the MCDF model has been given in Ref. 4. Here, we only outline the essential points. The total dielectronic recombination coefficient for the initial state i in the isolated resonance approximation can be written as⁶

$$\alpha_{\text{DR}}(i; \text{total}) = \frac{1}{2g_i} \left[\frac{4\pi R}{kT} \right]^{3/2} a_0^3 \sum_d \sum_f \exp \left[-\frac{e_2}{kT} \right] g_d \times A_a(d \rightarrow i) \omega_d, \quad (1)$$

with

$$\omega_d = A_r(d \rightarrow f) / [\Gamma_r(d) + \Gamma_a(d)]. \quad (2)$$

Here g_d and g_i are the statistical weight factors for intermediate state d and initial state i , respectively; R is the Rydberg energy and a_0 is the Bohr radius; $A_a(d \rightarrow i)$ is the Auger rate, and e_2 is the Auger energy; $A_r(d \rightarrow f)$ is the radiative rate; Γ_r and Γ_a are the total radiative and Auger rates, respectively, for the intermediate state d . A Maxwellian distribution of energy is assumed for the free electrons.

The relativistic Auger transition probability is calculated from perturbation theory.⁷ The transition probability from initial state i to final state f in a frozen-orbital approximation is given by

$$A_a = \frac{2\pi}{\hbar} \left| \left\langle \Psi_f \right| \sum_{\substack{\alpha, \beta \\ \alpha < \beta}} V_{\alpha\beta} \left| \Psi_i \right\rangle \right|^2 \rho(\epsilon). \quad (3)$$

Here $\rho(\epsilon)$ is the density of final states; the two-electron operator $V_{\alpha\beta}$ is taken to be the sum of Coulomb and generalized Breit operators and is given in atomic units by⁸

$$V_{12} = \frac{1}{r_{12}} - \alpha_1 \cdot \alpha_2 \frac{\cos(\omega r_{12})}{r_{12}} + (\alpha_1 \cdot \nabla_1)(\alpha_2 \cdot \nabla_2) \frac{\cos(\omega r_{12}) - 1}{\omega^2 r_{12}}. \quad (4)$$

The radiative electric dipole transition probability is given in perturbation theory by⁹

$$A_r(i \rightarrow f) = \frac{2\pi}{3(2J_i + 1)} |\langle f || T_1 || i \rangle|^2. \quad (5)$$

The calculation of the relativistic reduced dipole-matrix element $\langle f || T_1 || i \rangle$ in the framework of the MCDF model has been described in Refs. 7 and 9.

In calculations of detailed Auger and radiative rates, the required energy levels and bound-state wave functions were evaluated in intermediate coupling with configuration interaction using the MCDF model in the extended average-level scheme.¹⁰

TABLE I. Theoretical total dielectronic recombination rate coefficients for He-like ions (in multiples of 10^{-13} cm³/sec).

| Temperature (keV) | B ³⁺ | C ⁴⁺ | N ⁵⁺ | O ⁶⁺ | F ⁷⁺ |
|----------------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0.04 | 1.78 | 0.451 | 0.0657 | 0.006 22 | |
| 0.06 | 4.79 | 2.55 | 0.847 | 0.187 | 0.0314 |
| 0.08 | 6.95 | 5.41 | 2.79 | 0.977 | 0.264 |
| 0.10 | 8.05 | 7.91 | 5.32 | 2.50 | 0.915 |
| 0.12 | 8.46 | 9.71 | 7.82 | 4.49 | 2.03 |
| 0.14 | 8.44 | 10.85 | 9.95 | 6.60 | 3.49 |
| 0.16 | 8.22 | 11.47 | 11.62 | 8.60 | 5.13 |
| 0.18 | 7.88 | 11.74 | 12.84 | 10.36 | 6.78 |
| 0.20 | 7.50 | 11.77 | 13.69 | 11.84 | 8.35 |
| 0.24 | 6.71 | 11.38 | 14.53 | 13.96 | 11.05 |
| 0.30 | 5.64 | 10.36 | 14.51 | 15.50 | 13.76 |
| 0.50 | 3.40 | 7.08 | 11.53 | 14.59 | 15.64 |
| 1.00 | 1.46 | 3.34 | 6.09 | 8.77 | 10.86 |
| 2.00 | 0.568 | 1.37 | 2.63 | 4.05 | 5.39 |
| 3.00 | 0.320 | 0.781 | 1.54 | 2.41 | 3.28 |
| 4.00 | 0.211 | 0.519 | 1.03 | 1.63 | 2.26 |
| 5.00 | 0.152 | 0.378 | 0.752 | 1.20 | 1.67 |
| 6.00 | 0.117 | 0.203 | 0.580 | 0.930 | 1.30 |

Dielectronic recombination from a He-like ground state to a state of a Li-like ion can be represented by

$$1s^2 + e^- \rightleftharpoons 1s nl n' l' \rightarrow 1s^2 n'' l'' + h\nu.$$

In the present work, we carried out explicit calculations for the intermediate states with $n=2$ and $n' \leq 15$, $l' \leq 4$.

For the $1s 2p nl$ Rydberg states, the Coster-Kronig transition $1s 2p nl \rightarrow 1s 2s + e^-$ becomes energetically possible for certain large n . In the present calculations, Coster-Kronig transitions were included in the evaluations of fluorescence yields [Eq. (2)]. For the $1s 2p nl$ configuration with $n > 15$, the DR coefficients were estimated by using an n^{-3} extrapolation of the Auger rates.

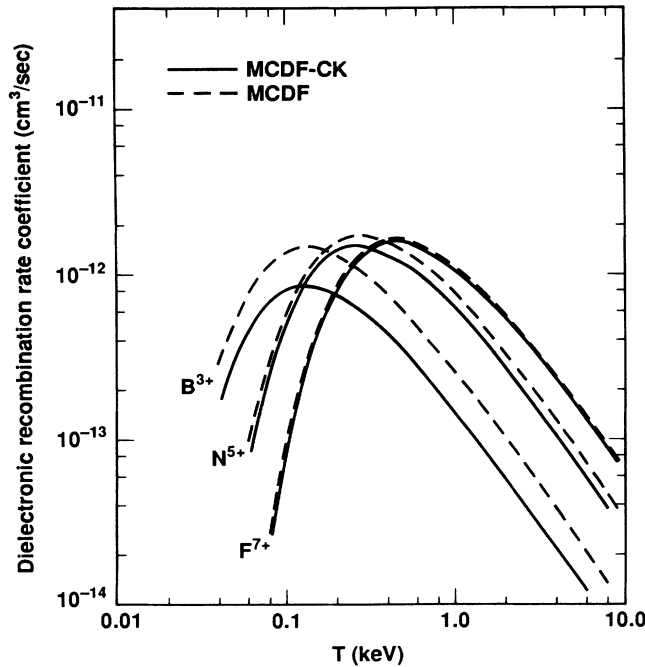


FIG. 1. Total dielectronic recombination rate coefficients as functions of electron temperature. Solid curves represent the present MCDF results including the effect of Coster-Kronig transitions. Dashed curves indicate the values from the MCDF calculations without Coster-Kronig transitions.

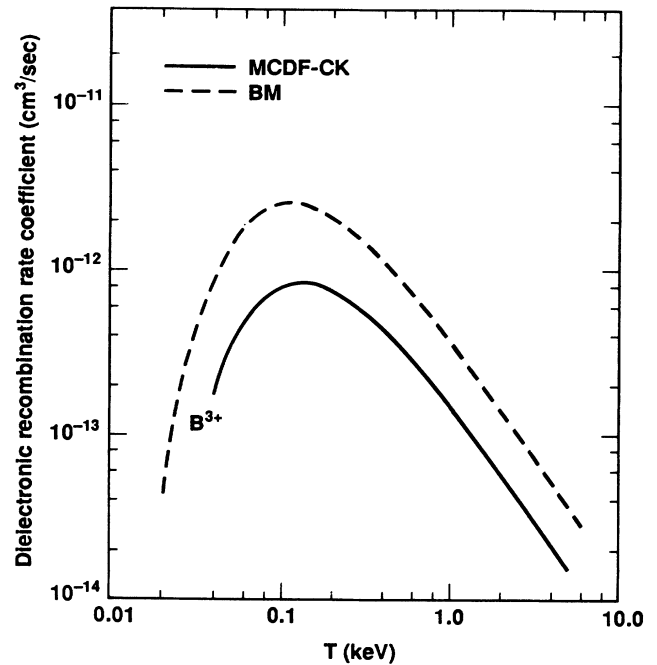


FIG. 2. Total dielectronic recombination rate coefficients for the B³⁺ ion as functions of electron temperature. Solid curve displays the present MCDF results with Coster-Kronig transitions and dashed curve represents values derived from the Burgess-Merts formula.

III. RESULTS AND DISCUSSION

Dielectronic recombination coefficients for the He isoelectronic sequence were calculated for B^{3+} , C^{4+} , N^{5+} , O^{6+} , and F^{7+} ions using the MCDF model. The calculations include Coster-Kronig transitions to the excited states of the recombining ion. The total dielectronic recombination coefficients are listed in Table I.

From our previous work,⁴ we have shown that our MCDF results without Coster-Kronig transitions agree reasonably well with other theoretical calculations. We will not repeat the comparison here. For the B^{3+} ion, the low-lying $1s\ 2l\ nl'$ ($n \leq 3$) states contribute only 20% of the total DR coefficient while the same states contribute 50% for the F^{7+} ion at the peak temperature. The onset of the $2s\text{-}2p\ nl$ Coster-Kronig transition for the B^{3+} ion is at $n=5$. As Z increases, the Coster-Kronig transition becomes energetically favorable at much higher n (e.g., $n=9$ for the F^{7+} ion). The total DR coefficients for B^{3+} , N^{5+} , and F^{7+} ions are reduced by 60, 13, and 4%, respectively, at the peak values due to inclusion of the Coster-Kronig transitions (see Fig. 1). This behavior is caused by the fact that the contributions from high- n states decrease and the onset of the Coster-Kronig transitions occurs at higher n as Z increases. Therefore, the re-

sults from our previous calculations⁴ are affected only for ions with $Z \leq 9$. The effect of including Coster-Kronig transitions on the total DR rate coefficients for He-like ions with $Z \geq 10$ is negligible.

The present MCDF results for the B^{3+} ion, including the effect of Coster-Kronig transitions, are compared with the predictions from the Burgess-Merts formula^{11,12} in Fig. 2. The values from the Burgess-Merts formula were obtained by using hydrogenic oscillator strengths and excitation energies. At electron temperature $T=100$ eV, the results from the present work is smaller than the value from the Burgess-Merts formula by a factor of 3 for the B^{3+} ion which is in contrast to the earlier findings for low- Z ions.^{1,4} The fact that the Burgess-Merts formula does not take into account the opening of the Coster-Kronig channels for high- n Rydberg states contributes heavily to the above-mentioned discrepancies.

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