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K-shell width, fluorescence yield, and K_β/K_α intensity ratio calculation for Fe in the Dirac-Fock approach

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Synopsis K-shell fluorescence yield, width, and K_β/K_α intensity ratio for Fe are calculated using the Dirac-Fock approach. Results are compared with available data.

The knowledge of accurate values of atomic decay rates and fluorescence yields is fundamental in quantitative analysis in X-ray spectroscopy, plasma physics, nuclear physics, dosimetry, radiation protection, among many other areas [1]. Despite the increasing number of theoretical and experimental work concerning the determination of fluorescence yields for several elements, the available data are still scarce. Iron is one of the most abundant elements in the universe and is of extreme importance in the analysis of stellar objects like stars and galaxies. Iron spectral lines are used in plasma diagnostics and help us to know physical properties such as temperature and electron density as well as for abundance studies [2].

In this work, we present a relativistic calculation of the K-shell width, fluorescence yield and K_β/K_α intensity ratio in Fe using the multi-configuration Dirac-Fock (MCDF) code of Desclaux and Indelicato [3, 4]. The code was used in a single-configuration approach, with Breit interaction and the vacuum polarization terms included in the self-consistent field calculations, and other QED effects included as perturbations.

Table 1. K-shell fluorescence yield (ω_K), width (eV), and K_β/K_α intensity ratio for iron

	ω_K	width	K_β/K_α
This work	0.378	1.14	0.134
McGuire [5]	0.386		
Krause [6]	0.34		
Campbell [7]		1.19	
Carreras *et al* [8]			0.14
Scofield [9]			0.139
Jankowsky *et al* [10]			0.134
Bé *et al* [11]			0.142

Since iron has an open outer shell ($3d^6$), electron coupling leads to 348105 possible radiative and radiationless transitions from the initial K hole configuration. Preliminary results for the K-shell fluorescence yield, width and K_β/K_α intensity ratio are consistent with the available data (Table 1).

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