Atomic data for the X-rays

Science & Technology Facilities Council

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Calculations of basic atomic data

1) **Direct-ionization by electron impact**:

Dere (2007) calculated ab-initio cross-sections of impact with ions and compared them with available experimental data for a large number of ions.

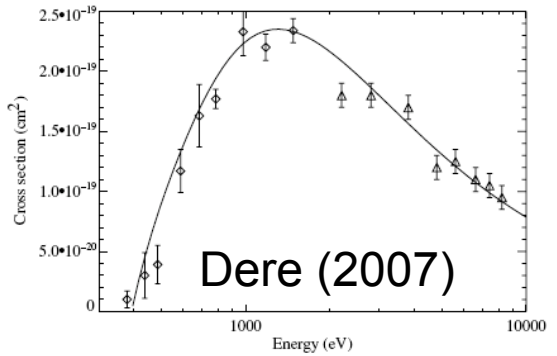


Fig. 3. FAC DI cross sections for C V and the measurements of Crandall et al. (1979a) (diamonds) and Donets & Ovsyannikov (1981) (triangles, plotted with an arbitrary 10% experimental error).

2) **Radiative recombination**: Badnell (2006)

3) **Dielectronic recombination**: after Badnell et al. (2003), a number of papers.

4) **Electron impact excitation**: a large number of papers from Iron Project, UK-Rmax network.

We now have an STFC-funded **APAP Network**

http://www.apap-network.org/

to automatically calculate data for ***all*** astrophysically-important ions.
(cf. Witthoeft Whiteford Badnell 2007 for F-like ions).

Atomic Data and Databases

1) Atomic data from the **APAP Network** will be available through:

SADA: Server of Atomic Data for Astrophysics

2) Atomic data have been included into the **CHIANTI database:** **www.chianti.rl.ac.uk** Unfortunately, CHIANTI is not funded by STFC anymore.

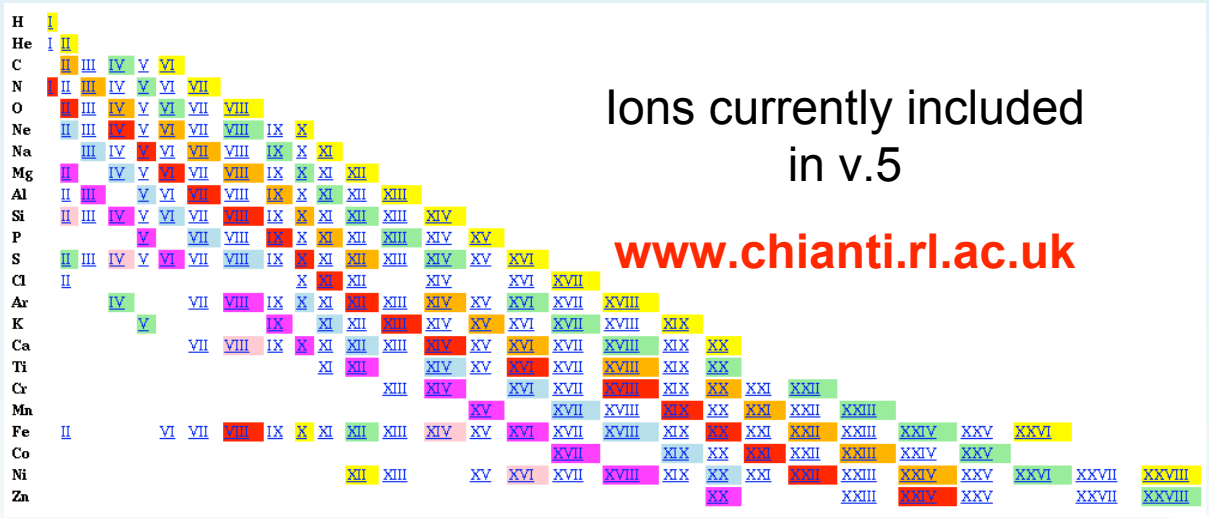
3) Basic atomic data and spectral line emissivities for plasma modelling have been imported from CHIANTI into a MySQL database accessible via **AstroGrid:** **www2.astrogrid.org** and **VOSpec.** Unfortunately, AstroGrid is not funded by STFC anymore. However, Del Zanna & Mason have obtained funding from the EU for provision of atomic data (VAMDC international collaboration)

4) Basic atomic data from e.g. CHIANTI are included in many other spectral codes. Photoionization (XSTAR, CLOUDY, MOCASSIN) and others (ATOMDB, XSPEC, ISIS, PINTofALE).

For the survival of atomic physics calculations it is essential that **appropriate references are given in the literature !**

CHIANTI: have we made it too easy ?

CHIANTI Provides all atomic data and IDL programs necessary for modelling spectra from collisionally-ionised plasmas for the XUV. About 1000 citations.



Ions currently included in v.5

www.chianti.rl.ac.uk

V.6, to be released April 2009 (Dere et al.2009) contains **new ionization and recombination rates** (to study non-equilibrium), and new ionization equilibrium:

and many new datasets for excitation data

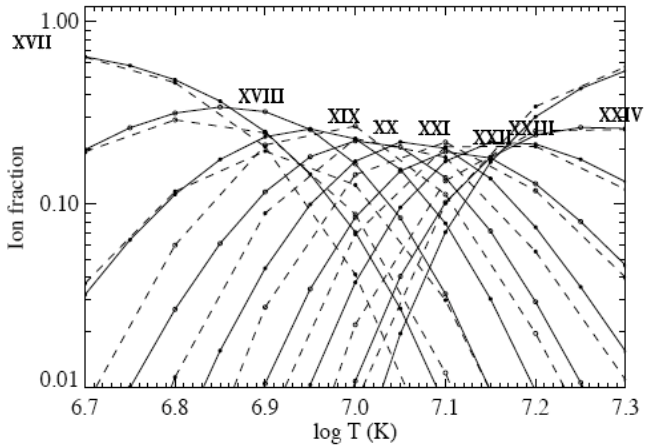


Fig. 3. Ionization equilibria for Fe XVII-XXIV. Full line - current calculations, dashed line = Mazzotta et al. (1998).

Benchmarking atomic data for astrophysics

In a series of papers, I have calculated and benchmarked atomic data for the XUV. The benchmark approach is novel.
Atomic structure calculations and comparisons between observed and theoretical line intensities for a wide range of astrophysical and laboratory plasmas using the emissivity ratios:

$$F_{ji}(N_e, T_e) = C \frac{I_{ob} N_e}{N_j(N_e, T_e) A_{ji}}$$

have resulted in a large number of revised wavelengths, new identifications and new diagnostic applications. For example:

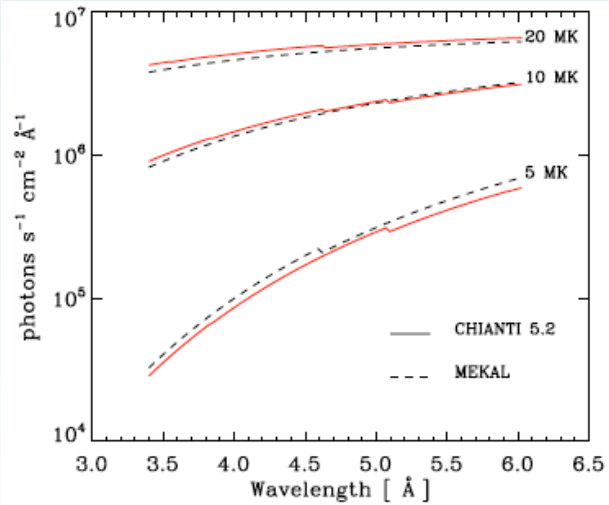
- Fe XVII: Loch et al. (2006); **benchmark:** Del Zanna (2008,2009)
- Fe XVIII: Witthoeft et al. (2006); **benchmark:** Del Zanna (2006b)
- Fe XX: Witthoeft, Del Zanna, Badnell (2007)
- Fe XXIII: Chidichimo Del Zanna et al. (2005); **benchmark:** Del Zanna et al. (2005)
- Fe XXIV: Whiteford et al. (2002); **benchmark:** Del Zanna (2006a)

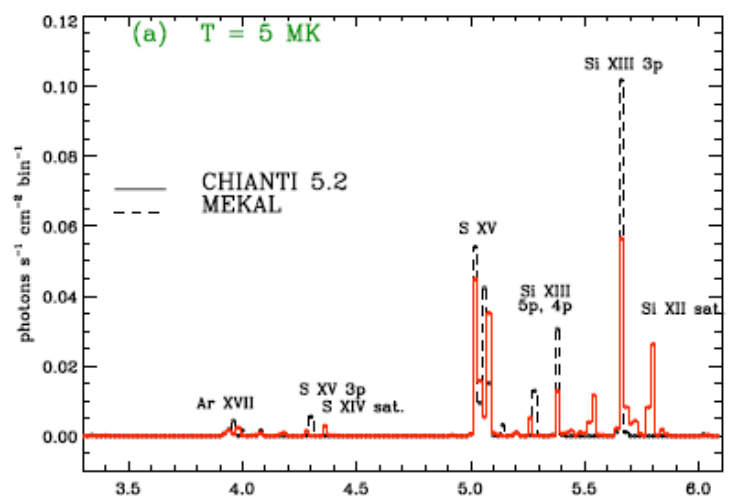
- New atomic data included in v.6 of CHIANTI for:
- O VIII, C VI, Ar XVII, S XV, Ca XIX, Fe XXV, Ne IX

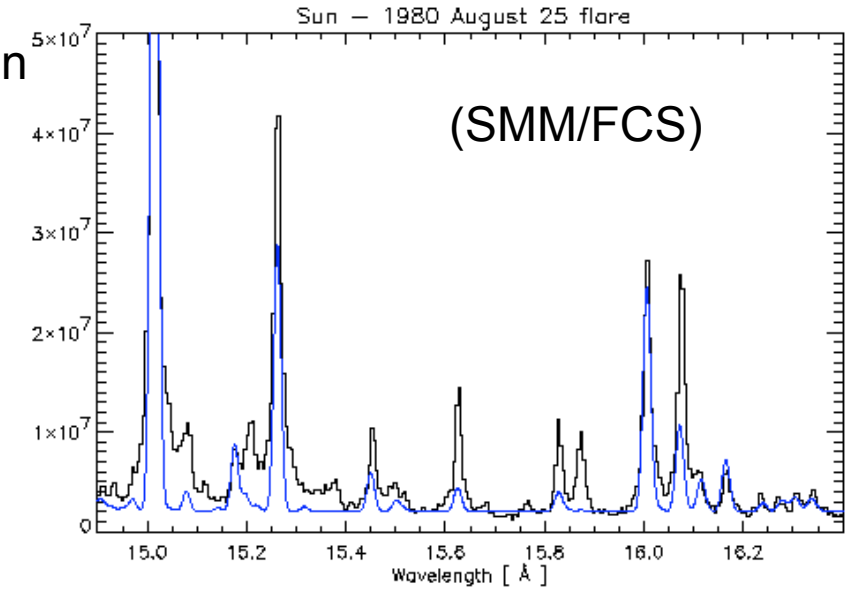
Preliminary benchmarks for the X-rays

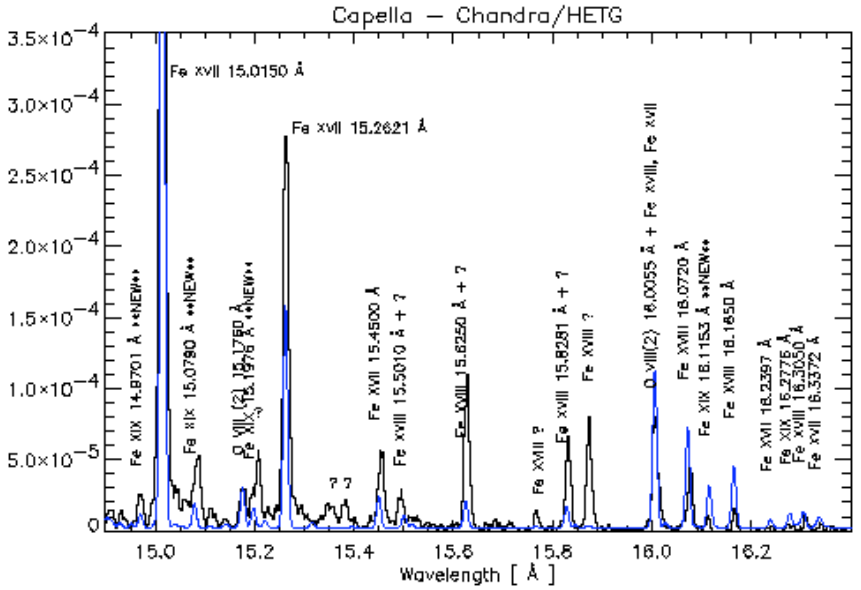
A lot of benchmark work went into the preparation of CHIANTI v.4, released in 2003 (e.g. Del Zanna G. 2002):

and for v.5 (cf. Chifor, Del Zanna et al. 2007):





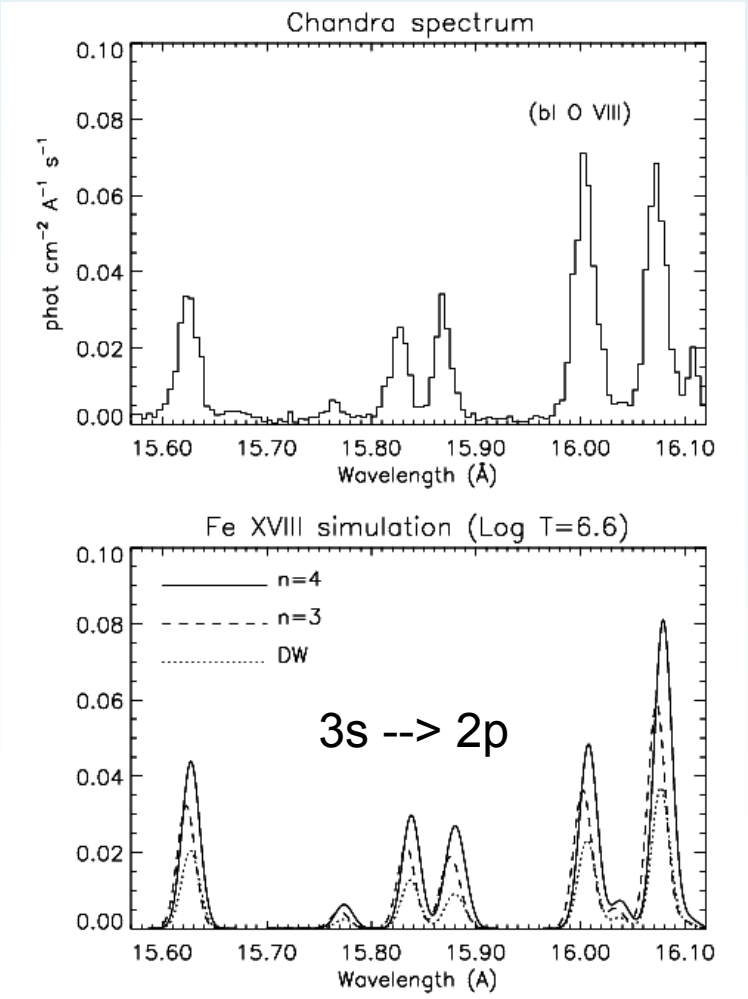


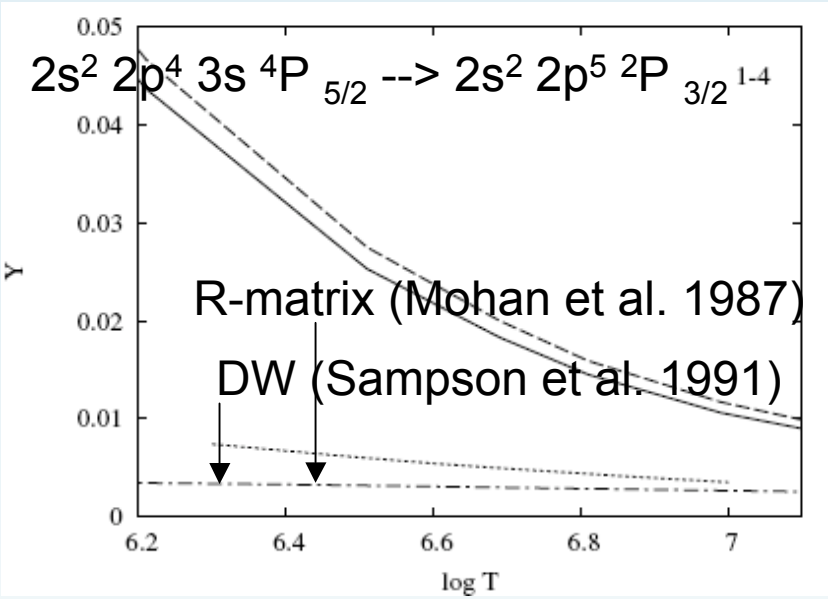


Fe XVIII: the new atomic data do make a big difference!

First R-matrix e- scattering calculation by

Witthoeft, Badnell, Del Zanna et al. (2006)





The large discrepancies between observed and theoretical intensities for the strong 3s--> 2p transitions are now resolved.

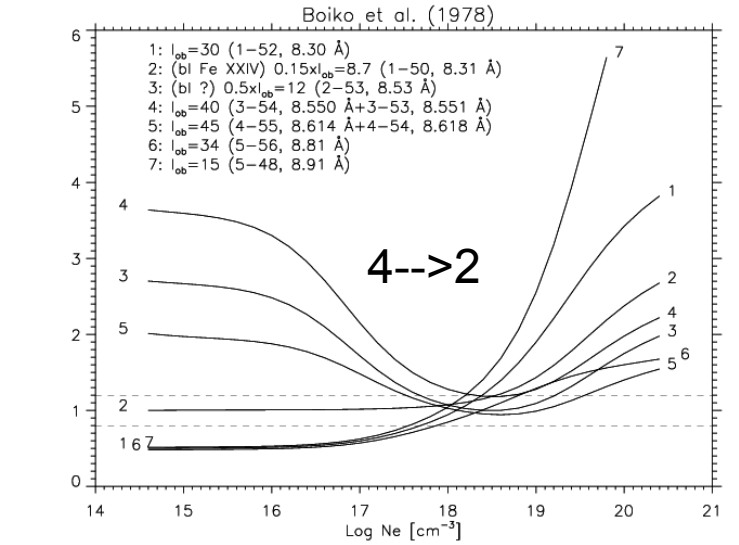
New diagnostics to measure electron temperatures and densities are now available (Del Zanna 2006).

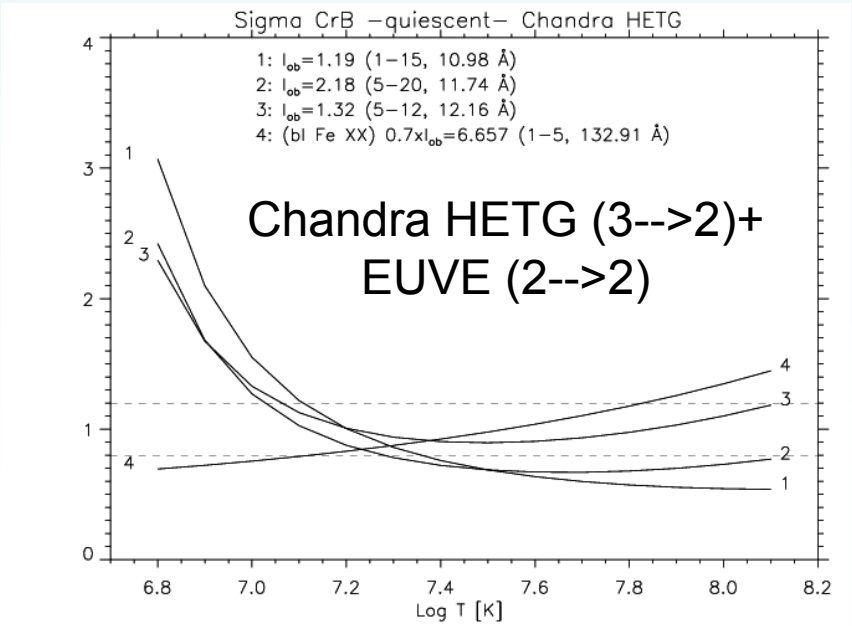
Fe XXIII: new diagnostics

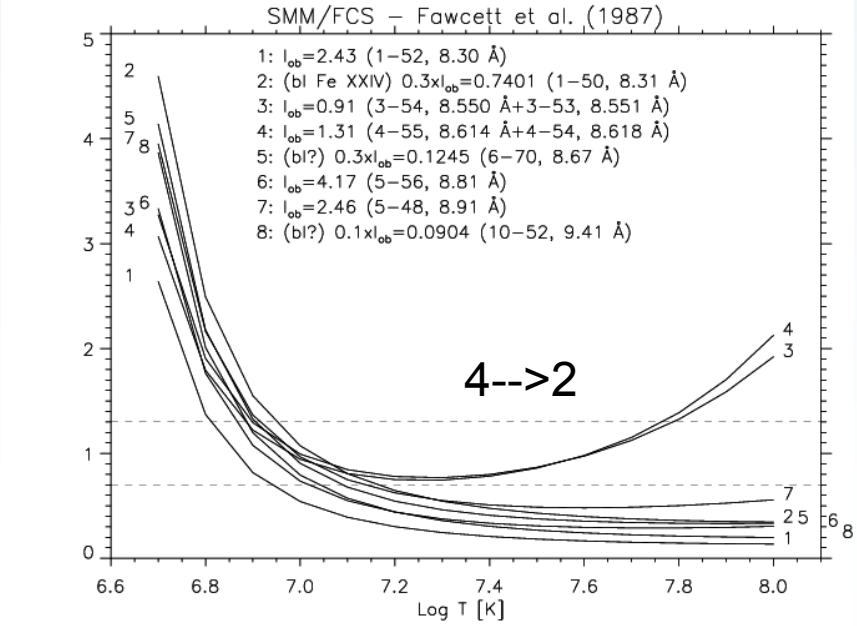
Fe XXIII: New electron impact excitation by Chidichimo et al. (2005).

Del Zanna et al. (2005):

New diagnostics to measure electron temperatures and densities.







Conclusions

Excellent agreement (within 10%) between theoretical and observed line intensities is found when appropriate atomic data are used.

A novel on-going benchmark work has already established a large number of new line identifications and spectral diagnostics for collisionally-ionised plasmas, however a large amount of work is still needed, especially now that we are providing a large new set of data.

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