Dielectronic recombination for oxygenlike ions relevant to astrophysical applications

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In the modeling of the astrophysical plasmas, the relative elemental abundance inferred from solar and stellar upper atmosphere can be affected by as much as a factor of 5 due to the uncertainties in the current dielectronic recombination (DR) rate coefficients used to analyze the spectra [Savin and Laming, Astrophys. J. **566**, 1166 (2002)]. DR rate coefficients for oxygenlike ions have been identified as the most urgent needs for the astrophysical applications. In this work, we report on the calculations of DR rate coefficients for Mg V, Si VII, S IX, and Fe XIX ions which are important for the modeling of the astrophysical plasmas. The calculations are carried out in isolated resonance and distorted-wave approximations. The relevant atomic data are calculated using the multiconfigurational Dirac-Fock method. We include $2s-2p$, $2p_{1/2}-2p_{3/2}$, $2\ell-3\ell'$, and $1s-2p$ excitations and cover temperatures ranging from 0.001 eV to 10 000 eV. For low temperatures, it is essential to have accurate DR resonance energies and to include fine-structure excitations in order to obtain reliable DR rate coefficients. Good agreement with experiment has been found for Fe XIX. For Mg V, Si VII, and S IX, significant discrepancies are noted between this work and recommended rate coefficients.

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I. INTRODUCTION

Dielectronic recombination (DR) is one of the most important recombination processes in high-temperature plasmas [1–3]. Accurate DR rate coefficients are needed to carry out successful modeling of astrophysical and laboratory produced plasmas. Recently, a critical evaluation of the uncertainties of the existing theoretical DR rate coefficients has been performed [4]. It was found that the uncertainties can be as large as a factor of 2–5 for some ions. In the modeling of the astrophysical plasmas, the relative elemental abundance inferred from solar and stellar upper atmosphere can be affected by as much as a factor of 5 due to these uncertainties in the DR rate coefficients employed to analyze the spectra [4]. DR rate coefficients for oxygenlike ions have been identified as the most urgent needs for the astrophysical applications [4]. For Mg V, Si VII, S IX, and Fe XIX, a few theoretical investigations have been done [5–10]. Fe XIX is the only ion for which several different calculations exists. The only reliable experiment is also for Fe XIX ion [10]. In the work of Jacobs *et al.* [5–7], the calculations were carried out in LS coupling and the autoionization rates were obtained from the theoretical values of the partial-wave electron-impact excitation cross sections by means of the quantum-defect theory. Roszman [8] performed a nonrelativistic single configuration Hartree-Fock calculation in LS coupling while Dasgupta and Whitney [9] used Cowan's Hartree-Fock code [11] with relativistic corrections. All of these earlier calculations neglected the contributions from the fine-structure ($2p_{1/2}-2p_{3/2}$) excitation which has been shown to be very important for low-temperature DR rate coefficients [10,12]. Thus, including fine-structure excitation is essential to produce reliable DR rate coefficients applicable for modeling the photoionized gas. In addition, LS coupling calculations are known not to include all possible autoionizing states contributing to the DR process which could lead to serious errors in their results [13–16]. The most recent calculations for Fe XIX were carried out in intermediate coupling and include fine-structure excitation using semirelativistic multiconfiguration Breit-Pauli (MCBP) and fully relativistic multiconfiguration Dirac-Fock (MCDF) methods. These calculations yield satisfactory agreement with experiment [10,12].

In this work, we report on the relativistic calculations of total DR rate coefficients for Mg V, Si VII, S IX, and Fe XIX for the ground state and the excited states of the ground configuration. These calculations are performed using the MCDF method [17,18] in intermediate coupling with configuration interaction from the same complex and include contributions from $2s-2p$, $2p_{1/2}-2p_{3/2}$, $2\ell-3\ell'$, and $1s-2p$ excitations. The MCDF method which has been benchmarked by experiments [10,12] should give reliable total DR rate coefficients. These data are also fitted by analytic functions for easy use in the modeling of both collisionally-ionized and photoionized plasmas. We find significant discrepancies between present results and the recommended values [5–7] for Mg V, Si VII, and S IX.

II. THEORETICAL CALCULATION

DR resonance strengths and rate coefficients are calculated in the independent processes and isolated resonance approximations [1]. The total rate coefficient for an initial state i after averaging over the Maxwellian distribution of the plasma electrons is given by [1],

$$\alpha_{DR}(i)=\frac{1}{2g_i}\left(\frac{4\pi R}{kT}\right)^{3/2}a_0^3\sum_{d,f}\exp(-E_d/kT)\times g_d A_A(d\rightarrow i)A_r(d\rightarrow f)/[\Gamma_r(d)+\Gamma_A(d)]. \quad (1)$$

Here, the sums on d and f are over the intermediate autoionizing states d and the stabilized final states f, respectively; g_d and g_i are the statistical weight factors; R is the Rydberg energy and a_0 is the Bohr radius; $A_A(d\rightarrow i)$ is the Auger rate

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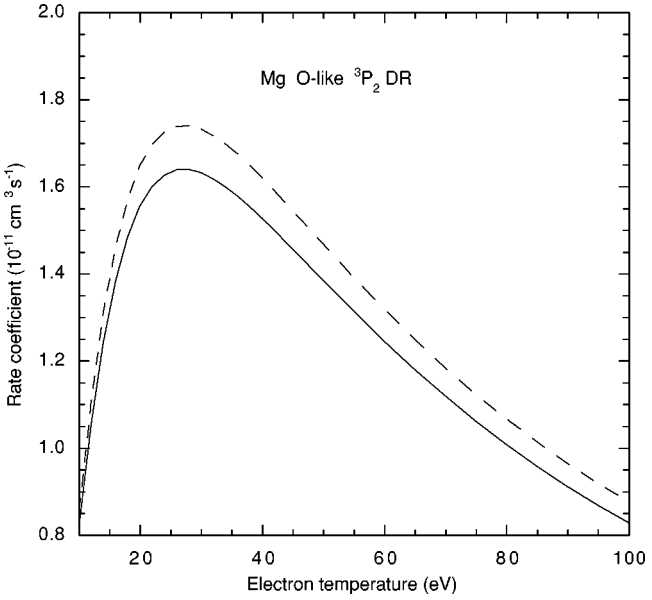

FIG. 1. DR rate coefficients for ground-state $^3P_2$ in Mg^{4+} as functions of electron temperature. The solid curve displays the results including cascade corrections while the dashed curve is the values without cascade corrections.

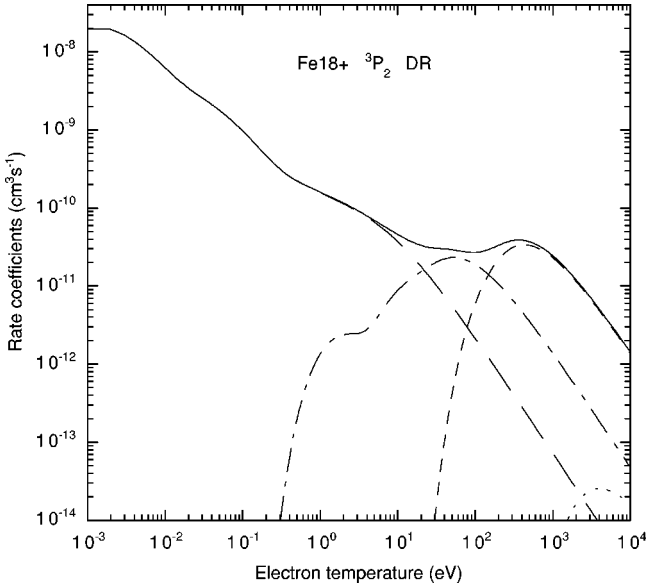

FIG. 2. DR rate coefficients for $^3P_2$ state of Fe^{18+} as functions of electron temperature. The dash-dotted, long-dashed, short-dashed, and dotted curves represent the results from the $2s-2p$, $2p_{1/2}-2p_{3/2}$, $2\ell-3\ell'$, and $1s-2p$ excitations, respectively. The solid curve displays the total DR rate coefficients.

and $A_r(d\to f)$ is the radiative rate; E_d is the Auger energy; k is the Boltzmann constant; T is the electron temperature; and $\Gamma_r(d)$ and $\Gamma_A(d)$ are the total radiative and Auger rates for state d, respectively.

The required transition energies, Auger and radiative transition rates are evaluated using the MCDF method [17,18]. From perturbation theory, the Auger transition rate in a frozen-orbital approximation is [17]

$$A_A(d\to i)=\frac{2\pi}{\hbar}|\langle\psi_i|H-E|\psi_d\rangle|^2\rho(\varepsilon), \tag{2}$$

where $\rho(\varepsilon)$ is the density of final states. It is worthwhile to note that the Auger operator in the present calculations is not just the Coulomb operator but includes also the one-electron operator as contained in the unperturbed Hamiltonian H. This is necessary because the Auger transitions involving the fine-structure levels results in a situation that the initial-state and final-state wave functions differ by only one orbital. Thus, the orthogonality of the orbital wave functions does not eliminate the contributions from the one-electron operator. The spontaneous electric-dipole radiative transition rate for each autoionizing state is also calculated using the first-order perturbation theory [17,19].

In the present work, total DR rate coefficients include the contributions from $2s-2p$, $2p_{1/2}-2p_{3/2}$, $2\ell-3\ell'$, and $1s-2p$ excitations. They can be represented schematically by

$$2s^22p^4+e\to 2s2p^5n\ell\to(2s^22p^4n\ell+2s^22p^5+2s2p^6+2s2p^5n'\ell')+h\nu, \tag{3}$$

$$2s^22p^4J+e\to 2s^22p^4J'n\ell\to(2s^22p^5+2s^22p^4n'\ell')+h\nu, \tag{4}$$

$$2s^22p^4+e\to(2s2p^43\ell n'\ell'+2s^22p^33\ell n'\ell')\to(2s^22p^4n''\ell''+2s2p^5n''\ell'')+h\nu, \tag{5}$$

$$1s^22s^22p^4+e\to 1s2s^22p^5n\ell\to(1s^22s^22p^4n\ell+1s^22s^22p^5)+h\nu. \tag{6}$$

All possible Coster-Kronig transitions and radiative transitions to bound states are included in the calculations.

For the $\Delta n=0$ transitions with $2s-2p$ [Eq. (3)] and $2p_{1/2}-2p_{3/2}$ [Eq. (4)] excitations, explicit calculations are performed for intermediate states $n_0\leqslant n\leqslant 30$ and $\ell\leqslant 12$. Here the onset values n_0 for $2p_{1/2}-2p_{3/2}$ excitation are 5, 7, 7, and 11 and those for $2s-2p$ excitation are 3, 3, 4, and 6 for $Z=12,14,16$, and 26, respectively. Since many important resonances for the $\Delta n=0$ DR have very small energies, the resonance energies are adjusted by using the known experimental excitation energies [20] between $n=2$ states to achieve better than 0.1 eV accuracy. The amount of adjustment is less than 2.7 eV for all resonances. For the case of $2s-2p$ excitation, the radiative decay of $2p$ electron can lead to a autoionizing state. For these DR transitions, a one-step cascade correction is included. The contributions from the high-n Rydberg states up to $n=600$ are taken into account using a n^{-3} scaling for the appropriate Auger and radiative transition rates. This high-n cutoff has been checked to give better than 1% convergence in total DR rate coefficients.

For the $2\ell-3\ell'$ excitations [Eq. (5)], detailed calculations are carried out for autoionizing states $3\leqslant n'\leqslant 15$ and

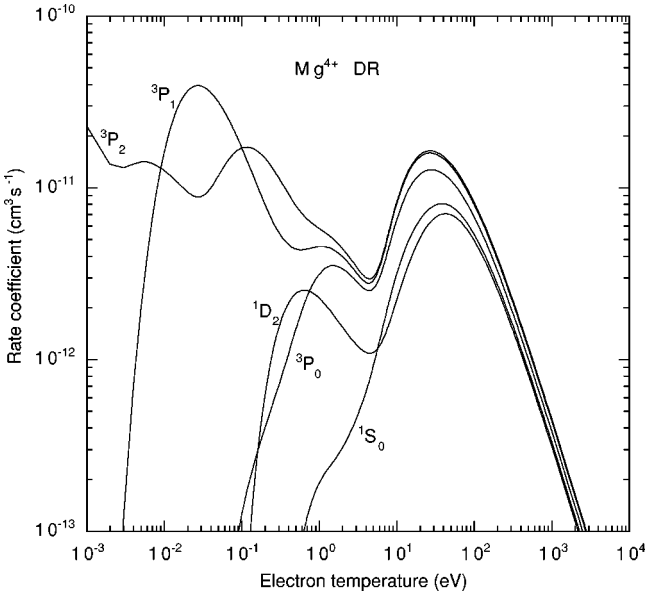

FIG. 3. Total DR rate coefficients for ground and excited states of Mg^{4+} as functions of electron temperature. The curves are labeled by their initial states.

$\ell' \leqslant 6$. No energy adjustment is done for this case because the resonance energies are more than 100 eV. The radiative decay of $3\ell'$ electron can also result in a autoionizing state. For these transitions, we also apply a one-step cascade correction. Similar n^{-3} scaling procedure is used to obtain the contributions from high-n Rydberg states up to $n=200$.

For K-shell excitation [Eq. (6)], we include only intermediate states with $n \leqslant 8$ and $\ell \leqslant 3$. The contributions to the total DR rate coefficients from K-shell excitation are less than 2% for all temperatures covered in this study.

For $2\ell - 4\ell'$ excitation, the existence of the extra $n=3$ Auger channels and the fact that $n=4$ to $n=3$ radiative decay leads to another autoionization state, these DR channels are expected to have rather small contributions to the total DR rate coefficients. This was confirmed by a recent experiment which did not observed any appreciable $2\ell - 4\ell' n\ell''$ DR resonances [10]. Therefore, these DR channels are neglected in the present work.

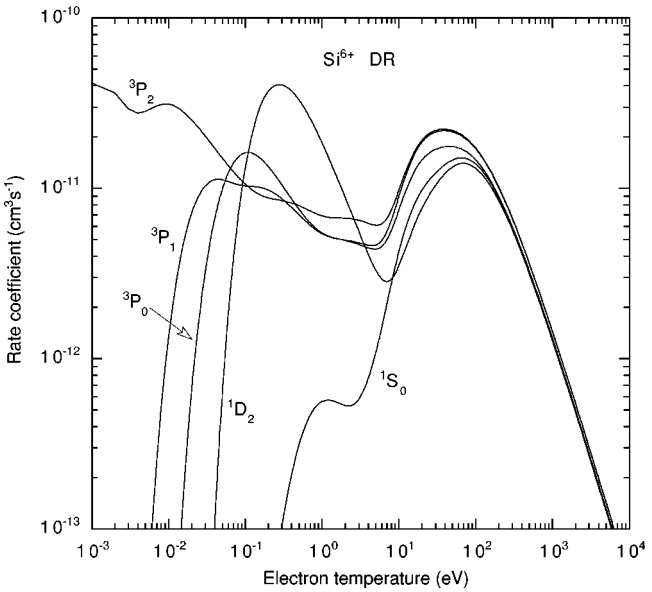

FIG. 4. Total DR rate coefficients for ground and excited states of Si^{6+} as functions of electron temperature. The curves are labeled by their initial states.

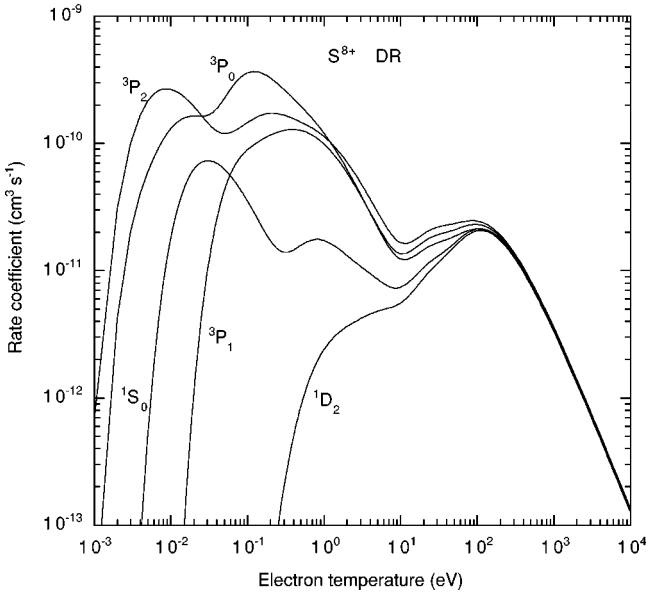

FIG. 5. Total DR rate coefficients for ground and excited states of S^{8+} as functions of electron temperature. The curves are labeled by their initial states.

III. RESULTS AND DISCUSSION

We have calculated the total DR rate coefficients for the $^3P_{0,1,2}$, $^1D_2$, and $^1S_0$ states of the ground configuration for

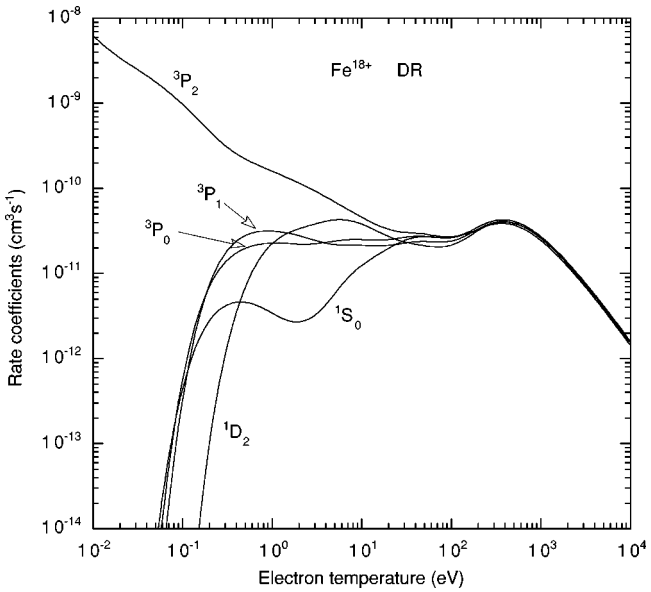

FIG. 6. Total DR rate coefficients for ground and excited states of Fe^{18+} as functions of electron temperature. The curves are labeled by their initial states.

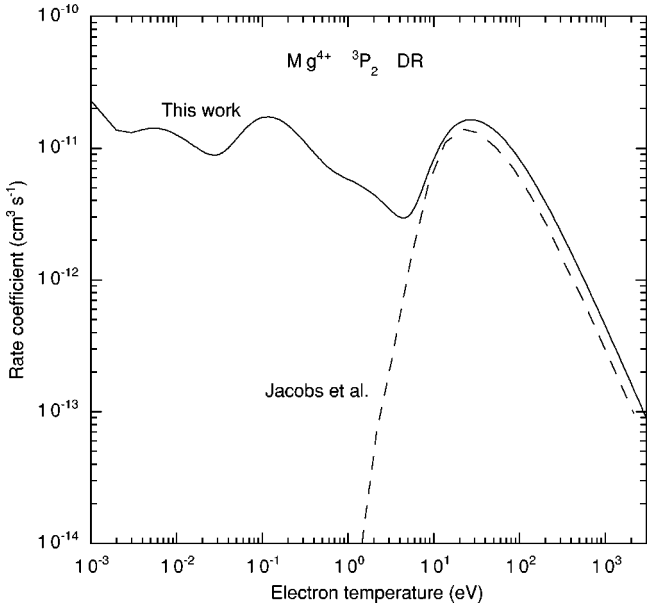

FIG. 7. Total DR rate coefficients for $^3P_2$ state of Mg^{4+} as functions of electron temperature. The solid curve is from this work and the dashed curve displays the results from Jacobs *et al.* (Ref. [7]).

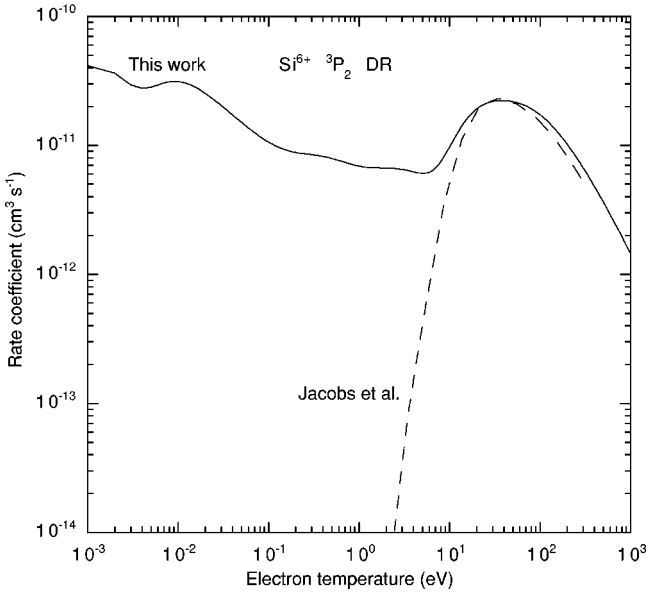

FIG. 8. Total DR rate coefficients for $^3P_2$ state of Si^{6+} as functions of electron temperature. The solid curve is from this work and the dashed curve displays the results from Jacobs *et al.* (Ref. [6]).

Mg V, Si VII, S IX, and Fe XIX. The calculations cover electron temperatures $0.001 \leqslant T \leqslant 10\,000$ eV. The numerical tables for DR rate coefficients for the ground state are available electronically from EPAPS storage [21]. The cascade correction can reduce the DR cross sections for some resonances by more than one order of magnitude but it reduces the total DR rate coefficients for ground state ($^3P_2$) by less than 10% (Fig. 1). The effect is much larger ($\sim$20%) for the excited states. Similar to the findings in our previous work on *B*-like ions [22], the *n* dependence of the DR rate coefficients behaves quite irregularly for the $\Delta n = 0$ transitions due to the opening of the new DR channels as n increases. When all channels are open, normal ordering (i.e., DR rate coefficients scale as n^{-3}) returns.

In Fig. 2, DR rate coefficients for ground state of Fe^{18+} from various excitation channels are shown. Similar behavior is found for Mg V, Si VII, and S IX ions. For temperatures less than 10 eV, the fine-structure excitations are the dominate DR channels. Calculations that neglect these channels, such as the earlier ones in LS coupling, will not predict the low-temperature behavior correctly. Between 10 eV and 100 eV, $2s-2p$ excitations take over and above 100 eV, $2\ell - 3\ell'$ excitations become the most important channels. In Figs. 3–6, total DR rate coefficients for the ground state and excited states are displayed. For electron temperatures less than 10 eV, the rate coefficients for different initial states can differ by as much as a few orders of magnitude. We also notice that the LS coupling is not a good scheme in such low-temperature regime even for low-*Z* ions. The reason for this is that the low-temperature DR rate coefficients are dominated by the low-energy $\Delta n = 0$ resonances. These resonances could have very different resonance energies for different fine-structure states or they may not even open for some initial states. Therefore, accurate descriptions for these resonances are needed to yield reliable results.

In Figs. 7–9, the DR rate coefficients for the ground state from this work are compared with the theoretical predictions from Jacobs *et al.* [5–7] which were recommended for use in the modeling of astrophysical plasmas [23]. Between 10 to 1000 eV, the discrepancies can be as large as 33%, 22%, and a factor of 3 for Mg V, Si VII, and S IX, respectively. These deviations are partly due to inaccurate resonance energies, the use of LS coupling, neglect of fine-structure excitations and the procedure to obtain Auger rates from extrapolating threshold excitation cross sections in the calculations of Ja-

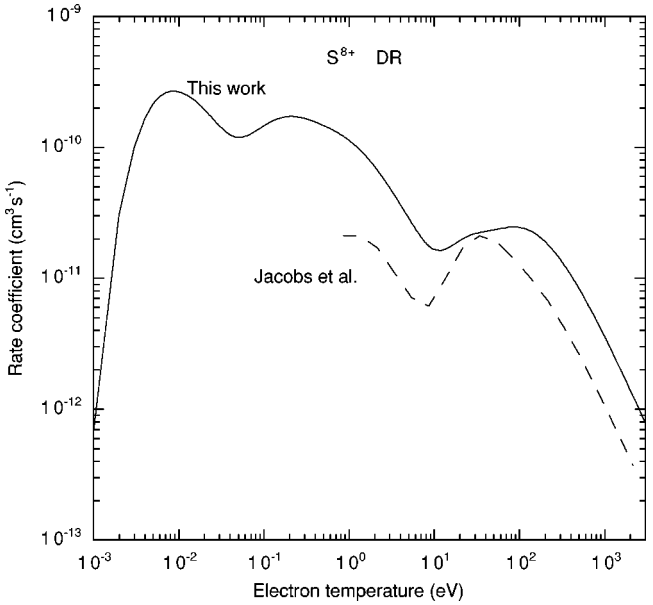

FIG. 9. Total DR rate coefficients for $^3P_2$ state of S^{8+} as functions of electron temperature. The solid curve is from this work and the dashed curve displays the results from Jacobs *et al.* (Ref. [7]).

TABLE I. Dielectronic recombination rate coefficient fit parameters. Numbers in square brackets indicate power of ten.

	Mg^{4+}		Si^{6+}		S^{8+}		Fe^{18+}	
i	c_i	E_i	c_i	E_i	c_i	E_i	c_i	E_i
1	7.42[−10] [a]	0.0 [b]	1.93[−8]	2.84[−3]	1.13[−6]	1.21[−2]	5.65[−6]	2.00[−3]
2	1.28[−8]	5.37[−3]	2.73[−7]	2.54[−2]	3.13[−6]	8.17[−2]	7.28[−6]	8.57[−3]
3	6.14[−8]	2.09[−2]	1.98[−6]	2.27[−1]	6.72[−5]	2.97[−1]	4.34[−5]	5.93[−2]
4	1.66[−6]	1.42[−1]	1.77[−5]	1.09[+0]	2.10[−4]	1.10[+0]	2.67[−5]	2.46[−1]
5	2.97[−6]	2.66[−1]	1.91[−4]	5.70[+0]	2.86[−4]	2.83[+0]	4.43[−4]	1.33[+0]
6	2.52[−5]	2.05[+0]	8.12[−3]	3.58[+1]	7.37[−3]	3.72[+1]	1.38[−3]	5.19[+0]
7	3.01[−5]	5.05[+0]	1.20[−2]	6.00[+1]	2.23[−2]	7.65[+1]	5.01[−3]	2.25[+1]
8	6.12[−3]	3.24[+1]	4.51[−2]	1.59[+2]	1.43[−1]	2.29[+2]	4.88[−2]	9.24[+1]
9	4.59[−3]	4.76[+1]					3.10[−1]	3.67[+2]
10	8.38[−3]	1.02[+2]					1.55[+0]	7.86[+2]

[a]In units of $cm^3\ s^{-1}\ K^{1.5}$.
[b]In units of eV.

cobs *et al.* [5–7]. For $T<10$ eV, the results from Jacobs *et al.* are a few orders of magnitude lower than the present values due to the neglect of the contributions from the fine-structure excitations in their work. The comparison between theory and experiment for Fe XIX has been discussed in Ref. [10]. Our MCDF results have been found to agree with experiment and with the MCBP predictions while the results from earlier theoretical work [8,9] have poor agreement with experiment.

IV. RATE FORMULA FOR PLASMA MODELING

We have fitted our theoretical total DR rate coefficints for ground state using the formula [23]

$$\alpha_{DR}(T)=T^{-3/2}\sum_i c_i e^{-E_i/kT}, \tag{7}$$

where c_i and E_i are the strength parameter and the energy parameter, respectively, for the ith fitting function component. The best fit values are listed in Table I. For Mg V, the fit is good to better than 1% for $T\geqslant 0.03$ eV. For $0.004\leqslant T\leqslant 0.03$ eV, the fit is better than 4%. For Si VII, the fit is within 3% for $T\leqslant 0.35$ eV and is better than 5% for $0.01<T<0.35$ eV. For S IX, the fit is better than 2.5% for $T\geqslant 0.01$ eV and within 7% for $0.003\leqslant T<0.01$ eV. The fitting parameters for the MCDF values of Fe XIX from Ref. [10] are also listed in Table I for completeness.

V. SUMMARY

We have calculated the total DR rate coefficients for $^3P_2$, $^3P_1$, $^3P_0$, $^1D_2$, and $^1S_0$ states in Mg V, Si VII, S IX, and Fe XIX ions including contributions from $2s-2p$, $2p_{1/2}-2p_{3/2}$, $2\ell-3\ell'$, and $1s-2p$ excitations. As in the case of *B*-like ions [22], we find that accurate resonance energies for $\Delta n=0$ DR are critical to obtain reliable DR rate coefficients. We also find that the fine-structure excitation channels are very important in predicting the behavior of the low-temperature DR rate coefficients for all ions covered in this study.

ACKNOWLEDGMENT

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[21] See EPAPS Document No. E-PLRAAN-66-010212 for tables of dielectronic recombination rate coefficients for the ground state of Mg V, Si VII, S IX, and Fe XIX. A direct link to this document may also be reached via the EPAPS homepage (http://www.aip.org/pubservs/epaps.html) or from ftp.aip.org in the directory /epaps/. See the EPAPS homepage for more information.
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