

§12. Evaluation of Effective Collision Strengths of Electron-impact Excitation for Fe Atom and Ions

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Reliable atomic data for electron impact excitation rates of Fe ions are important for population kinetic models for plasma diagnostics. These data mostly rely on theoretical calculations and the development of computer power and atomic codes over the last decades has made it possible to obtain more detailed calculations. After an assessment meeting in 1992¹⁾, Pradhan and Zhang²⁾ reviewed available atomic data of electron impact excitation published by 1999 and gave recommended data for many Fe ions. The rate coefficients of electron impact excitation for 12 ions had been calculated using several R-matrix methods. During the decade since the review of Pradhan and Zhang, new data were calculated using various R-matrix methods and we assess the available information for electron impact excitation rates for Fe ions.

We made a list of recommended data for electron impact excitation effective collision strengths³⁾ which are obtained by averaging the collision strengths with Maxwellian distribution for electron velocity. We selected the data which were (1) calculated with an R-matrix method, (2) with many levels included, (3) by checking the treatment of configuration interaction, partial waves, relativistic effects, and energy range of calculations. As for a relativistic effect, Berrington et al.⁴⁾ compared the effective collision strengths of Fe¹⁴⁺ calculated by Breit-Pauli R-matrix method and Dirac R-matrix method with the same number of target states and the same energy mesh which gives very fine resolution to resolve the resonances. The results by both methods agree well and the average difference between the effective collision strengths is about 6%. This means that the difference in relativity treatment is not important for moderately ionized iron if all other conditions are the same.

There exist updated data produced for most of Fe ions since the review of Pradhan and Zhang. Recent trends are that the collision cross sections are calculated by (1) Breit-Pauli R-matrix method (BPRM), (2) Dirac R-matrix method (DARC), or (3) intermediate-coupling frame transformation (ICFT) R-matrix method⁵⁾. The ICFT method is equivalent to full Breit-Pauli R-matrix approach and computationally less demanding, so big calculations with many levels can be performed. The relativistic effects are included. Most of the data are available electronically via internet.

Figures show some examples of effective collision strengths between fine structure levels of excited states as a function of electron temperature for Fe⁴⁺ (Fe V) and Fe²³⁺ (Fe XXIV) ions.

- 1) Lang, J., Atomic Data and Nucl. Data Tables, **57** (1994) 1.
- 2) Pradhan, A. K. and Zhang, H. L., *Photon and Electron Interactions with Atoms, Molecules and Ions*, Landolt-Boernstein New Series I/17B, Ed. Y. Itikawa (Springer-Verlag, 2001), p.3-1.
- 3) Murakami, I. et al., accepted to IAEA Atomic and Plasma-Material Interaction Data for Fusion (2010).
- 4) Berrington, K. A., et al., J. Phys. B, **38** (2005) 1667.
- 5) Griffin, D. C. et al., J. Phys. B, **31** (1998) 3713.

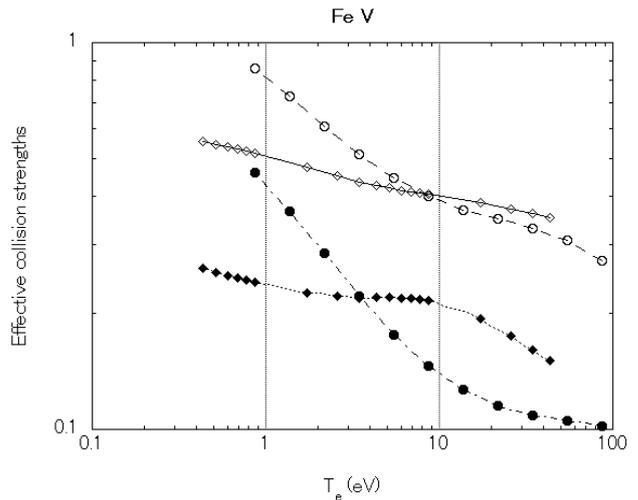


Figure 1 Effective collision strengths of the Fe V $3d^4\ ^5D_0 - 3d^4\ ^5D_1$ (open symbols) and the $3d^4\ ^5D_0 - 3d^4\ ^5D_2$ (filled symbols) transitions obtained by Berrington (1995) (circles) and Ballance and Griffin (2007) (diamonds, recommended) as a function of electron temperature.

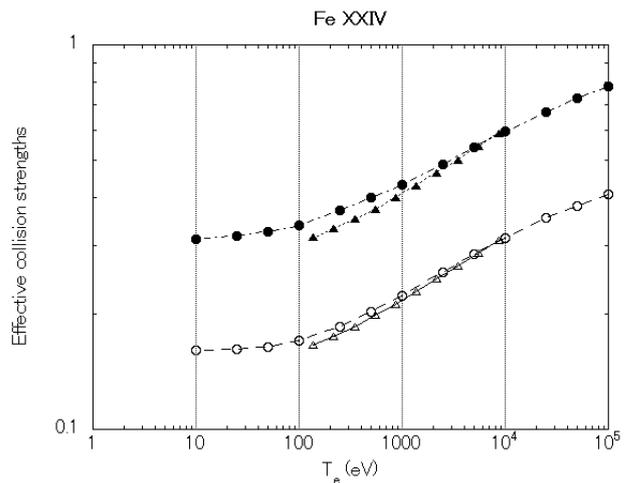


Figure 2. Effective collision strengths of the Fe XXIV $2s\ ^2S_{1/2} - 2p\ ^2P_{1/2}$ (open symbols) and the $2s\ ^2S_{1/2} - 2p\ ^2P_{3/2}$ (filled symbols) transitions obtained by Berrington and Tully (1997) (triangles) and Whiteford et al. (2002) (circles, recommended) as a function of electron temperature.