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K-line X-ray fluorescence from highly charged iron ions under dense astrophysical plasma conditions

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In the present work, we report an investigation of plasma environment effects on the atomic parameters associated with the K-vacancy states in highly charged iron ions within the astrophysical context of accretion disks around black holes. More particularly, the sensitivity of K-line X-ray fluorescence parameters (wavelengths, radiative transition probabilities, and Auger rates) in Fe XVII–Fe XXV ions has been estimated for plasma conditions characterized by an electron temperature ranging from 10^5 to 10^7 K and an electron density ranging from 10^{18} to 10^{22} cm^{-3}. In order to do this, relativistic multiconfiguration Dirac-Fock atomic structure calculations have been carried out by considering a time averaged Debye-Hückel potential for both the electron–nucleus and electron–electron interactions.

1 | INTRODUCTION

In the inner-radius region of a black-hole accretion disk, high plasma densities ($\geq 10^{20}$ cm^{-3}) are likely to exist.[1] This would affect all atomic parameters, either by changing the atomic structures and associated rates or by lowering the ionization potentials, increasing the importance of collisional processes. It is, therefore, imperative that models of X-ray spectra from astrophysical sources include plasma environment effects in the atomic data. Addressing the problem of high-density plasma is important also in modeling other astrophysical media such as the accretion disks of neutron stars, the atmospheres of white dwarfs, and partially ionized outflows from galactic black holes.[2] In these X-ray sources, the plasma densities approach or exceed the limits of applicability for many of the rates in current atomic databases[1]; thus, new atomic calculations tailored for high density plasmas are urgently needed. In this context, the importance of K-shell atomic processes has been appreciated since the launch of X-ray observatories *Chandra* and *XMM-Newton*. In particular, iron K lines emitted by accretion disks around black holes are widely used to investigate Doppler and gravitational effects and to measure the black-hole spin.[3] However, the accuracy of these spin estimates is called into question because the models used to determine those parameters from observations require inexplicably large iron abundances, several times the solar value (Garcia[4] and references therein). The most likely explanation for these iron overabundances is a deficiency in the models, and the main reason might be that current models are inapplicable at densities above 10^{18} cm^{-3}. Recently, we have started a systematic investigation of plasma environment effects on the K-line parameters in iron ions.[5,6] In the present paper, we focus on the calculation of K-edge energies, line wavelengths, fluorescence yields, and natural level widths in three particular ions, that is, Fe XVII, Fe XVIII, and Fe XIX, under plasma conditions characterized by an electron temperature ranging from 10^5 to 10^7 K and an electron density ranging from 10^{18} to 10^{22} cm^{-3}.

2 | THEORETICAL APPROACH

The atomic structure calculations were carried out by using the fully relativistic multiconfiguration Dirac-Fock method,[7] as implemented in the GRASP92[8] and RATIP[9] codes. In this approach, each atomic state function is represented as a linear combination of configuration state functions of the same parity (P) and total angular momentum (J, M) :

$$\left|\Psi_\alpha(PJM)\right> = \sum_{k=1}^{n_c} c_k(\alpha)\left|\gamma_k PJM\right>, \tag{1}$$

where the configuration state functions are antisymmetrized products of a common set of orthonormal orbitals, which are optimized self-consistently based on the Dirac-Coulomb Hamiltonian

$$H_{DC} = \sum_i h_D(\mathbf{r}_i) + \sum_{i>j} \frac{1}{r_{ij}}, \tag{2}$$

with the one-electron Dirac operator, h_D.

In order to model the effects of the plasma screening on the atomic properties, we used a Debye-Hückel potential. This technique has already been used in several studies to

TABLE 1 Computed level energies, fluorescence yields, and natural widths for K-vacancy states in Fe XVII–XIX ions as a function of the plasma screening parameter μ, in a.u

		Energy (keV)		ω_k (s^{-1})		Γ_k (eV)	
Ion	**Level**	$\mu = 0.0$	$\mu = 0.25$	$\mu = 0.0$	$\mu = 0.25$	$\mu = 0.0$	$\mu = 0.25$
Fe XVII	$1s2s^22p^63s\ ^3S_1$	7.151	7.143	0.44	0.44	5.70	5.66
	$1s2s^22p^63s\ ^1S_0$	7.156	7.148	0.43	0.43	5.90	5.85
	$1s2s^22p^63p\ ^3P_0$	7.183	7.176	0.44	0.45	5.66	5.58
	$1s2s^22p^63p\ ^3P_1$	7.184	7.176	0.45	0.45	5.46	5.38
	$1s2s^22p^63p\ ^3P_2$	7.186	7.179	0.46	0.46	5.46	5.42
	$1s2s^22p^63p\ ^1P_1$	7.190	7.182	0.49	0.50	5.89	5.83
Fe XVIII	$1s2s^22p^6\ ^2S_{1/2}$	6.437	6.435	0.29	0.29	8.86	8.75
Fe XIX	$1s2s^22p^5\ ^3P_2$	6.470	6.468	0.34	0.35	5.07	5.02
	$1s2s^22p^5\ ^3P_1$	6.477	6.474	0.38	0.38	5.28	5.23
	$1s2s^22p^5\ ^3P_0$	6.485	6.482	0.35	0.35	4.98	4.94
	$1s2s^22p^5\ ^1P_1$	6.497	6.495	0.51	0.51	6.34	6.30
	$1s2s2p^6\ ^3S_1$	6.587	6.585	0.45	0.45	5.75	5.71
	$1s2s2p^6\ ^1S_0$	6.615	6.613	0.36	0.36	7.33	7.24

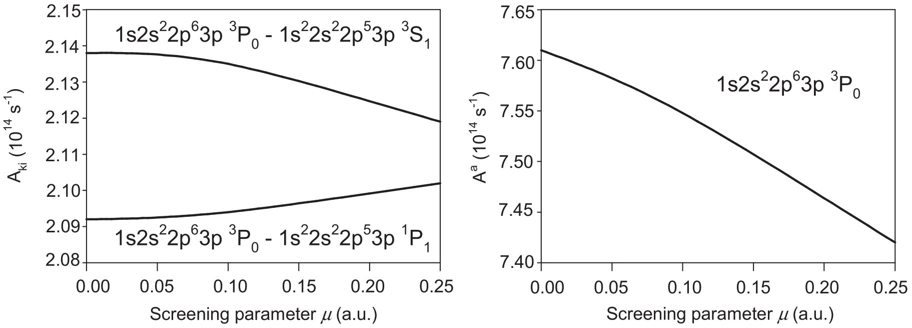

FIGURE 1 Variation of the radiative (*left panel*) and Auger (*right panel*) rates with the plasma screening parameter for the K-vacancy $1s2s^22p^63p$ text$^3P_0$ state in Fe XVII

simulate the plasma environment (see, e.g., Saha *et al.*[10–12]). This model potential reads, in atomic units (a.u.), as

$$V^{DH}(r,\mu) = -\sum_{i}^{N} \frac{Ze^{-\mu r_i}}{r_i} + \sum_{i>j}^{N} \frac{e^{-\mu r_{ij}}}{r_{ij}}, \tag{3}$$

where N is the number of bound electrons, r_i is the distance of the ith electron from the nucleus, and r_{ij} is the distance between the electrons i and j. Moreover, the plasma screening parameter, μ, is the inverse of the Debye shielding length, λ_{De}, and can be expressed in terms of the electron density, n_e, and temperature, T_e, of the plasma as (in a.u.)

$$\mu = \frac{1}{\lambda_{De}} = \sqrt{\frac{4\pi n_e}{kT_e}}. \tag{4}$$

Hence, any given values of both the temperature and the electron density of the plasma correspond to a certain value of the screening parameter μ. In the astrophysical context of an accretion disk around black hole, the physical conditions can be expected to be such as $T_e = 10^5 - 10^7$ K and $n_e = 10^{18} - 10^{22}$ cm^{-3}, which corresponds to screening parameter values up to about 0.25 a.u. Consequently, in our work, the plasma environment effects were estimated by means of a Debye-Hückel potential with a screening parameter μ ranging from 0 (isolated ion case) to 0.25 a.u.

3 | RESULTS AND DISCUSSION

3.1 | Fluorescence yields and natural level widths

For a K-vacancy level (i.e., a level belonging to a configuration with one hole in the K-shell), k, the fluorescence yield, ω_k and the natural width, Γ_k, are respectively given by

$$\omega_k = \frac{\sum_i A^r_{ki}}{\sum_i A^r_{ki} + A^a_k}, \tag{5}$$

and

$$\Gamma_k = \sum_i A^r_{ki} + A^a_k, \tag{6}$$

where A^r_{ki} represents the radiative transition probability to the lower level i, and A^a_k is the Auger rate.

The ω_k and Γ_k values calculated in our work for K-vacancy states in Fe XVII–Fe XIX using two different plasma screening parameters, that is, $\mu = 0$ and 0.25 a.u., are reported in Table 1. It is clear that the influence of the plasma environment on the results is rather small, the fluorescence yields being unchanged whereas the natural level widths appear to systematically decrease (by 1% on average), although the changes in radiative and Auger rates do not exhibit any systematic trend. This is illustrated in Figure 1 where the behaviour of some calculated A^r and A^a values in Fe XVII is plotted against the plasma screening parameter. We also note from Table 1 that the energies of K-vacancy level are lowered by about 8, 2, and 3 eV, in Fe XVII, Fe XVIII, and Fe XIX, respectively.

TABLE 2 Computed K-edge energies, in keV, for Fe XVII–XIX ions as a function of the plasma screening parameter μ, in a.u

Ion	$\mu = 0.0$	$\mu = 0.25$	Shift
Fe XVII	7.698	7.582	−0.116
Fe XVIII	7.827	7.705	−0.122
Fe XIX	7.960	7.831	−0.129

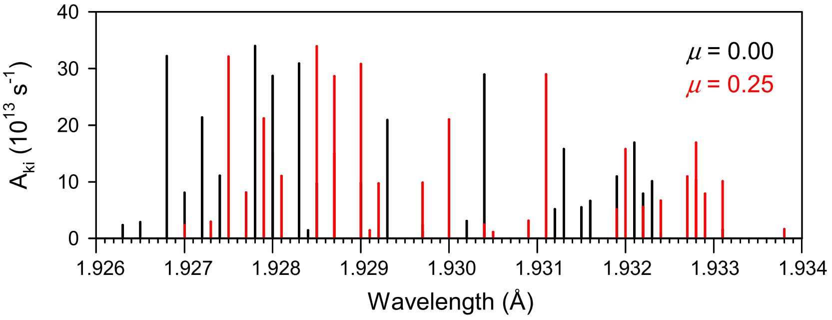

FIGURE 2 Variation of the calculated wavelengths with the plasma screening parameter ($\mu = 0$ a.u. in black; $\mu = 0.25$ a.u. in red) for the strongest Kα lines in Fe XVII

3.2 | K-edge energies and emission line wavelengths

The K-edge energy is set by the binding energy of the K-shell electrons of an atomic system. The effects of the plasma environment on the K-edge energies in Fe XVII, Fe XVIII, and Fe XIX are shown in Table 2. They are reduced by 116, 122, and 129 eV, respectively, when going from $\mu = 0$ to $\mu = 0.25$ a.u. This lowering could change the X-ray spectrum and the identification of those ions, which is often based on the position of the K-edges. The wavelengths computed in our work using $\mu = 0$ and 0.25 a.u. are compared in Figure 2 for emission K lines in Fe XVII. They all appear to be redshifted by about 1 mÅ.

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