

DIELECTRONIC RECOMBINATION OF Fe $3p^q$ IONS: A KEY INGREDIENT FOR DESCRIBING X-RAY ABSORPTION IN ACTIVE GALACTIC NUCLEI

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ABSTRACT

We have carried out multiconfiguration Breit-Pauli AUTOSTRUCTURE calculations for the dielectronic recombination (DR) of Fe^{8+} – Fe^{12+} ions. We obtain total DR rate coefficients for the initial ground level that are an order of magnitude larger than those corresponding to radiative recombination (RR), at temperatures where Fe $3p^q$ ($q = 2$ – 6) ions are abundant in photoionized plasmas. The resultant total (DR+RR) rate coefficients are then an order of magnitude larger than those currently in use by photoionized plasma modeling codes such as CLOUDY, ION, and XSTAR. These rate coefficients, together with our previous results for $q = 0$ and 1, are critical for determining the ionization balance of the M-shell Fe ions that give rise to the prominent unresolved-transition-array X-ray absorption feature found in the spectrum of many active galactic nuclei. This feature is poorly described by CLOUDY and ION, necessitating an ad hoc modification to the low-temperature DR rate coefficients. Such modifications are no longer necessary, and a rigorous approach to such modeling can now take place using these data.

Subject headings: atomic data — atomic processes — galaxies: active — galaxies: nuclei — X-rays: galaxies

1. INTRODUCTION

The iron M-shell ions (predominantly Fe^{7+} – Fe^{13+}) give rise to strong X-ray absorption lines due to $n = 2$ – 3 electronic inner-shell transitions. These are seen in the spectra of active galactic nuclei (AGNs) observed by *Chandra* and *XMM-Newton* (Sako et al. 2001) as an unresolved-transition-array (UTA). The shape of the UTA feature can be used as a powerful diagnostic—for a detailed discussion, see Behar et al. (2001), whose atomic database for describing it has been updated recently by Gu et al. (2006). However, Netzer et al. (2003) have pointed out problems in modeling this shape, and so Netzer (2004), using ION, and Kraemer et al. (2004), using CLOUDY, have suggested increasing the magnitude of the recombination rate coefficients for Fe ions, particularly the $3p^q$ ($q = 1$ – 6) ions Fe^{13+} – Fe^{8+} , by postulating ad hoc low-temperature dielectronic recombination (DR) rate coefficients. The net effect is to shift the ionization balance toward the neutral end. This brings the modeling results into accord with observation but is not rigorous, since there is little to constrain the DR rate coefficients that they use.

The extant recombination data is effectively all radiative (i.e., radiative recombination [RR]) at photoionized plasma temperatures.¹ The recommended DR data for these Fe ions (Arnaud & Raymond 1992) are based on the high-temperature electron-collisional plasma results of Jacobs et al. (1977) and Hahn (1989) that give essentially zero contribution from DR at photoionized plasma temperatures. There is much evidence from the Fe L shell, both experimental and theoretical (see, e.g., Savin et al. 2006), that a significant contribution can be expected from DR at low temperatures, due principally to “non-dipole” core excitations that were not (needed to be) considered by Jacobs et al. (1977) and Hahn (1989).

Recently, measurements by Schmidt et al. (2006)² on Fe^{13+} ($q = 1$) at the Heidelberg heavy-ion test storage ring have

found the contribution from DR to the total recombination rate coefficient to be an order of magnitude larger than that due to RR, at photoionized plasma temperatures. We have carried out a detailed theoretical analysis of these experimental results (Badnell 2006a). We found some disagreements, especially at energies that affect the DR rate coefficient at photoionized plasma temperatures. Nevertheless, our DR rate coefficient for Fe^{13+} is also an order of magnitude larger than our RR one, but it is up to a third smaller than the experimentally based one over 10^4 – 10^5 K. We now report on the results of calculations for the computationally demanding Fe $3p^q$ ($q = 2$ – 6) ions.

2. METHODOLOGY

Our recent comprehensive study (Badnell 2006a) of the DR of Fe^{13+} ($q = 1$), including detailed comparisons of our theoretical cross sections with those of the high-energy resolution measurements of Schmidt et al. (2006), provides us with a guide for our approach to the $3p^q$ ($q = 2$ – 6) ions. These ions are computationally more demanding, and there are no (published) experimental results for them. We give the essentials of the new work below and refer the reader to Badnell (2006a) for a more detailed exposition of the atomic physics. In particular, we note that a level-resolved treatment is critical for the determination of accurate DR rate coefficients at photoionized plasma temperatures but that the results of such calculations are sparse for the M shell.

2.1. Theory

The total dielectronic recombination rate coefficient, $\alpha_v^{\text{DR}}(T)$, from an initial state v of an N -electron ion is given, at a temperature T , by

$$\alpha_v^{\text{DR}}(T) = \left(\frac{4\pi a_0^2 I_H}{k_B T} \right)^{3/2} \sum_j \frac{\omega_j}{2\omega_v} e^{-E_c/(k_B T)} \times \frac{\sum_{i,l} A_{j \rightarrow v, E_c, l}^a A_{j \rightarrow i}^r}{\sum_h A_{j \rightarrow h}^r + \sum_{m,l} A_{j \rightarrow m, E_c, l}^a} \quad (1)$$

¹ When we refer to photoionized or electron-collisional plasma temperatures, we mean the temperatures at which Fe $3p^q$ ions are abundant in such plasmas—see Kallman & Bautista (2001; XSTAR) and Mazzotta et al. (1998), respectively.

² Schmidt et al. (2006) also give an up-to-date list of references of observations of the AGN X-ray absorption feature.

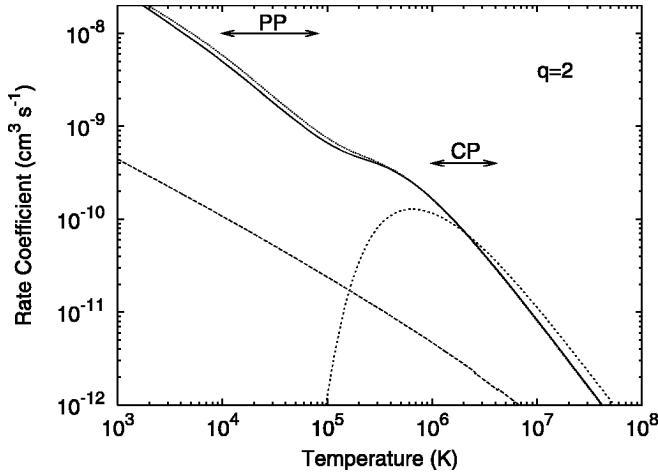


FIG. 1.—Total ground-level rate coefficients for Fe^{12+} ($q = 2$). Solid curve, DR (7CF); dotted curve, DR (8CF); long-dashed curve, RR; all present AUTOSTRUCTURE results. Short-dashed curve, Recommended DR data of Arnaud & Raymond (1992). PP and CP denote typical photoionized and electron-collisional plasma temperature ranges, respectively, for Fe^{12+} (Kallman & Bautista 2001 and Mazzotta et al. 1998).

(Burgess 1964), where ω_j is the statistical weight of the $(N+1)$ -electron doubly excited resonance state j , ω_i is the statistical weight of the initial state, and the autoionization (A'') and radiative (A') rates are in inverse seconds. Here, E_c is the energy of the continuum electron (with orbital angular momentum l), which is fixed by the position of the resonances, and I_H is the ionization potential energy of the hydrogen atom (both are in the same units of energy), k_B is the Boltzman constant, T is the electron temperature, and $(4\pi a_0^2)^{3/2} = 6.6011 \times 10^{-24} \text{ cm}^3$.

We have used AUTOSTRUCTURE (Badnell 1986) to carry out multiconfiguration Breit-Pauli calculations of all of the necessary rates and energies, as detailed next.

2.2. The $\text{Fe } 3p^q$ Target

We describe the N -electron target by the following configurations (assuming a closed-shell Ne-like core): (1) $3s^2 3p^q$, (2) $3s 3p^{q+1}$, (3) $3s^2 3p^{q-1} 3d$, (4) $3p^{q+2}$, (5) $3s 3p^q 3d$, (6) $3s^2 3p^{q-2} 3d^2$, (7) $3p^{q+1} 3d$. (If a given value of q results in an occupation number <0 or >6 , then that “configuration” does not exist for said ion.) This target expansion allows for both $3s$ and $3p$ $\Delta n = 0$ subshell promotions from the ground configuration, as well as including important interacting config-

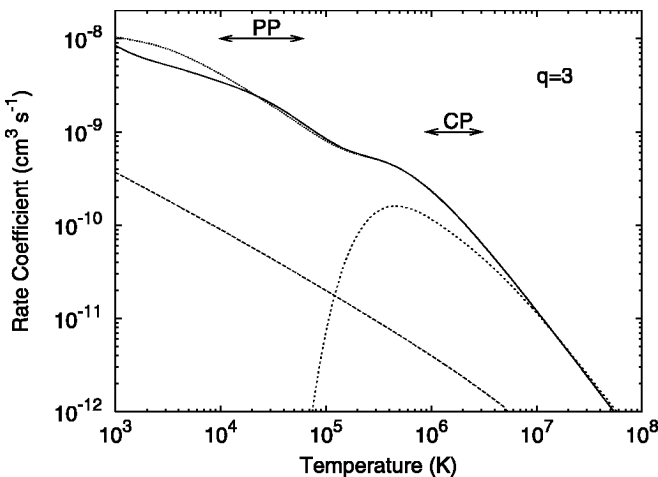


FIG. 2.—Same as Fig. 1, but for Fe^{11+} ($q = 3$).

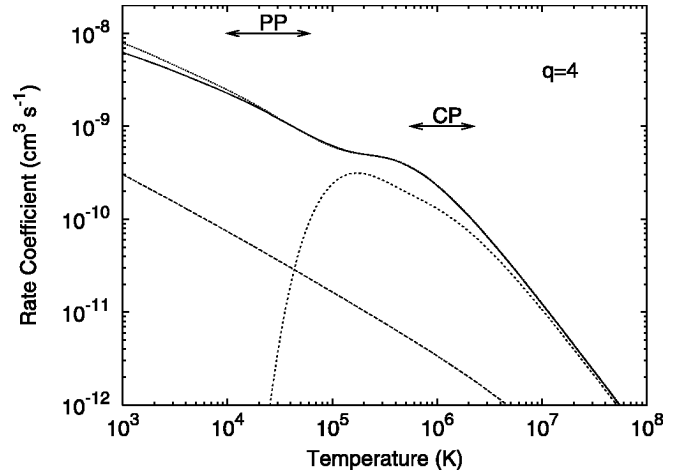


FIG. 3.—Same as Fig. 1, but for Fe^{10+} ($q = 4$).

urations. We denote it as “7CF.” We also investigated the accuracy of this representation for DR by carrying out a further calculation for each ion that included the additional configuration interaction due to $(8) 3s 3p^{q-1} 3d^2$. We denote the combined set as “8CF.”

The contribution from higher energy ($\Delta n = 1$) promotions has no effect at photoionized plasma temperatures, while in electron-collisional plasmas we expect such contributions to be less than 10% of the $\Delta n = 0$, following our results for $q = 1$ (Badnell 2006a). (The relative importance of $\Delta n = 1$ contributions decreases as q increases. This is because the inner-shell 2–3 contribution is further suppressed by additional core rearrangement autoionizing transitions, and the 3–4 outer-shell contribution peaks at a temperature that is closer to that of the $\Delta n = 0$ peak.)

All relevant $(N+1)$ -electron autoionization and radiative rates are then determined, for the given target expansion, for all Rydberg states up to $n = 1000$ and $l = 9$ –13, depending on q , and the total DR rate coefficient is then determined according to equation (1).

In addition, we use observed target energies wherever possible.³ This minimizes the sensitivity to the Maxwellian exponential factor at low temperatures, which is critical for application to photoionized plasmas. Since the observed energies are incomplete, we adopt the expedient strategy of using cal-

³ See the NIST Atomic Spectral Database, ver. 3.1.0, at <http://physics.nist.gov/PhysRefData/ASD>.

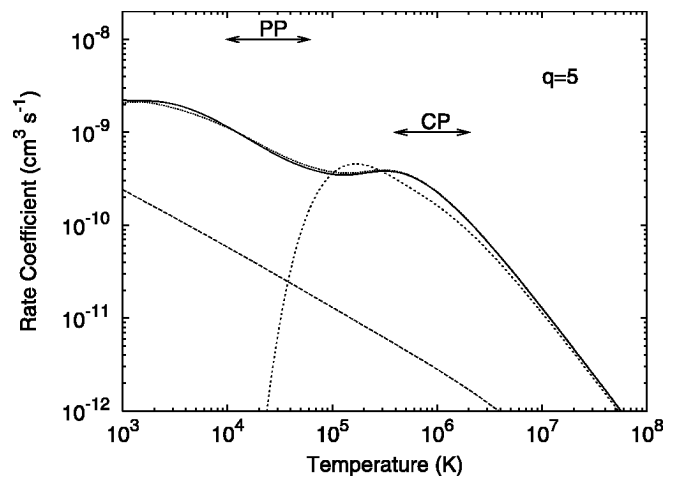
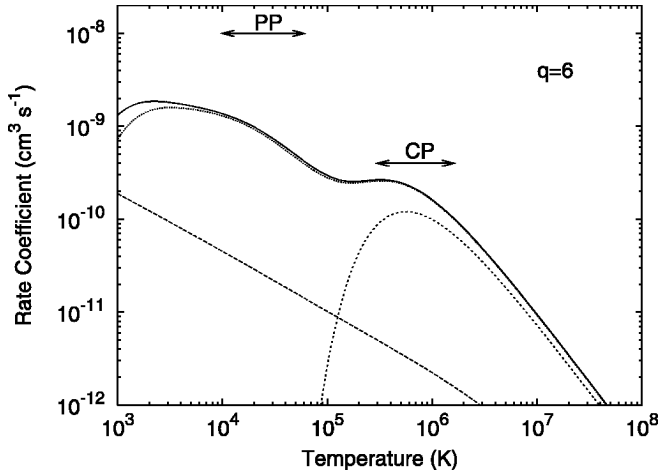


FIG. 4.—Same as Fig. 1, but for Fe^{9+} ($q = 5$).

FIG. 5.—Same as Fig. 1, but for Fe $^{8+}$ ($q = 6$).

culated level splittings to adjust the positions of the missing levels of a term, relative to an observed one. Similarly, we adjust (unobserved) terms to maintain the splitting with observed ones of the same symmetry. Finally, for higher energy configurations (typically, configuration 4 and above) where there are no observed level energies, we adjust the entire configuration position by considering the average shift of lower lying configurations.

Radiative recombination may be expected to be important at photoionized plasma temperatures, and so we have also calculated total RR rate coefficients, $\alpha_v^{\text{RR}}(T)$, with AUTO-STRUCTURE, following Badnell (2006b).

2.3. Fits

For ease of use, we fit our total recombination rate coefficients to the usual functional forms. For DR,

$$\alpha_v^{\text{DR}}(T) = T^{-3/2} \sum_i c_i \exp(-E_i/T), \quad (2)$$

where the E_i are in the units of temperature, T (K), and the c_i are in units of $\text{cm}^3 \text{s}^{-1} \text{K}^{3/2}$; for RR,

$$\alpha_v^{\text{RR}}(T) = A[\sqrt{T/T_0}(1 + \sqrt{T/T_0})^{1-B}(1 + \sqrt{T/T_1})^{1+B}]^{-1}, \quad (3)$$

where, for greater accuracy, B may be replaced as

$$B \rightarrow B + C \exp(-T_2/T). \quad (4)$$

Here, $T_{0,1,2}$ are in units of temperature (K), A is in units of $\text{cm}^3 \text{s}^{-1}$, and B and C are dimensionless.

3. RESULTS

In Figures 1–5 we present our recombination rate coefficients for the initial ground level of Fe $^{12+}$ –Fe $^{8+}$ ($q = 2$ –6) and

compare them with the DR rate coefficients recommended by Arnaud & Raymond (1992). These recommended data are based on the results of Jacobs et al. (1977) for $q = 2, 4, 5$ and Hahn (1989) for $q = 3, 6$, and they were for application to high-temperature electron-collisional plasmas. They have little in the way of a low-temperature contribution—a modest one may just be seen for $q = 4$ and 5 at around 10^5 K.

The main result, common to all ions, is the order-of-magnitude difference between the DR and RR rate coefficients at photoionized plasma temperatures. The strength and the temperature range of the “low- T ” DR rate coefficients are a reflection of the contribution from many low-lying resonances associated with many core excitations. This is similar to the situation found for $q = 1$ (Schmidt et al. 2006; Badnell 2006a). Thus, the ad hoc modifications proposed by Netzer (2004) and Kraemer et al. (2004) were conservative, increasing the total recombination rate coefficient by factors of only 2–4. These new rate coefficients (plus $q = 0, 1$ data) can be expected to have a significant effect on the ionization balance of Fe $^{7+}$ –Fe $^{13+}$ in photoionized plasmas and, in turn, the modeling of the UTA X-ray absorption feature in AGNs. On comparing our 7CF and 8CF results, we also note that sensitivity to near-threshold resonance positions at low temperatures does not appear to become an issue until $\lesssim 10^4$ K, i.e., below the main temperatures of interest for photoionized plasmas.

At electron-collisional plasma temperatures, we find reasonable agreement with the recommended data of Arnaud & Raymond (1992). The strength of the contribution from “low-temperature” resonances extends to enhancing the high-temperature peak in many cases. Even at 10^7 K, which is the far-off equilibrium, our present results are still (a little) larger than those recommended by Arnaud & Raymond (1992), except for the case of $q = 2$. Even in this case ($q = 2$) we expect the $\Delta n = 1$ contribution to result in no more than a 10% increase at a few times 10^6 K, rising to at most 20% by 10^7 K, and less for lower charge ions, based on our results for $q = 1$ (Badnell 2006a) and our comments in § 2.2. Thus, the present results can, and should, be used for modeling electron-collisional plasmas as well.

In Tables 1 and 2 we present our fit coefficients for these DR rate coefficients, and in Table 3 we present our fit coefficients for these RR rate coefficients—as defined by equations (2) and (3). For convenience, we include the results for $q = 1$ (Badnell 2006a) and $q = 0$ (Altun et al. 2006) as well. Results for all higher charge states may be found online (Badnell 2006c, 2006d), following the work of Badnell et al. (2003) and Badnell (2006b) for DR and RR, respectively.

4. CONCLUDING REMARKS

We have reported new DR rate coefficients for Fe $3p^q$ ($q = 2$ –6) ions that give rise to total recombination rate coefficients that are an order of magnitude larger at photoionized plasma temperatures than those currently recommended (Arnaud & Raymond 1992) and routinely used by modeling codes such as CLOUDY,

TABLE 1
DR FITTING COEFFICIENTS c_i ($\text{cm}^3 \text{s}^{-1} \text{K}^{3/2}$) FOR THE INITIAL GROUND LEVEL OF Fe $3p^q$ ($q = 0$ –6) IONS

q	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8
0	5.636E-4	7.390E-3	3.635E-2	1.693E-1	3.315E-2	2.288E-1	7.316E-2	...
1	1.090E-3	7.801E-3	1.132E-2	4.740E-2	1.990E-1	3.379E-2	1.140E-1	1.250E-1
2	3.266E-3	7.637E-3	1.005E-2	2.527E-2	6.389E-2	1.564E-1
3	1.074E-3	6.080E-3	1.887E-2	2.540E-2	7.580E-2	2.773E-1
4	9.073E-4	3.777E-3	1.027E-2	3.321E-2	8.529E-2	2.778E-1
5	5.335E-4	1.827E-3	4.851E-3	2.710E-2	8.226E-2	3.147E-1
6	7.421E-4	2.526E-3	4.605E-3	1.489E-2	5.891E-2	2.318E-1

TABLE 2
DR FITTING COEFFICIENTS E_i (K) FOR THE INITIAL GROUND LEVEL OF Fe $3p^q$ ($q = 0-6$) IONS

q	E_1	E_2	E_3	E_4	E_5	E_6	E_7	E_8
0	3.628E3	2.432E4	1.226E5	4.351E5	1.411E6	6.589E6	1.030E7	...
1	1.246E3	1.063E4	4.719E4	1.952E5	5.637E5	2.248E6	7.202E6	3.999E9
2	1.242E3	1.001E4	4.466E4	1.497E5	3.919E5	6.853E5
3	1.387E3	1.048E4	3.955E4	1.461E5	4.010E5	7.208E5
4	1.525E3	1.071E4	4.033E4	1.564E5	4.196E5	7.580E5
5	2.032E3	1.018E4	4.638E4	1.698E5	4.499E5	7.880E5
6	3.468E3	1.353E4	3.690E4	1.957E5	4.630E5	8.202E5

ION, and XSTAR. These new rate coefficients can be expected to significantly change the ionization balance of the Fe M-shell ions that give rise to the important UTA X-ray absorption feature seen in the spectra of AGNs observed by *Chandra* and *XMM-Newton*, and they will enable rigorous modeling of this feature to be carried out now using these data.

Similarly, large low-temperature DR contributions can be

expected for $3p^q$ ions of other elements of astrophysical importance, e.g., Si, S, Ar, Ni. A move into the $3d$ subshell of lower charge Fe ions, using a level-resolved approach, is also desirable.

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TABLE 3
RR FITTING COEFFICIENTS FOR THE INITIAL GROUND LEVEL OF Fe $3p^q$ ($q = 0-6$) IONS

q	A ($\text{cm}^2 \text{s}^{-1}$)	B	T_0 (K)	T_1 (K)	C	T_2 (K)
0	1.179E-9	0.7096	4.508E2	3.393E7	0.0154	3.977E6
1	1.050E-9	0.6939	4.568E2	3.987E7	0.0066	5.451E5
2	9.832E-10	0.7146	3.597E2	3.808E7	0.0045	3.952E5
3	8.303E-10	0.7156	3.531E2	3.554E7	0.0132	2.951E5
4	1.052E-9	0.7370	1.639E2	2.924E7	0.0224	4.291E5
5	1.338E-9	0.7495	7.242E1	2.453E7	0.0404	4.199E5
6	1.263E-9	0.7532	5.209E1	2.169E7	0.0421	2.917E5

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