

Dielectronic recombination plasma rate coefficients of Na-, Mg-, and Al-like iron ions: The role of the $2(s + p) \rightarrow 4l, n'l'$ and $3(s + p) \rightarrow 5l, n'l'$ resonances

G. Visentin^{1,2} , S. Schippers^{3,4}, and S. Fritzsche^{1,2,5}

¹ Helmholtz-Institut Jena, Fröbelstieg 3, 07743 Jena, Germany

² GSI Helmholtzzentrum für Schwerionenforschung, Planckstrasse 1, 64291 Darmstadt, Germany
 e-mail: g.visentin@hi-jena.gsi.de

³ Institut für Atom- und Molekülphysik, Justus-Liebig-Universität Giessen, 35392 Giessen, Germany

⁴ Helmholtz Forschungsakademie Hessen für FAIR, Campus Giessen, 35392 Giessen, Germany

⁵ Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

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ABSTRACT

Dielectronic recombination (DR) is the major electron-ion recombination process in many astrophysical and laboratory plasmas. This process has been thoroughly studied for several charged species, in particular for M-shell iron ions. Previous investigations into the DR of such ions have mostly focused on the valence $3l \rightarrow 3l, n'l'$ and the core $2(s + p) \rightarrow 3l, n'l'$ DR resonances, while neglecting the $2(s + p) \rightarrow 4l, n'l'$ and $3(s + p) \rightarrow 5l, n'l'$ DR resonances. These were predicted to contribute to the broad unresolved transition array detected in several active galactic nuclei at reasonably high temperatures and column densities. In this work, we systematically assessed the importance of $2(s + p) \rightarrow 4l, n'l'$ and $3(s + p) \rightarrow 5l, n'l'$ resonances in the DR of three M-shell iron ions, Fe^{15+} , Fe^{14+} , and Fe^{13+} , with the multi-configuration Dirac-Hartree-Fock (MCDHF) method. Above the collisionally ionized plasma temperatures, these high-energy resonances contribute to the overall DR of Fe^{15+} , Fe^{14+} , and Fe^{13+} by up to 21%, 40%, and 22%, respectively.

Key words. atomic data – atomic processes – plasmas – relativistic processes

1. Introduction

Dielectronic recombination (DR) can be described as a two-step process, involving an N -electron ion and a free electron. In the first step, the free electron is resonantly captured into an $(N + 1)$ -electron resonance level embedded into the continuum of the initial ion. In the second step, the resonance level can either decay radiatively to some final states below the ionization threshold of the ion or re-autoionize back to the initial charge state.

The DR process dominates the electron-ion recombination dynamics in many astrophysical and laboratory plasmas (Beiersdorfer et al. 1992; Kallman & Palmeri 2007; Pütterich et al. 2008; Wu et al. 2015); thus, its knowledge is crucial for the investigation of plasma properties such as the level population and the ionization balance (Beiersdorfer 2003; Huang et al. 2018; Khan et al. 2018).

Experimental as well as theoretical studies have been systematically performed in support of the astronomical observations (see, for instance, Schippers et al. 2010), and repositories were created, in which the DR rate coefficients are tabulated for several electron temperatures (Summers 2003). DR rate coefficients can be retrieved from the cross sections measured at heavy-ion storage ring facilities (see, for instance, Badnell et al. 2003; Schuch and Böhm 2007, and Schippers 2009, 2015) or estimated theoretically by means of “ab initio” computations (see, for instance, Altun et al. 2006, 2007; Zatsarinny et al. 2006; Badnell et al. 2006; Abdel-Naby et al. 2012; Fritzsche 2021). Ab initio methods compute the DR rate coefficients by the additive inclusion of electron excitations. In turn, electron

excitations are classified as the difference $\Delta n = n' - n$, where n and n' mark the principal quantum numbers of the excited bound electron in the initial state and resonance levels, respectively (see, for instance, Fritzsche 2021). In turn, each electron excitation encompasses all the possible dielectronic capture resonances $nl \rightarrow n'l', n''l''$, in which a bound electron is excited from an initial shell, nl , to a final shell, $n'l'$, with the simultaneous capture of a free electron into a Rydberg shell, $n''l''$. As any electron excitation contributes to the total DR, theoretical investigations focus only on the supposedly most important ones.

Iron ions have been thoroughly targeted for DR investigations, as iron is the most astronomically abundant heavy element. Moreover, spectral lines ascribed to these ions were detected by several X-ray observatories (Khan et al. 2018). In particular, strong X-ray lines associated with L-shell iron ions were observed in binary star systems such as Capella (Canizares et al. 2000) and II Pegasi (Huenermoerder et al. 2001), and in the elliptical galaxy NGC 4636 (Xu et al. 2001). A broad unresolved transition array (UTA) occurring at 16–17 Å was detected in active galactic nuclei (AGN) in the vicinity of a supermassive black hole (Behar et al. 2001, 2003; Pounds et al. 2001; Pounds 2004; Kaspi et al. 2002; Kaspi 2004; Steenbrugge et al. 2003; Gallo et al. 2004; Netzer 2004; Krongold et al. 2005) and attributed mostly to M-shell Fe ions. These UTA lines were assigned to resonances involving $2l$ and $3l$ shells (Behar et al. 2001; Sako et al. 2001). In particular, the lines at 16 Å were attributed to $2p \rightarrow 3d$ core electron excitations, while the lines in the 14–16 Å region were ascribed to $2p \rightarrow 4d$ core electron excitations. The contribution of $2p \rightarrow 4d$ and high-energy $3l \rightarrow n'l'$ electron excitations to the equivalent width was

predicted to become important for ionic column densities larger than 10^{17} cm^{-2} (Behar et al. 2001).

Such astronomical observations demand experimental as well as theoretical investigations into the DR of L- and M-shell iron ions. For the DR of L-shell Fe ions, both theory and measurements have focused on the $2l \rightarrow 2l'$ and $2l \rightarrow 3l'$ valence electron excitations (see Zatsarinny et al. 2003, 2004a, 2006; Altun et al. 2005). For a few ionic species even the $2l \rightarrow 4l'$ (see Zatsarinny et al. 2004b) and the inner-core $1s \rightarrow 2l$ (see Chen 1991; Savin et al. 2006) electron excitations have been investigated.

The experimental investigations into the DR of M-shell Fe ions have mostly covered the free-electron energies due to the lowest lying resonances, corresponding to the $3l \rightarrow 3l'$ and $3l \rightarrow 4l'$ valence electron excitations (see Schippers et al. 2010 and references therein). As an exception to this approach, recent measurements of the DR of the Mg-like Fe^{14+} ions (Bernhardt et al. 2014) have focused on the free-electron energies due to the $2(s+p) \rightarrow 3l$ core electron excitations. For the remaining M-shell Fe ions, the DR contributions due to these core electron excitations have only been determined theoretically (see, for instance, Badnell et al. 2006; Altun et al. 2006, 2007). Unlike the theoretical investigations of the L-shell Fe ions, the $\Delta n = 2$ electron excitations have never been included in the modeling of DR for M-shell Fe ions.

For this study, we assessed the importance of the $\Delta n = 2$ electron excitations in the DR process of M-shell Fe ions. Specifically, we modeled the DR of the Na-like Fe^{15+} , Mg-like Fe^{14+} and Al-like Fe^{13+} ions upon additive inclusion of the core $2(s+p) \rightarrow 4l$ and the valence $3l \rightarrow 5l'$ excitations alongside the $\Delta n = 0$ (i.e., $3l \rightarrow 3l'$) and $\Delta n = 1$ (i.e., $2(s+p) \rightarrow 3l$ and $3l \rightarrow 4l'$) electron excitations. The importance of such $\Delta n = 2$ electron excitations in the overall DR was then quantified by the computation of the related plasma DR rate coefficients.

Our work is organized as follows: in Sect. 2, we describe the theory of DR in plasmas and the computational strategy employed in the present calculations; Sect. 3 is devoted to discussing the plasma DR rate coefficients computed for Na-like, Mg-like, and Al-like Fe ions. Our findings and related perspectives are summarized as concluding remarks in Sect. 4.

2. Plasma dielectronic recombination rates in multiply charged ions

2.1. Theoretical background

The DR of an ion in a given charge state involves an initial state, $i = (\alpha_i \mathbb{J}_i)$, a resonance (doubly excited) level embedded within the continuum of the initial ion, $d = (\alpha_d \mathbb{J}_d)$, and a final state, $f = (\alpha_f \mathbb{J}_f)$, into which the recombined system may decay radiatively. Both states and levels are labeled in terms of their total angular momentum and parity, $\mathbb{J} \equiv J^P$, while all further quantum numbers are referred to as α . In plasmas, electron-ion recombination is temperature-dependent, due to the Maxwellian distribution of the free electrons that are captured by the ions (Massey and Bates 1942). For a single ion per unit volume in the initial state, i , the explicit rate to recombine with a Maxwell-distributed electron at electron temperature, T , is called the DR plasma rate coefficient, $\alpha^{(\text{DR})}(T; i)$, and reads as (Fritzsche 2021)

$$\alpha^{(\text{DR})}(T; i) = \frac{4}{(k_B T)^{3/2} \sqrt{2\pi m}} \int_0^\infty dE E \sigma^{(\text{DR})}(E; i \rightarrow \{d\}) \times \exp\left(-\frac{E}{k_B T}\right). \quad (1)$$

Here, $\sigma^{(\text{DR})}(E; i \rightarrow \{d\})$ stands for the total cross section associated with the capture of the colliding electron into a span of intermediate levels, $\{d\}$. This quantity can be written in terms of the resonance strength, $S(i \rightarrow d)$ (Griffin 1989; Tu et al. 2016), and the kinetic energy of the colliding electron, $\varepsilon_d = E_d - E_i$, thus yielding (Hahn 1985)

$$\sigma^{(\text{DR})}(E; i \rightarrow \{d\}) = \sum_d S(i \rightarrow d) \delta(E - \varepsilon_d), \quad (2)$$

with

$$S(i \rightarrow d) = \frac{\pi^2 \hbar (2J_d + 1)}{k_d^2 (2J_i + 1)} \sum_f \frac{A_a(d \rightarrow i) A_r(d \rightarrow f)}{\Gamma_d}. \quad (3)$$

In Eq. (3) the resonance strength is expressed in terms of the Auger (A_a) and radiative (A_r) rates of the resonance level, d , as well as its half-width, Γ_d .

If we substitute Eq. (2) into (1), the total DR plasma rate coefficient can be expressed as a sum over the partial DR plasma rate coefficients, $\alpha^{(\text{DR})}(T; i \rightarrow d)$. Each partial rate coefficient refers to a specific $i \rightarrow d$ dielectronic capture resonance,

$$\alpha^{(\text{DR})}(T; i) = \sum_d \alpha^{(\text{DR})}(T; i \rightarrow d), \quad (4)$$

with

$$\alpha^{(\text{DR})}(T; i \rightarrow d) = \frac{4}{(k_B T)^{3/2} \sqrt{2\pi m}} (E_d - E_i) \times S(i \rightarrow d) \exp\left(-\frac{E_d - E_i}{k_B T_e}\right). \quad (5)$$

2.2. Computational strategy

We modeled the Hamiltonian of all the ions with the multi-configuration Dirac-Hartree-Fock (MCDHF) method in the intermediate coupling, as implemented in the Jena Atomic Calculator (JAC) toolbox (Fritzsche 2019; JACb 2023). Electron-electron correlations are described by means of a Dirac-Coulomb interaction term and only electric-dipole radiative decays are allowed. With this approach we first computed the partial DR plasma rate coefficients for the $\Delta n = 0, 1$, and 2 core and valence electron excitations and subsequently summed them to yield the total plasma DR rate coefficients, as described in Eq. (4). All the calculations were performed over a range of electron temperatures spanning from 10^4 up to 10^9 K in order to encompass both the photoionized (approximately $10^4 \text{ K} \leq T \leq 10^5 \text{ K}$) and the collisionally ionized (approximately $10^6 \text{ K} \leq T \leq 10^7 \text{ K}$) plasma temperatures (Mazzotta et al. 1998; Kallman and Bautista 2001).

The partial plasma rate coefficients associated with the low-energy $\Delta n = 0$ electron excitations need to be computed with reasonable accuracy, since they dominate the photoionized plasma region (Fritzsche 2021). This requirement led us to adopt two different computational strategies to calculate them: i) in the photoionized plasma region we included only the lowest-lying resonance levels in the calculations, but improved the modeling of the electron-electron correlations; ii) beyond the photoionized plasma region we computed the plasma rate coefficients with a dielectronic capture cascade computation. Such a cascade begins from the capture of the free electron into various nl shells and then models the subsequent electron and photon emission

as a stepwise decay of the ion toward its ground configuration. The relevant configurations are either treated independently or combined into moderate groups of configurations. Indeed, this approach provides a relatively simplified modeling of the electron-electron correlations, but enables the inclusion of a larger number of resonance states compared to strategy i).

The remaining $\Delta n = 1, 2$ core and valence electron excitations were computed by the sole dielectronic cascade computation, as described in ii).

3. Results and discussion

3.1. Plasma rate coefficients of Na-like Fe

We chose the electronic ground state of Fe^{15+} , $1s^2 2s^2 2p^6 3s^2 S_{1/2}$ as the initial state from which the DR process starts. We followed the approach of Altun et al. (2006) in the choice of the bound electron excitations, and thus, by $\Delta n = 0$, we mean the excitation of a $3s \rightarrow 3(p+d)$ bound electron and the capture of a free electron into a high-lying nl shell. This reads as:

$$\begin{aligned} & \text{Fe}^{15+} [2s^2 2p^6 3s^2 S_{1/2}] + e^- \\ \Rightarrow & \begin{cases} \text{Fe}^{14+} [2s^2 2p^6 3p^2 P_{1/2,3/2}] & (10l + \dots + 20l) \\ \text{Fe}^{14+} [2s^2 2p^6 3d^2 D_{3/2,5/2}] & (7l + \dots + 20l) \end{cases} \end{aligned}$$

$\Delta n = 1$ includes those DR resonances in which the bound electron is excited either from the $3s$ orbital to the $4l$ shell or from the $2(s+p)$ orbitals to the $3l$ shell, while a free electron is captured into a high-lying nl' shell:

$$\begin{aligned} & \text{Fe}^{15+} [2s^2 2p^6 3s^2 S_{1/2}] + e^- \\ \Rightarrow & \begin{cases} \text{Fe}^{14+} [2s^2 2p^6 4l] & (4l' + \dots + 15l') \\ \text{Fe}^{14+} [2s^2 2p^5 3s 3l] & (3l' + \dots + 15l') \\ \text{Fe}^{14+} [2s 2p^6 3s 3l] & (3l' + \dots + 15l'). \end{cases} \end{aligned}$$

Besides the above resonances, we added the $\Delta n = 2$ electron excitations:

$$\begin{aligned} & \text{Fe}^{15+} [2s^2 2p^6 3s^2 S_{1/2}] + e^- \\ \Rightarrow & \begin{cases} \text{Fe}^{14+} [2s^2 2p^6 5l] & (5l' + \dots + 15l') \\ \text{Fe}^{14+} [2s^2 2p^5 3s 4l] & (4l' + \dots + 15l') \\ \text{Fe}^{14+} [2s 2p^6 3s 4l] & (4l' + \dots + 15l'). \end{cases} \end{aligned}$$

The resonance energies associated with the $\Delta n = 0$ electron excitations were shifted by -0.228 eV, in order to match the strongest resonances measured by Linkemann et al. (1995).

In Fig. 1, we compare our plasma rate coefficients for the $3s \rightarrow 3l, nl'$ and $3s \rightarrow 4l, nl'$ DR resonances with the intermediate-coupling multi-configuration Breit-Pauli (MCBP) computations of Altun et al. (2006) and the experimentally derived results by Schippers et al. (2010). Our results compare favorably with the experimentally derived data in the photoionized plasma region: between 2×10^4 and 10^5 K the discrepancy between our computed plasma rate coefficients and the analogs by Schippers et al. amounts at most to a factor of 1.2. Similar deviations from the experimental benchmark affect the MCBP computations. The largest discrepancy in the photoionized plasma region occurs at around 10^4 K, where our plasma rate coefficients are 1.4 times larger than the experimentally derived analogs, in analogy with the results of Altun et al. For electron temperatures between 10^5 and 10^6 K our results align with the theoretical reference.

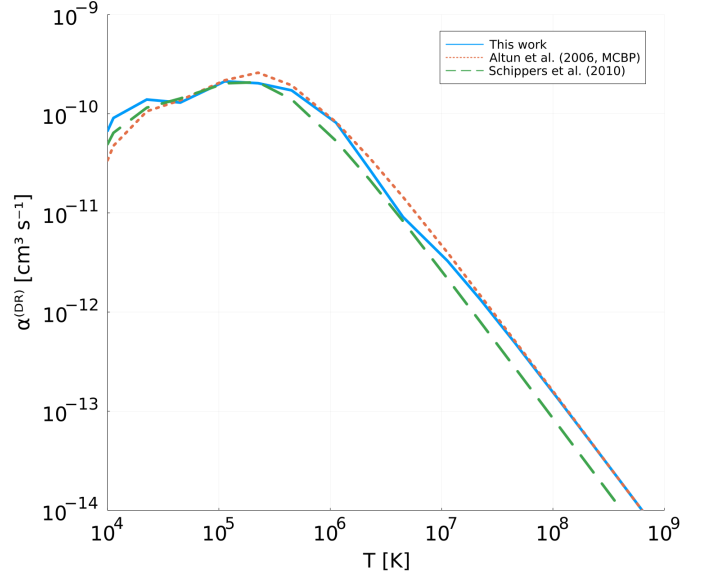


Fig. 1. $\Delta n = 0, 1$ plasma DR rate coefficients for initially sodium-like Fe^{15+} ions. The present results (thick blue line) are compared with the MCBP computations of Altun et al. (2006; dashed orange line) and the results experimentally derived by Schippers et al. (2010; dotted green line).

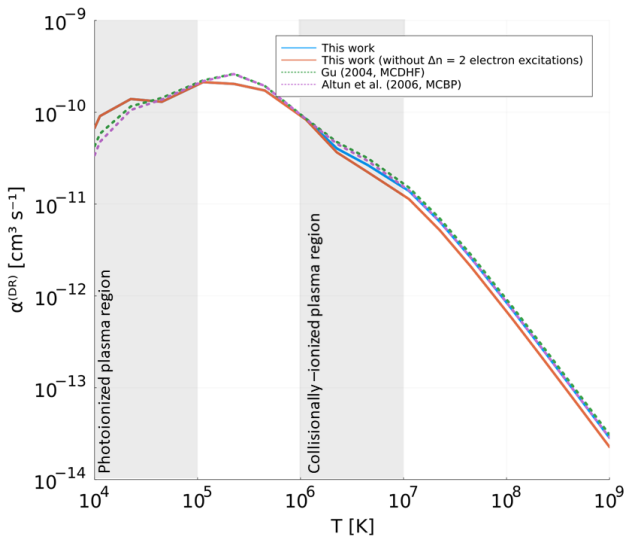
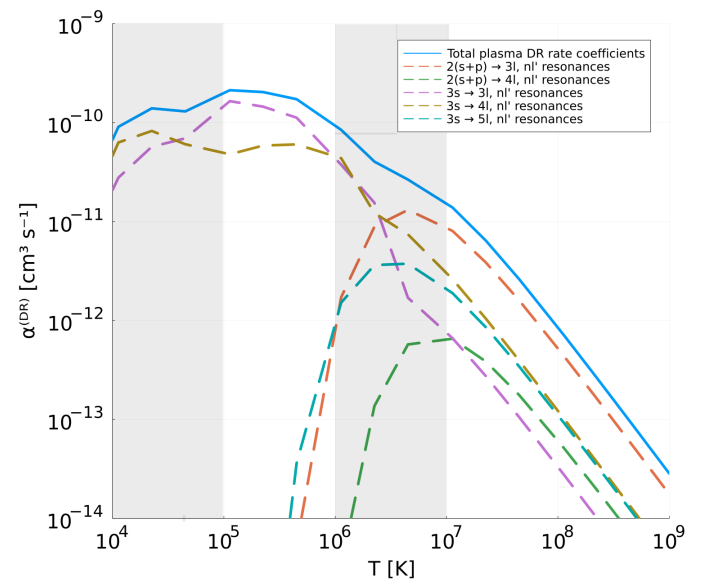
Our plasma rate coefficients at the collisionally ionized plasma temperatures lie between the experimental and theoretical references. At around 5×10^6 K our results attain the best agreement with the experimentally derived data. However, we interpret this good agreement as fortuitous. In fact, our plasma rate coefficient at this electron temperature is significantly smaller than both its analog at about 2×10^6 and 10^7 K. This feature suggests that a better account for electron-electron correlation would be necessary at such an electron temperature. Above the collisionally ionized plasma temperatures, our computed plasma rate coefficients overlap with the MCBP calculations.

We now compare our results for the $\Delta n = 0, 1$ electron excitations with the MCBP and MCDHF computations of Altun et al. and Gu (2004), respectively. This comparison is illustrated in Fig. 2. Our results are presented in two sets, with only the $\Delta n = 0, 1$ (thick orange line) and with the additional $\Delta n = 2$ (thick blue line) electron excitations. Let us focus on the electron temperatures beyond the photoionized plasma region, as there resonances for core electron excitations and excitations from the valence shells to shells with $n > 4$ become important. Our results align with the references between 10^5 and about 10^6 K. At higher electron temperatures our plasma rate coefficients are 1.25 times smaller than the references. This deviation may be attributed to the lower number of resonance levels included in our calculations compared to the reference. However, the comparison depicted in Fig. 1 also shows that the benchmark computations may be significantly overestimated with respect to the data retrieved experimentally. Therefore, we ascribe this reasonable discrepancy partly to the intrinsic limits of our computational approach and partly to the overestimating trend in the theoretical literature.

Let us now focus on the $\Delta n = 2$ electron excitations: the comparison of our two sets of results shows a significant increase in the plasma rate coefficients upon the inclusion of the $2(s+p) \rightarrow 4l, nl'$ and $3s \rightarrow 5l, nl'$ DR resonances. We evaluate the importance of such contributions in Fig. 3, which shows the

Table 1. Total and partial DR plasma rate coefficients of initially Fe¹⁵⁺ ions.

T [K]	$\alpha^{(\text{DR})}(T; i \rightarrow d) [\text{cm}^3 \text{s}^{-1}]$					$\alpha^{(\text{DR})}(T; i) [\text{cm}^3 \text{s}^{-1}]$
	$2(s+p) \rightarrow 3l, nl'$	$2(s+p) \rightarrow 4l, nl'$	$3s \rightarrow 3l, nl'$	$3s \rightarrow 4l, nl'$	$3s \rightarrow 5l, nl'$	Total
1.13E+04	<1E-18	<1E-18	2.7800E-11	6.3038E-11	<1E-18	9.0838E-11
2.25E+04	<1E-18	<1E-18	5.6988E-11	8.2379E-11	<1E-18	1.3937E-10
4.50E+04	<1E-18	<1E-18	6.9368E-11	6.0478E-11	<1E-18	1.2985E-10
1.13E+05	<1E-18	<1E-18	1.6480E-10	4.7860E-11	<1E-18	2.1266E-10
2.25E+05	3.1442E-18	1.8372E-28	1.4502E-10	5.8616E-11	5.4525E-17	2.0364E-10
4.50E+05	5.4181E-15	2.0315E-20	1.1218E-10	6.0236E-11	3.6190E-14	1.7246E-10
1.13E+06	1.7143E-12	3.3166E-15	3.7555E-11	4.3709E-11	1.5166E-12	8.4498E-11
2.25E+06	8.8830E-12	1.3694E-13	1.5471E-11	1.2195E-11	3.6334E-12	4.0319E-11
4.50E+06	1.3122E-11	5.7288E-13	1.6955E-12	7.4083E-12	3.7498E-12	2.6548E-11
1.13E+07	8.0415E-12	6.5397E-13	6.6236E-13	2.6188E-12	1.8904E-12	1.3867E-11
2.25E+07	3.8614E-12	3.8500E-13	2.7458E-13	1.0458E-12	8.5447E-13	6.4213E-12
4.50E+07	1.5898E-12	1.7562E-13	1.0498E-13	3.9206E-13	3.4146E-13	2.6039E-12
1.13E+08	4.3803E-13	5.1461E-14	2.7665E-14	1.0208E-13	9.2429E-14	7.1167E-13
2.25E+08	1.6071E-13	1.9267E-14	1.0003E-14	3.6760E-14	3.3715E-14	2.6046E-13
4.50E+08	5.7699E-14	6.9885E-15	3.5646E-15	1.3074E-14	1.2069E-14	9.3395E-14
1.13E+09	1.4634E-14	1.7835E-15	9.0011E-16	3.2972E-15	3.0558E-15	2.3671E-14

**Fig. 2.** Total plasma DR rate coefficients for initially sodium-like Fe¹⁵⁺ ions. The present results include the $\Delta n = 0, 1$ (thick orange line) and 2 (thick blue line) core excitations and are compared to the MCBP computations of Altun et al. (2006; dotted purple line) and the MCDHF computations of Gu (2004; dotted green line).**Fig. 3.** Total (thick blue line) and partial (dashed lines) DR plasma rate coefficients for initially sodium-like Fe¹⁵⁺ ions. Each partial rate coefficient is associated with a different resonance, respectively: $2(s+p) \rightarrow 3l, nl'$ (orange line), $2(s+p) \rightarrow 4l, nl'$ (light green line), $3s \rightarrow 3l, nl'$ (purple line), $3s \rightarrow 4l, nl'$ (golden line), and $3s \rightarrow 5l, nl'$ (dark green line). The two dark areas between 10^4 and 10^5 K and between 10^6 and 10^7 K indicate the photoionized and collisionally ionized plasma regions, respectively.

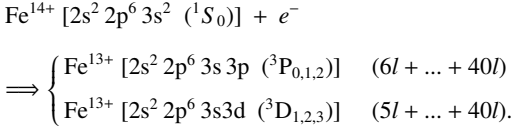
partial plasma rate coefficients associated with each DR resonance, alongside the total plasma rate coefficients. A detailed insight into the contribution of each resonance is provided in Table 1, where the partial plasma rate coefficients are listed across a set of electron temperatures. These electron temperatures coincide with those reported in the ADAS (Summers 2003) repository for the DR of Na-like Fe ions. It can be observed from Fig. 3 that the photoionized plasma region is dominated by the $3s \rightarrow 3l, nl'$ and $3s \rightarrow 4l, nl'$ DR resonances. The resonances associated with the $2(s+p) \rightarrow 3l$ core electron excitations and the $\Delta n = 2$ electron excitations contribute significantly in the collisionally ionized plasma region. Here, the $2(s+p) \rightarrow 3l, nl'$ DR resonances are dominant: their contribution accounts for 49% of the total DR at 4.5×10^6 K and steadily grows as the electron

temperature increases, up to 62% at 10^9 K. The importance of these contributions to the total plasma rate coefficients at high electron temperatures was already reported by several authors, among them Linkemann et al. (1995); Altun et al. (2006), and Lestinsky et al. (2009). The contribution from the $\Delta n = 2$ electron excitations becomes significant at the end of the collisionally ionized plasma region (16% of the total DR plasma rate coefficients between 4.5×10^6 and 10^7 K) and grows alongside the electron temperature up to 20% at 10^9 K. The $3s \rightarrow 5l, nl'$ resonances always contribute more than the $2(s+p) \rightarrow 4l, nl'$,

although the difference between the two contributions becomes smaller as the electron temperature increases.

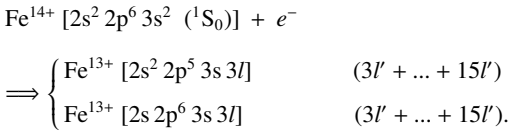
3.2. Plasma rate coefficients of Mg-like Fe

The DR process of Mg-like Fe ions starts from the electronic ground state, $1s^2 2s^2 2p^6 3s^2 \ ^1S_0$. The choice of the bound electron excitations follows the approach of [Altun et al. \(2007\)](#). Accordingly, the $\Delta n = 0$ electron excitations account for the $3s \rightarrow 3l$ excitations of the bound electron, while a free electron is captured in a high-lying nl' shell:



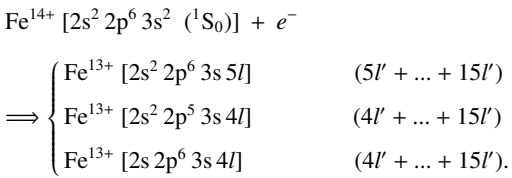
These resonances were computed together in both the atomic and the cascade calculations, in order to include further electron-electron correlations.

For $\Delta n = 1$ a core electron is excited from the $2(s+p)$ shell up to the $3l$ shell, while the free electron is captured in an nl' shell with $n \geq 3$. This reads as



These resonances were modeled together by means of a cascade computation.

We added the contributions due to the $\Delta n = 2$ electron excitations to the partial plasma rate coefficients thus computed. These electron excitations involve the $3s \rightarrow 5l$ and $2(s+p) \rightarrow 4l$ bound electron excitations and the free electron captured into an nl' shell. This process can be summarized as



The most recent literature works available on Fe^{14+} include the above-mentioned MCBP computations of [Altun et al. \(2007\)](#) and the experimentally derived plasma rate coefficients of [Bernhardt et al. \(2014\)](#). The latter measured the DR contributions due to the $\Delta n = 0, 1$ electron excitations.

We first adjusted the $3s \rightarrow 3l, nl'$ resonance energies by -0.03 eV. In this way, the strongest low-lying resonances were put in good agreement with the measured analogs. In the second step, we compared our plasma rate coefficients with the theoretical and experimental benchmarks. This comparison is illustrated in Fig. 4, where our results are presented as two sets: the first set includes only the $\Delta n = 0, 1$ electron excitations (thick orange line), while the second set includes the $\Delta n = 2$ electron excitations (thick blue line).

Our plasma rate coefficients are smaller than the experimentally derived data in the photoionized plasma region. Similar underestimations also appears in the state-of-the-art MCBP computations of Altun et al. . Our discrepancy with the experimental reference lies between a factor of 1.6 at about 10^4 K and a factor of 1.3 at about 10^5 K. Our agreement with the data of Bernhardt et al. improves beyond the photoionized plasma region

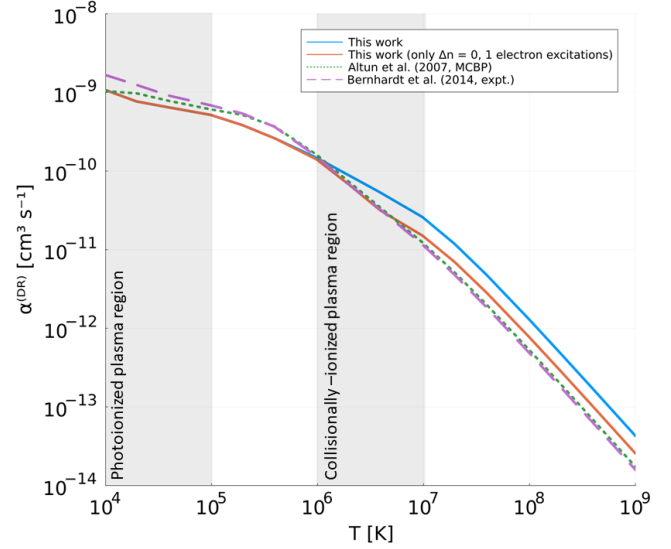


Fig. 4. Total plasma DR rate coefficients for initially magnesium-like Fe^{14+} ions. The present results include the $2(s+p) \rightarrow 3l$ and $3s$ resonances ($\Delta n = 1$ core excitations, thick orange line) and the $\Delta n = 2$ (thick blue line) core excitations, and are compared to the MCBP computations of [Altun et al. \(2007\)](#); green dotted line) and the experimentally derived data of [Bernhardt et al. \(2014\)](#); purple dashed line).

and aligns with the MCBP computations in the collisionally ionized region. There, both our results and the theoretical reference overlap with the experimentally derived plasma rate coefficients. The discrepancy with the references increases again at electron temperatures higher than 10^7 K. In this region our computed plasma rate coefficients are 1.5 times larger than the experimentally derived plasma rate coefficients of Bernhardt et al. and the MCBP computations. This discrepancy is explained as being likely due to the modeling of the highest-lying continuum orbitals included in the computations. In particular, the hydrogenic approximation used by [Altun et al. \(2007\)](#) to model the free-electron capture into the high Rydberg shells is likely more accurate than the approximation employed in our cascade calculations. Nonetheless, the good overall agreement of our results with the references suggests that this reasonable discrepancy does not compromise the reliability of our approach.

We notice a significant increase of the plasma rate coefficients upon including the $\Delta n = 2$ electron excitations. Figure 4 shows that this increase is particularly remarkable in the collisionally ionized plasma region, while Fig. 5 displays the partial plasma rate coefficients for each resonance together with the total plasma rate coefficients. For a quantitative evaluation of these partial contributions across the whole electron temperature range, they are listed in Table 2. The temperatures reported in the table are the same as those listed in the ADAS ([Summers 2003](#)) data tables for the DR of the Mg-like Fe ions.

The photoionized plasma region is dominated by the $3s \rightarrow 3l, nl'$ resonances, while the partial plasma rate coefficients for the $\Delta n = 1$ and 2 electron excitations become important in the collisionally ionized plasma region. The contributions from the $2(s+p) \rightarrow 3l, nl'$ resonances are significantly smaller than their counterparts in the DR of Fe^{15+} and account, at most, for 40% of the total DR. Another striking difference with respect to Fe^{15+} regards the importance of the $\Delta n = 2$ electron excitations: in the electron temperature region from the collisionally ionized plasma temperatures up to 10^9 K, these electron excitations provide the largest contribution to the total DR. The $3s \rightarrow 5l, nl'$

Table 2. Total and partial DR plasma rate coefficients of initially Fe¹⁴⁺ ions.

T [K]	$\alpha^{(DR)}(T; i \rightarrow d)$ [cm ³ s ⁻¹]				$\alpha^{(DR)}(T; i)$ [cm ³ s ⁻¹] Total
	$2(s+p) \rightarrow 3l, nl'$	$2(s+p) \rightarrow 4l, nl'$	$3s \rightarrow 3l, nl'$	$3s \rightarrow 5l, nl'$	
9.80E+03	<1E-18	<1E-18	1.0822E-09	<1E-18	1.0822E-09
1.96E+04	<1E-18	<1E-18	7.6819E-10	<1E-18	7.6819E-10
3.92E+04	<1E-18	<1E-18	6.4645E-10	<1E-18	6.4645E-10
9.80E+04	<1E-18	<1E-18	5.1817E-10	<1E-18	5.1817E-10
1.96E+05	<1E-18	<1E-18	3.8344E-10	3.6899E-17	3.8344E-10
3.92E+05	3.3931E-16	<1E-18	2.6159E-10	7.7647E-14	2.6167E-10
9.80E+05	6.8326E-13	7.1063E-16	1.3975E-10	7.3830E-12	1.4782E-10
1.96E+06	6.0325E-12	6.2989E-14	6.1782E-11	2.0853E-11	8.8731E-11
3.92E+06	1.1689E-11	3.8906E-13	1.9793E-11	2.1315E-11	5.3186E-11
9.80E+06	8.5323E-12	5.6611E-13	6.5196E-12	1.0282E-11	2.5900E-11
1.96E+07	4.3269E-12	3.6070E-13	2.6587E-12	4.5148E-12	1.1861E-11
3.92E+07	1.8349E-12	1.7139E-13	1.0144E-12	1.7794E-12	4.8002E-12
9.80E+07	5.1800E-13	5.1790E-14	2.6907E-13	4.8053E-13	1.3194E-12
1.96E+08	1.8997E-13	1.9429E-14	9.6668E-14	1.7364E-13	4.7970E-13
3.92E+08	6.8408E-14	7.0761E-15	3.4455E-14	6.2063E-14	1.7200E-13
9.80E+08	1.7498E-14	1.8223E-15	8.7588E-15	1.5803E-14	4.3882E-14
1.96E+09	6.2090E-15	6.4811E-16	3.1018E-15	5.5995E-15	1.5558E-14

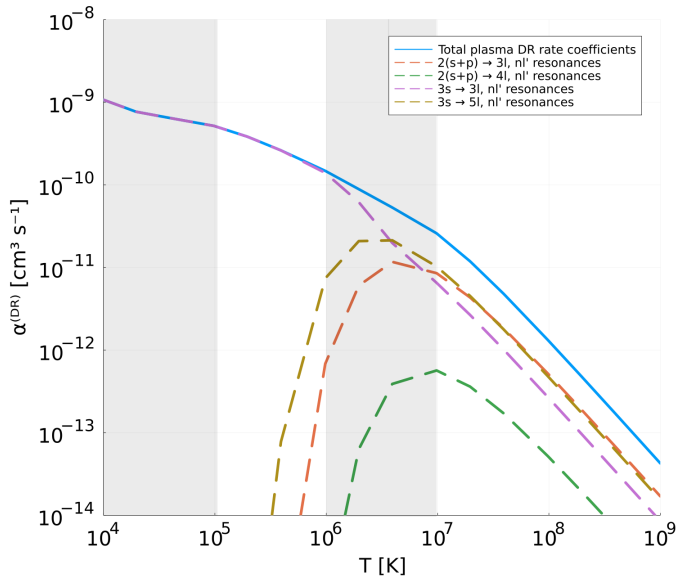


Fig. 5. Total (thick blue line) and partial (dashed lines) DR plasma rate coefficients for initially magnesium-like Fe¹⁴⁺ ions. Each partial rate coefficient is associated with a different resonance: $2(s+p) \rightarrow 3l'$ (orange line), $2(s+p) \rightarrow 4l$ (light green line), $3s \rightarrow 3l$ (purple line), $3s \rightarrow 4l$ (golden line), and $3s \rightarrow 5l$ (dark green line), respectively. The two dark areas between 10^4 and 10^5 K and between 10^6 and 10^7 K indicate the photoionized and collisionally ionized plasma regions, respectively.

resonances always prevail over the $2(s+p) \rightarrow 4l, nl'$ ones, and their contribution reaches 40% of the total plasma rate coefficients in the collisionally ionized plasma region. This explains the substantial increase in the plasma rate coefficients in this electron temperature range. By contrast, the contribution due to the $2(s+p) \rightarrow 4l, nl'$ electron excitations is never larger than approximately 4%. Overall, the $\Delta n = 2$ electron excitations account for 40% of the total plasma rate coefficients in the electron temperature region between 10^7 and 10^9 K. This value is

roughly twice the contribution of these electron excitations in the DR of Fe¹⁵⁺ ions and can be easily explained in terms of the electron configuration of Fe¹⁴⁺: in fact, in the DR of this ion, two $3s$ electrons can be excited to the $5l$ shell. In summary, the contributions from the $\Delta n = 2$ electron excitations to the total DR plasma rate coefficients is much more important for Fe¹⁴⁺ than for Fe¹⁵⁺, due to the closed-shell electron configuration of the former.

3.3. Plasma rate coefficients of Al-like Fe

The DR process for Fe¹³⁺ begins from the electronic ground state, $1s^2 2s^2 2p^6 3s^2 3p^2 P_{1/2}^o$. The modeling of the $\Delta n = 0, 1$ electron excitations follows the approach of Badnell et al. (2006). Thus, $\Delta n = 0$ includes the excitation of one valence electron from the $3s$ or $3p$ orbitals into the $3p$ or $3d$ orbitals. In summary,

$$\text{Fe}^{13+} [2s^2 2p^6 3s^2 3p^2 ({}^2P_{1/2}^o)] + e^- \Rightarrow \begin{cases} \text{Fe}^{12+} [2s^2 2p^6 3s^2 3p^2 ({}^2P_{3/2}^o)] & (8l + \dots + 40l) \\ \text{Fe}^{12+} [2s^2 2p^6 3s3p^2] & (7l + \dots + 40l) \\ \text{Fe}^{12+} [2s^2 2p^6 3s^2 3d] & (6l + \dots + 40l) \\ \text{Fe}^{12+} [2s^2 2p^6 3s3p3d] & (5l + \dots + 40l). \end{cases}$$

Due to the strong configuration mixing within the $3l$ shell (see Badnell et al. 2006; Schmidt et al. 2006; Abdel-Naby et al. 2012), modeling these core excitations by means of one atomic calculation is hardly feasible. Therefore, we modeled the $3(s+p) \rightarrow 3p, nl'$ and $3(s+p) \rightarrow 3d, nl'$ resonances by two atomic computations and then summed them. By contrast, in the cascade computations these resonances were modeled together, due to the smaller cost of this approach compared to the correlated atomic computations.

The $\Delta n = 1$ electron excitations involve the $3(s+p) \rightarrow 4l$ valence electron excitations and the $2(s+p) \rightarrow 3l$ core electron excitations:

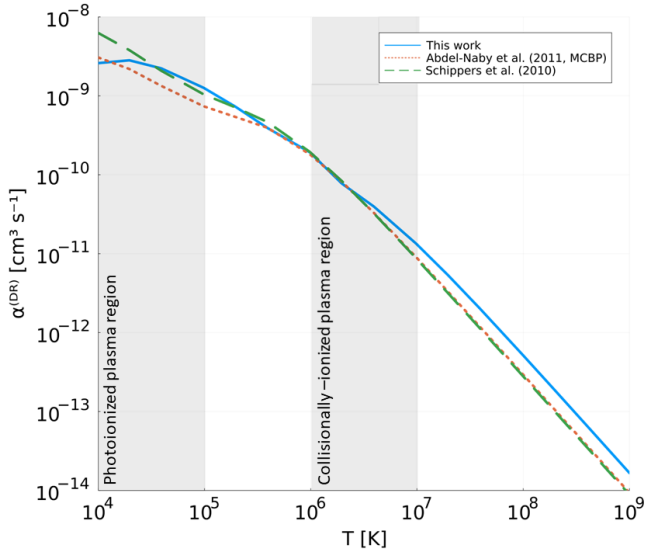


Fig. 6. $3(s+p) \rightarrow 3(p+d)$ and $3(s+p) \rightarrow 4l$ plasma DR rate coefficients for initially aluminum-like Fe^{13+} ions. The present results (thick blue line) are compared with state-of-the-art MCBP computations (Abdel-Naby et al. 2012; orange dotted line) and the heavy-ion storage ring measurements by Schippers et al. (2010; green dashed line).

$$\text{Fe}^{13+} [2s^2 2p^6 3s^2 3p (^2P_{1/2}^o)] + e^-$$

$$\Rightarrow \begin{cases} \text{Fe}^{12+} [2s^2 2p^6 3s^2 4l] & (4l' + \dots + 10l') \\ \text{Fe}^{12+} [2s^2 2p^6 3s 3p 4l] & (4l' + \dots + 10l') \\ \text{Fe}^{12+} [2s^2 2p^5 3s^2 3p (3p+3d)] & (3l + \dots + 15l) \\ \text{Fe}^{12+} [2s 2p^6 3s^2 3p (3p+3d)] & (3l + \dots + 15l). \end{cases}$$

For the $\Delta n = 2$ bound electron excitations we considered the $3(s+p) \rightarrow 5l$ valence electron excitation and the $2(s+p) \rightarrow 4l$ core electron excitations, while a free electron was resonantly captured into a span of Rydberg shells:

$$\text{Fe}^{13+} [2s^2 2p^6 3s^2 3p (^2P_{1/2}^o)] + e^-$$

$$\Rightarrow \begin{cases} \text{Fe}^{12+} [2s^2 2p^6 3s^2 5l] & (5l' + \dots + 20l') \\ \text{Fe}^{12+} [2s^2 2p^6 3s 3p 5l] & (5l' + \dots + 20l') \\ \text{Fe}^{12+} [2s^2 2p^5 3s^2 3p 4l] & (4l' + \dots + 20l') \\ \text{Fe}^{12+} [2s 2p^6 3s^2 3p 4l] & (4l' + \dots + 20l'). \end{cases}$$

We first assess our results for the partial plasma rate coefficients associated with the $3(s+p) \rightarrow 3(p+d)$, nl and $3(s+p) \rightarrow 4l$, nl' DR resonances. Our calculations are benchmarked with respect to the experimentally derived results of Schippers et al. (2010) and the MCBP computations of Abdel-Naby et al. (2012). We display our partial plasma rate coefficients alongside the experimentally derived and theoretical benchmarks in Fig. 6. Our plasma rate coefficients in the photoionized plasma temperature range are in excellent agreement with the experimentally derived data. The only exception to this trend occurs between 2×10^4 and 3.9×10^4 K: in this electron temperature range our results are 1.7 times smaller than the data of Schippers et al. Nevertheless, this discrepancy is comparable with the analogous deviation affecting the data of Abdel-Naby et al. (2012). The discrepancy with the experimentally derived data increases, starting from the collisionally ionized plasma temperatures: there, our

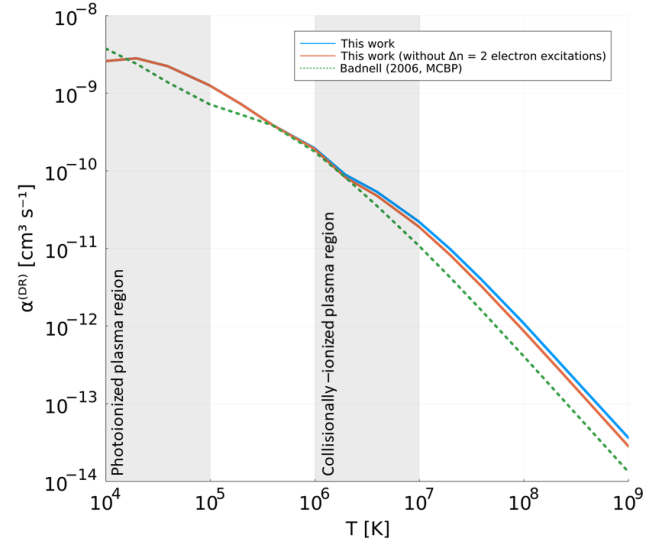


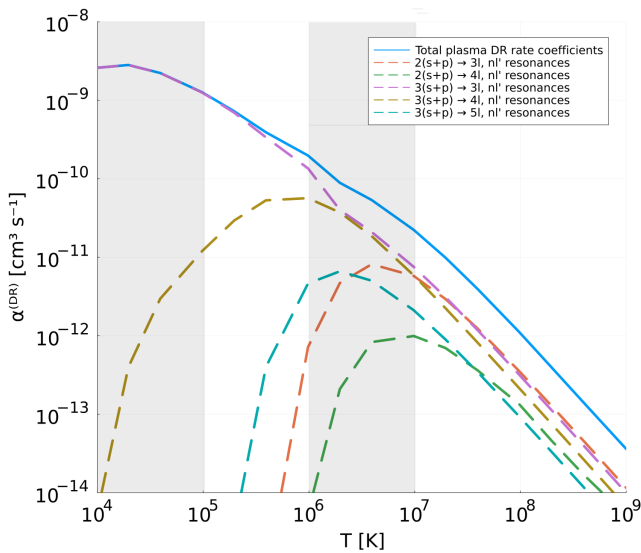
Fig. 7. Total plasma DR rate coefficients for initially aluminum-like Fe^{13+} ions. The present results include the $\Delta n = 0, 1$ (thick orange line) and 2 (thick blue line) core excitations and are compared to the MCBP computations of Badnell et al. (2006; green dotted line).

plasma rate coefficients deviate from the experimental reference by a factor of 1.2 at most. This discrepancy increases up to a factor of 1.3 in the electron temperature range between 4×10^7 and 10^9 K. Such a deviation is reasonable, but should be ascribed to the different modeling of the high-lying resonance states in our approach compared to the approach of Abdel-Naby and co-workers. In their work, the authors modeled these resonance levels by means of a hydrogenic approximation, whereas our atomic cascade approach includes part of the configuration interaction for all the resonance levels computed. Their modeling is likely more accurate for high nl shells compared to ours.

The second step in the validation of our approach is illustrated in Fig. 7, where we compare our plasma rate coefficients for the $\Delta n = 0, 1$ electron excitations (thick orange line) with the MCBP computations of Badnell et al. (2006). In the figure we also show the total plasma rate coefficients computed for the $\Delta n = 0, 1, 2$ electron excitations (thick blue line). At the photoionized plasma temperatures our results lie up to 1.5 times higher than the MCBP reference. At these electron temperatures the plasma rate coefficients are dominated by the lowest-lying $3(s+p) \rightarrow 3(p+d)$, nl DR resonances. The comparison of these resonances with the experimentally derived data of Schippers et al. (see Fig. 6) already validates the accuracy of our approach in the photoionized plasma region. Our results and the references are in very good agreement between 3.92×10^5 and 3.92×10^6 K, where the highest discrepancy amounts to a factor of 1.2. At higher electron temperatures the discrepancy increases and becomes significant beyond 3.92×10^7 K, where our results lie 1.7 times higher than the reference. Two factors may affect this substantial deviation. First, the modeling of the highest-lying resonance states. As for the plasma rate coefficients associated with the lowest-lying DR resonances (Fig. 6), the hydrogenic approximation may provide a better description of the most energetic DR resonances than our limited account of the configuration-interaction effects. As the second factor, we should also consider that Badnell's results turned out to underestimate the experimentally derived plasma rate coefficients, at least at the photoionized plasma temperatures. Thus, it is also possible that some underestimation affects Badnell's plasma

Table 3. Total and partial DR plasma rate coefficients of initially Fe¹³⁺ ions.

T [K]	$\alpha^{(\text{DR})}(T; i \rightarrow d) [\text{cm}^3 \text{s}^{-1}]$					$\alpha^{(\text{DR})}(T; i) [\text{cm}^3 \text{s}^{-1}]$ Total
	$2(s+p) \rightarrow 3l, nl'$	$2(s+p) \rightarrow 4l, nl'$	$3s \rightarrow 3l, nl'$	$3s \rightarrow 4l, nl'$	$3s \rightarrow 5l, nl'$	
1.96E+04	<1E-18	<1E-18	2.8204E-09	3.9871E-13	<1E-18	2.8208E-09
3.92E+04	<1E-18	<1E-18	2.2251E-09	2.9681E-12	<1E-18	2.2281E-09
9.80E+04	<1E-18	<1E-18	1.2527E-09	1.2060E-11	<1E-18	1.2648E-09
1.96E+05	<1E-18	<1E-18	6.9692E-10	2.9384E-11	3.4830E-15	7.2631E-10
3.92E+05	8.7883E-16	<1E-18	3.3767E-10	5.3225E-11	4.0142E-13	3.9130E-10
9.80E+05	7.2032E-13	5.5426E-15	1.3573E-10	5.6737E-11	4.6467E-12	1.9784E-10
1.96E+06	4.7034E-12	2.0947E-13	4.0167E-11	3.7259E-11	6.6297E-12	8.8969E-11
3.92E+06	8.1695E-12	8.3221E-13	2.1019E-11	1.8624E-11	5.0370E-12	5.3682E-11
9.80E+06	5.7895E-12	9.9451E-13	7.5621E-12	5.8761E-12	2.1147E-12	2.2337E-11
1.96E+07	2.9314E-12	6.9758E-13	3.0987E-12	2.2414E-12	8.9588E-13	9.8649E-12
3.92E+07	1.2443E-12	3.6456E-13	1.1876E-12	8.2345E-13	3.4768E-13	3.9675E-12
9.80E+07	3.5165E-13	1.3311E-13	3.1605E-13	2.1320E-13	9.3104E-14	1.1071E-12
1.96E+08	1.2903E-13	4.6518E-14	1.1369E-13	7.5964E-14	3.3553E-14	3.9875E-13
3.92E+08	4.6474E-14	1.7245E-14	4.0549E-14	2.6962E-14	1.1977E-14	1.4321E-13
9.80E+08	1.1889E-14	5.2220E-15	1.0312E-14	6.8367E-15	3.0475E-15	3.7307E-14
1.96E+09	4.2191E-15	1.6028E-15	3.6522E-15	2.4190E-15	1.0795E-15	1.2973E-14

**Fig. 8.** Total (thick blue line) and partial (dashed lines) DR plasma rate coefficients for initially aluminum-like Fe¹³⁺ ions. Each partial rate coefficient is associated with a different resonance, respectively: $2(s+p) \rightarrow 3l, nl'$ (orange line), $2(s+p) \rightarrow 4l, nl'$ (light green line), $3s \rightarrow 3l, nl'$ (purple line), $3s \rightarrow 4l, nl'$ (golden line) and $3s \rightarrow 5l, nl'$ (dark green line). The two dark areas between 10^4 and 10^5 K and between 10^6 and 10^7 K indicate the photoionized and collisionally ionized plasma regions, respectively.

rate coefficients. Upon accounting for this intrinsic underestimation, the inaccuracy of our results at high electron temperatures appears quite reasonable.

The inclusion of the $2(s+p) \rightarrow 4l, nl'$ and $3(s+p) \rightarrow 5l, nl'$ resonances into the DR process increases the total plasma rate coefficients. To estimate such a growth, we list the partial plasma rate coefficients for each resonance in Fig. 8, alongside the total DR plasma rate coefficients. We also list each partial plasma rate coefficient in Table 3, across a set of electron temperatures that coincide with those reported in the ADAS repository for this ionic species.

The lowest-lying $3(s+p) \rightarrow 3(p+d), nl$ resonances are dominant at the photoionized plasma temperatures and the electron temperature interval between the photoionized and the collisionally ionized plasma regions. The DR contributions due to the higher-lying $3(s+p) \rightarrow 4l, nl'$ resonances become comparable to the $3(s+p) \rightarrow 3(p+d), nl$ analogs only at the collisionally ionized plasma temperatures. There, they contribute at most 42% of the total DR. Beyond this electron temperature region the $2(s+p) \rightarrow (3l+4l), nl'$ and $3(s+p) \rightarrow 5l, nl'$ resonances become non-negligible. The $2(s+p) \rightarrow 3l, nl'$ DR resonances provide the largest contribution to the total DR in this electron temperature interval, in analogy with the DR of Fe¹⁵⁺. These resonances contribute as much as 33% of the total DR at electron temperatures between 2×10^8 and 4×10^8 K, approximately. This contribution is slightly smaller than the analogous contribution to the DR of Mg-like Fe ions. The DR contributions due to the $\Delta n = 2$ core and valence electron excitations are less important than the $2(s+p) \rightarrow 3l, nl'$ resonance, but their contribution is anyway non-negligible and can reach up to 22% of the total DR at about 10^9 K. The importance of these electron excitations in the DR of Al-like Fe ions is comparable to the role of their counterparts in the Fe¹⁵⁺ DR. This analogy is explained if we consider that for both ions the valence orbital is occupied by one electron. Unlike the DR of Na-like iron ions, in the DR of the Al-like Fe the $2(s+p) \rightarrow 4l, nl'$ resonances contribute more than the $3(s+p) \rightarrow 5l, nl'$ ones between 10^8 and 10^9 K. In fact, in this electron temperature region the contribution of the $2(s+p) \rightarrow 4l, nl'$ resonances to the total plasma rate coefficients ranges from 12% (at about 10^8 K) up to 14% (at about 10^9 K), while the contribution of the $3(s+p) \rightarrow 5l, nl'$ resonances never exceeds 8.5%. We can tentatively explain this behavior in terms of the larger resonance level density of Fe¹³⁺ compared to Fe¹⁵⁺, but further investigations into the DR of Fe ions with $3d^1$ (K-like) and $4s^1$ (Mn-like) would be helpful to validate this hypothesis.

4. Concluding remarks

We investigated the importance of the high-energy $2(s+p) \rightarrow 4l, nl'$ and $3l \rightarrow 5l', nl''$ resonances ($\Delta n = 2$ electron excitations) in the DR plasma rate coefficients of Fe¹⁵⁺,

Fe^{14+} , and Fe^{13+} across the electron temperature interval that encompasses both the photoionized and collisionally ionized plasma temperatures. Our results for the resonances involving the excitation of a valence electron to the $3l$ or $4l$ shells and of a core $2(s+p)$ electron to the $3l$ shell ($\Delta n = 0, 1$ electron excitations) show a reasonable overall agreement with the available experimentally derived data and the state-of-the-art atomic calculations. The favorable comparison of our $\Delta n = 0, 1$ plasma rate coefficients with the benchmarks validates our theoretical approach. The inclusion of the $\Delta n = 2$ electron excitations is found to raise the total plasma rate coefficients up to a non-negligible extent in the electron temperature interval between the collisionally ionized plasma temperatures and 10^9 K. We further estimate the $2(s+p) \rightarrow 4l, nl'$ and $3l \rightarrow 5l', nl''$ resonances to account, at most, for approximately 21%, 40%, and 22% of the total DR plasma rate coefficients of Fe^{15+} , Fe^{14+} , and Fe^{13+} , respectively. The large contributions from these resonances in the DR of Mg-like Fe are explained in terms of the two $3s$ valence electrons that can be excited to the $5l$ shells. On the other hand, the similarity between the $\Delta n = 2$ contributions in the DR of Na- and Al-like Fe ions is ascribed to their similar electron configurations, which feature one electron in the outermost orbital. The slightly larger contribution of these resonances in the DR of Fe^{13+} compared to Fe^{15+} may be due to the two subvalence $3s$ electrons featuring the former's electron configuration. However, we would need a systematic investigation into the DR of Fe ions with $3d$ and $4s$ singly occupied valence orbitals in order to confirm this explanation.

On this ground, we expect these highly energetic resonances to contribute to the plasma DR more and more remarkably as the valence $3l$ orbitals are filled, with the highest contributions to be attained for closed-shell iron ions. Thus, such resonances contribute substantially to the DR of M-shell iron ions and cannot be neglected in the modeling of this process at high electron temperatures. Furthermore, our results support the predictions of Sako et al. (2001) and Behar et al. (2001), that the high-energy $2(s+p) \rightarrow 4l, nl'$ and $3l \rightarrow 5l', nl''$ resonances can significantly shape the UTA observed in active galactic nuclei at reasonably high temperatures.

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