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 multi-configuration 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 which 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 which 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 — see Behar et al. (2001) for a detailed discussion, and 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 towards the neutral end. This brings the modeling results towards accord with observation, but it is not rigorous since there is little to constrain the DR rate coefficients which they use.

The extant recombination data is effectively all radiative (RR) at photoionized plasma temperatures [1]. The recommended DR data for these Fe ions (Arnaud & Raymond 1992) is based upon the high-temperature electron-collisional plasma results of Jacobs et al. (1977), which 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 which were not (needed to be)

considered by Jacobs et al. (1977).

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 which 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.

The remainder of the paper is organized as follows: in Section 2 we describe our methodology, in Section 3 we present our results and make comparisons with the results of earlier works, and then make some concluding remarks.

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 are both 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. But, we note in particular that a level-resolved treatment is critical for the determination of accurate DR rate coefficients at photoionized plasma temperatures, but the results of

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[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 and 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.

such calculations are sparse for the M-shell.

2.1. Theory

The total dielectronic recombination rate coefficient, $\alpha_\nu^{\mathrm{DR}}(T)$, from an initial state ν of an N-electron ion is given, at a temperature T, by (Burgess 1964)

$$\alpha_\nu^{\mathrm{DR}}(T) = \left(\frac{4\pi a_0^2 I_{\mathrm{H}}}{k_{\mathrm{B}}T}\right)^{3/2} \sum_j \frac{\omega_j}{2\omega_\nu} \, \mathrm{e}^{-E_c/(k_{\mathrm{B}}T)}$$

$$\times \frac{\sum_{i,l} A_{j\to\nu,E_c l}^{\mathrm{a}} \, A_{j\to i}^{\mathrm{r}}}{\sum_h A_{j\to h}^{\mathrm{r}} + \sum_{m,l} A_{j\to m,E_c l}^{\mathrm{a}}} \, , \qquad (1)$$

where ω_j is the statistical weight of the $(N+1)$-electron doubly-excited resonance state j, ω_ν is the statistical weight of the initial state and the autoionization (A^{a}) and radiative (A^{r}) 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 in the same units of energy), k_{B} is the Boltzman constant, T the electron temperature and $(4\pi a_0^2)^{3/2} = 6.6011 \times 10^{-24}$ cm^3.

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

2.2. The Fe $3p^q$ target

We describe the N-electron target by the following configurations (assuming a closed Ne-like core):

1 : $3s^2 3p^q$,   2 : $3s3p^{q+1}$,   3 : $3s^2 3p^{q-1} 3d$,

4 : $3p^{q+2}$,   5 : $3s3p^q 3d$,   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 $\Delta n = 0$ sub-shell promotions from the ground configuration, as well as including important interacting configurations. We denote it as '7CF'. We also investigated the accuracy of this representation for DR by carrying-out a further calculation for each ion which included the additional configuration interaction due to

8 : $3s3p^{q-1} 3d^2$.

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 re-arrangement autoionizing transitions and the $3-4$ outer-shell contribution peaks at a temperature which 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 (NIST v3) wherever possible. 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 calculated level splittings to adjust the position of 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 number 4 and above) where there are no observed level energies, we adjust the entire configuration position by consideration of 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, $\alpha_\nu^{\mathrm{RR}}(T)$, with AUTOSTRUCTURE, following Badnell (2006b).

2.3. Fits

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

$$\alpha_\nu^{\mathrm{DR}}(T) = T^{-3/2} \sum_i c_i \exp\left(-E_i/T\right) , \qquad (2)$$

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

$$\alpha_\nu^{\mathrm{RR}}(T) = A \qquad\qquad\qquad (3)$$

$$\times \left[\sqrt{T/T_0} \left(1 + \sqrt{T/T_0}\right)^{1-B} \left(1 + \sqrt{T/T_1}\right)^{1+B} \right]^{-1} ,$$

where, for greater accuracy, B may be replaced as

$$B \to B + C \exp(-T_2/T). \qquad (4)$$

Here, $T_{0,1,2}$ are in units of temperature (K), the units of A are cm^3 s^{-1}, while 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). The data of Arnaud & Raymond (1992) are based principally upon the results of Jacobs et al. (1977), but include an estimate of the contribution from $2p - 3d$ inner-shell transitions as well — these were not included by Jacobs et al. (1977). The work of Jacobs et al. (1977) was for application to high-temperature electron-collisional plasmas and their results 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. 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 by 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 upon 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 note also 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 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-upon our results for $q = 1$ (Badnell 2006a) and our comments in Section 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 and RR rate coefficients, respectively, 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,d), 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 which give rise to total recombination rate coefficients which 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, ION and XSTAR. These new rate coefficients can be expected to change significantly the ionization balance of the Fe M-shell ions which give rise to the important UTA X-ray absorption feature seen in the spectra of AGNs observed by *Chandra* and *XMM-Newton*, and to enable rigorous modeling of it 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 sub-shell of lower-charge Fe ions, using a level-resolved approach, is also desirable.

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TABLE 1
DR FITTING COEFFICIENTS, c_i (cm^{3}s^{-1}K$^{3/2}$) AND E_i(K), 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	5.636(−4)[a]	7.390(−3)	3.635(−2)	1.693(−1)	3.315(−2)	2.288(−1)	7.316(−2)	
1	1.090(−3)	7.801(−3)	1.132(−2)	4.740(−2)	1.990(−1)	3.379(−2)	1.140(−1)	1.250(−1)
2	3.266(−3)	7.637(−3)	1.005(−2)	2.527(−2)	6.389(−2)	1.564(−1)		
3	1.074(−3)	6.080(−3)	1.887(−2)	2.540(−2)	7.580(−2)	2.773(−1)		
4	9.073(−4)	3.777(−3)	1.027(−2)	3.321(−2)	8.529(−2)	2.778(−1)		
5	5.335(−4)	1.827(−3)	4.851(−3)	2.710(−2)	8.226(−2)	3.147(−1)		
6	7.421(−4)	2.526(−3)	4.605(−3)	1.489(−2)	5.891(−2)	2.318(−1)		

q	E_1	E_2	E_3	E_4	E_5	E_6	E_7	E_8
0	3.628(3)	2.432(4)	1.226(5)	4.351(5)	1.411(6)	6.589(6)	1.030(7)	
1	1.246(3)	1.063(4)	4.719(4)	1.952(5)	5.637(5)	2.248(6)	7.202(6)	3.999(9)
2	1.242(3)	1.001(4)	4.466(4)	1.497(5)	3.919(5)	6.853(5)		
3	1.387(3)	1.048(4)	3.955(4)	1.461(5)	4.010(5)	7.208(5)		
4	1.525(3)	1.071(4)	4.033(4)	1.564(5)	4.196(5)	7.580(5)		
5	2.032(3)	1.018(4)	4.638(4)	1.698(5)	4.499(5)	7.880(5)		
6	3.468(3)	1.353(4)	3.690(4)	1.957(5)	4.630(5)	8.202(5)		

[a]Note, (n) denotes $\times 10^n$.

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

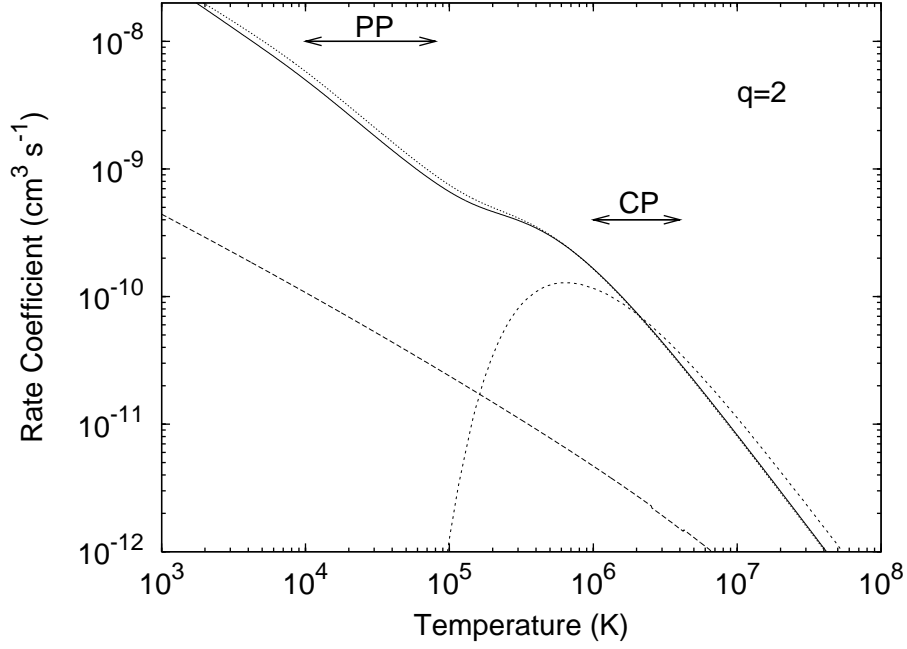| q	A (cm^{3}s^{-1})	B	T_0(K)	T_1(K)	C	T_2(K)
0	1.179(−9)	0.7096	4.508(2)	3.393(7)	0.0154	3.977(6)
1	1.050(−9)	0.6939	4.568(2)	3.987(7)	0.0066	5.451(5)
2	9.832(−10)	0.7146	3.597(2)	3.808(7)	0.0045	3.952(5)
3	8.303(−10)	0.7156	3.531(2)	3.554(7)	0.0132	2.951(5)
4	1.052(−9)	0.7370	1.639(2)	2.924(7)	0.0224	4.291(5)
5	1.338(−9)	0.7495	7.242(1)	2.453(7)	0.0404	4.199(5)
6	1.263(−9)	0.7532	5.209(1)	2.169(7)	0.0421	2.917(5)

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 and Bautista 2001) and (Mazzotta et al. 1998).
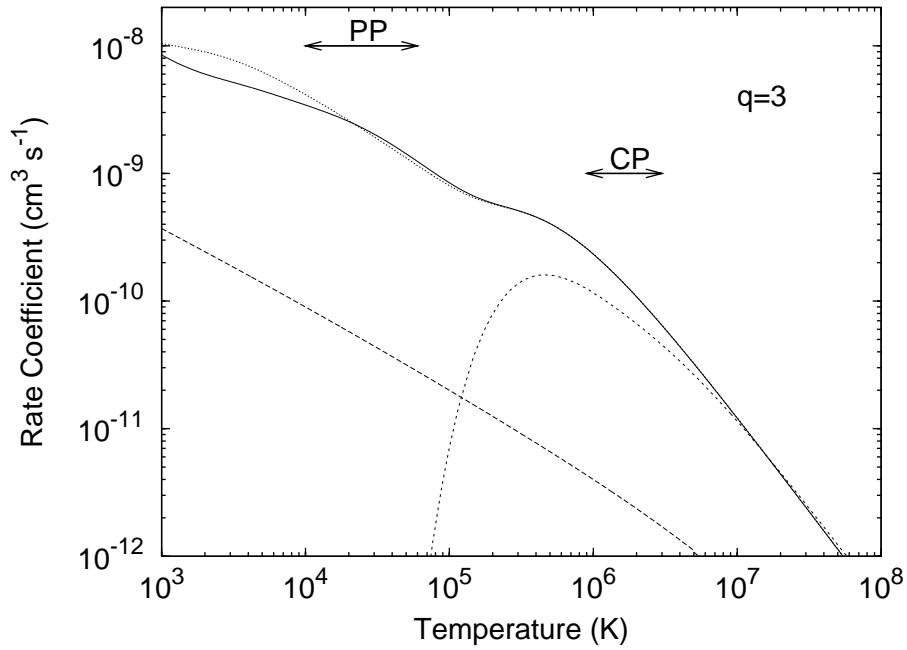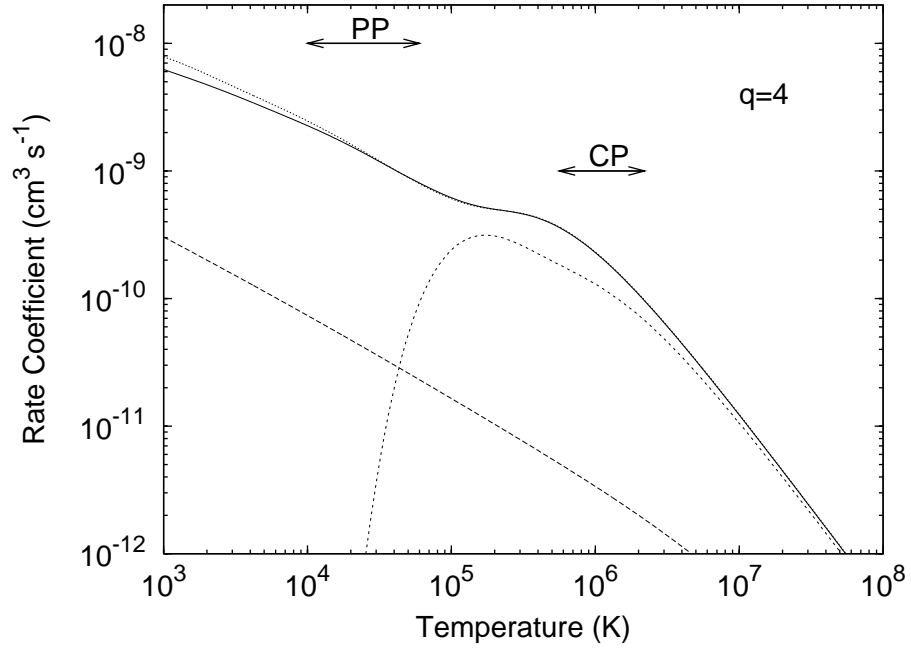

FIG. 2.— As Figure 1, but for Fe^{11+} ($q = 3$).

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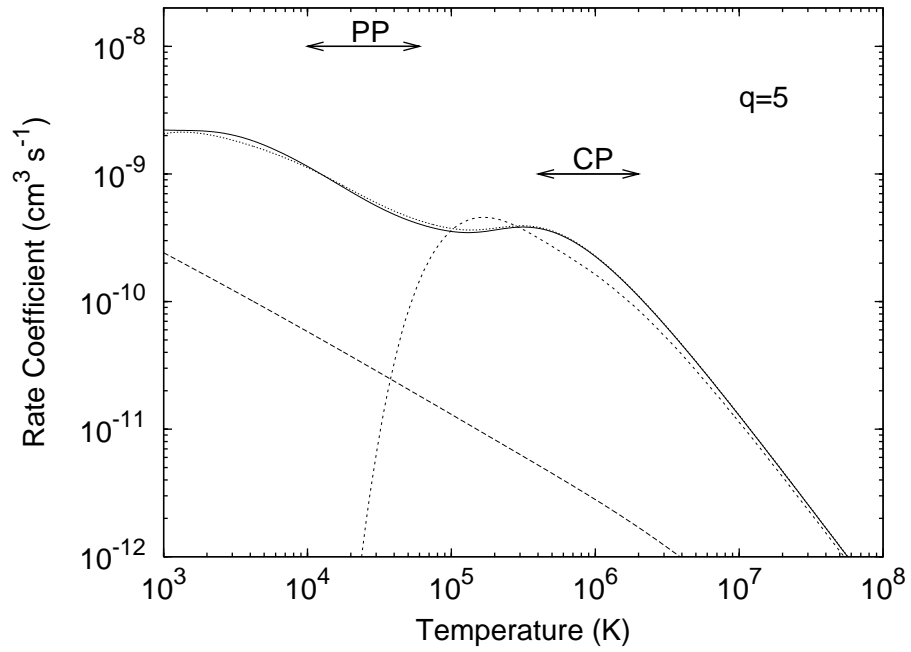FIG. 3.— As Figure 1, but for Fe^{10+} $(q = 4)$.
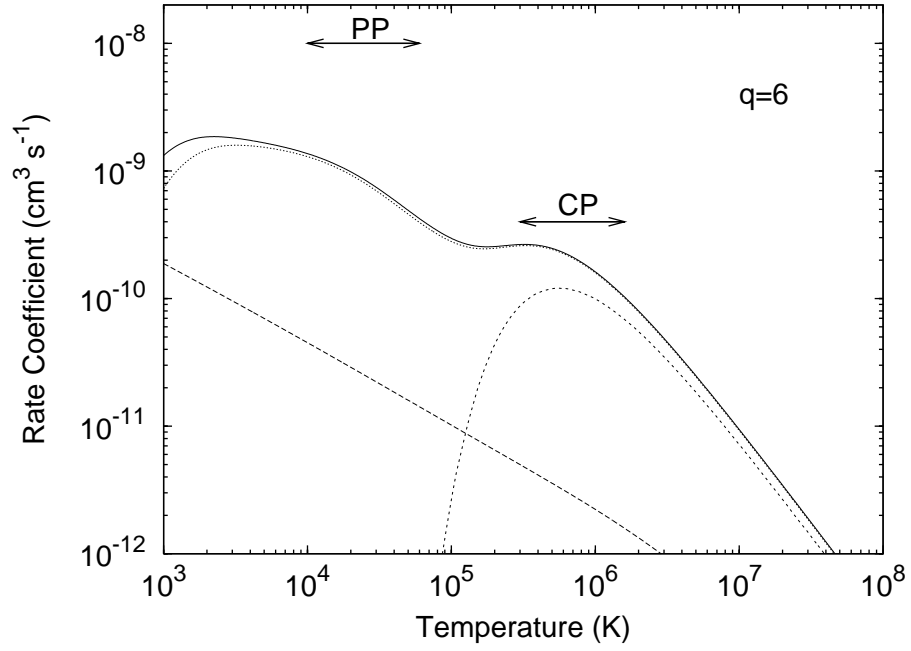

FIG. 4.— As Figure 1, but for Fe^{9+} $(q = 5)$.

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