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Systematic theoretical study of dielectronic recombination for helium-like isoelectronic sequence

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Abstract

Dielectronic recombination cross sections and rate coefficients of He-like isoelectronic sequence are systematically calculated employing the relativistic Flexible Atomic Code (FAC). The calculated DR resonance strengths, cross sections and rate coefficients are in good agreement with other experimental and theoretical results. The effects of radiative cascades on DR cross sections and the variation of DR branching ratio with different DR resonance and atomic numbers Z are studied. The n^{-3} scaling law is also checked and used to extrapolate rate coefficients. And analytic formulas are used to fit the total rate coefficients with respect to both T and Z for helium-like isoelectronic sequence.
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1. Introduction

Dielectronic recombination (DR) is an important atomic process contributing to ion balance in high-temperature low-density plasmas [1]. It is a two-step resonant process. When a free electron collides with an ion, it may be captured nonradiatively and transfer energy to a bound electron to form a doubly excited state. Subsequently, the state decays into a nonautoionizing state through radiative transition processes. These reactions have the form

$$(1s^2) + e^- \rightarrow (1snln'l') \rightarrow \cdots \rightarrow (1s^2n''l'') + h\nu.$$

Few experimental measurements have been reported on DR rate coefficients which are essential in the determination of charge distribution in plasma, especially in highly charged ions such as He-like ions. Fuchs et al. reported a measurement of DR cross sections for highly charged Krypton ions including He-like Kr^{34+}, and also gave theoretical results employing the Hebrew University Lawrence Livermore Atomic Code (HULLAC) [2]. Karim et al. calculated total DR rate coefficients for He-like ions with $Z = 10-28$ employing a self-consistent Hartree–Fock–Slater method with relativistic corrections [3]. Chen calculated the DR rate

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coefficients for the 13 He-like ions from C^{4+} to Mo^{40+} using multiconfiguration Dirac–Fock (MCDF) method, and pointed out that relativity had a nonnegligible effect on total DR rate coefficients [4]. Nilsen also gave the rate coefficients for He-like ions Ne, Si, Ar, Ti, Fe, Kr, Mo and Xe, and fitted the total rate coefficients using an analytic formula for each ion separately [5]. Based on the calculated rate coefficients from Chen's works, Teng et al. used another formula to fit the total rate coefficients, and also gave the analytic relations between the fit parameters and the nuclear numbers [6,7]. In Ref. [8], one of us also calculated the DR rate coefficients for He-like Mg, Si, S, Ar, Ca, Fe and Ni ions. And recently, Dasgupta and Whitney reported Z-scaling law for state-specific DR rate coefficients of He-like ions based on the data of Al^{11+}, Ti^{20+}, Ni^{26+}, Kr^{34+} and Mo^{40+} calculated by using the Hartree–Fock with relativistic corrections method of Cowan [9].

The Flexible Atomic Code (FAC), recently developed by one of us, has been successfully used to calculate radiative and dielectronic recombination, resonance excitation and collisional ionization rate coefficients [8,10,11]. In this paper, the DR cross sections and rate coefficients for highly charged He-like ions Ne^{8+}, Si^{12+}, Ar^{16+}, Ti^{20+}, Fe^{24+}, Ge^{30+}, Kr^{34+}, Mo^{40+}, Ag^{45+}, Sn^{48+}, Xe^{52+} are systematically calculated using FAC. The calculated Auger and radiative transition rates, resonance strengths, cross sections and rate coefficients are in good agreement with the experiments and other calculations. The effect of radiative cascades on DR cross sections is studied in detail. The variations of DR branching ratio with different DR resonances and atomic number Z are given. The validation of n^{-3} scaling law for extrapolation in the calculation of rate coefficients is discussed. The empirical formulas are used to fit the dependences of total rate coefficients on the temperature and nuclear number with high accuracy for He-like isoelectronic sequence.

2. Outline of the theory

The DR strength can be written as

$$S_{ij} = \frac{\pi^2\hbar^3}{m_e E_{ij}}\frac{g_j}{2g_i}A^a(j \to i)B^r_j, \tag{1}$$

where j represents a doubly excited intermediate state, i represents the initial ground state. E_{ij} is the resonant energy, g_i and g_j are the statistical weights of state i and j. $A^a(j \to i)$ is the autoionization rate from level j to level i. Considering radiative cascades, the radiative branching ratio B^r_j can be written as

$$B^r_j = \frac{1}{\Gamma_j}\sum_f\left[A^r(j \to f) + \sum_d A^r(j \to d)\frac{A^r(d \to f)}{\Gamma_d}\right], \tag{2}$$

with

$$\Gamma_j = \sum_f A^r(j \to f) + \sum_d A^r(j \to d) + \sum_k A^a(j \to k). \tag{3}$$

$A^a(j \to k)$ and $A^r(j \to f, d)$ are Auger and radiative rates of state j. k represents a final state of Auger process, f represents a nonautoionizing state, d represents a low-lying autoionizing doubly excited state, the radiative decays to level d lead to radiative cascades. Γ_d is the total decay rate of state d similar to Γ_j.

Ignoring the detailed structure of the resonance profiles, the DR cross section is

$$\sigma_{ij}(E) = S_{ij}\delta(E - E_{ij}). \tag{4}$$

In order to compare with experimental measurement, we convolve the above cross section with a Gaussian profile for the electron energy distribution.

In thermal plasmas, the rate coefficient is defined as

$$\alpha_i(T) = \sum_j \int_0^\infty vf(v,T)\sigma_{ij}(v)\,dv, \tag{5}$$

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