The Flexible Atomic Code (FAC)

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Single Electron Dirac Equations

The basis states are constructed by solving the single electron Dirac Equation for a suitable local central potential $V(r)$.

$$\begin{aligned}
\left(\frac{d}{dr} + \frac{\kappa}{r}\right) P_{n\kappa} &= \alpha \left(\varepsilon_{n\kappa} - V + \frac{2}{\alpha^2}\right) Q_{n\kappa} \\
\left(\frac{d}{dr} - \frac{\kappa}{r}\right) Q_{n\kappa} &= \alpha \left(-\varepsilon_{n\kappa} + V\right) P_{n\kappa},
\end{aligned} \tag{1}$$

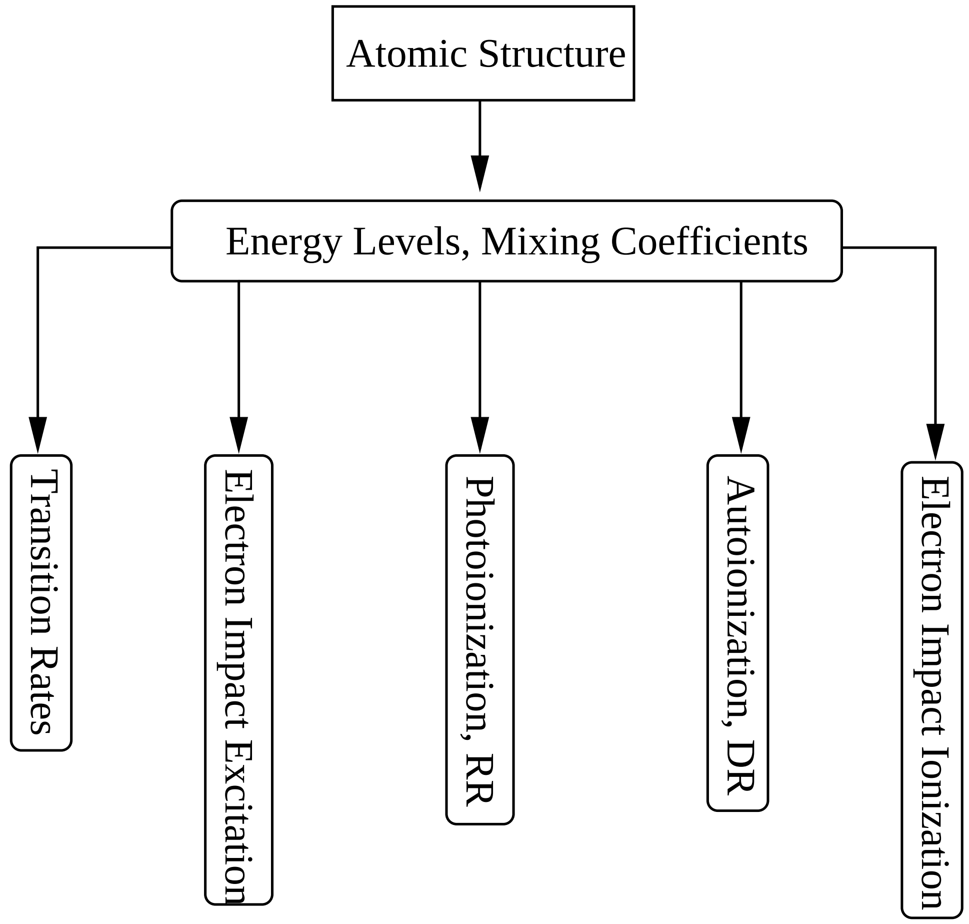

Figure 1: Flow chart of the FAC package

Example for Ne-like Fe Structure Calculation

Python Script:

```
# import the modules
from pfac import config, fac
fac.SetAtom('Fe')
# 1s shell is closed
config.closed('1s')
config.config('2*8', group = 'n2')
config.config('2*7 3*1', group = 'n3')

fac.OptimizeRadial('n2', 'n3')
fac.Structure()
fac.LevelTable('ne.lev')
fac.TransitionTable(['n2'], ['n3'], 'ne.tr', -1)
```

Comparison with Sampson & Zhang Code

	Level	FAC ΔE	FAC gf	SZ ΔE	SZ gf
2	$(2p_{3/2}3s_{1/2})_1$	726.99	0.1214	727.22	0.1102
4	$(2p_{1/2}3s_{1/2})_1$	739.24	0.1049	739.50	0.0937
16	$(2p_{3/2}3d_{3/2})_1$	802.42	0.0103	802.64	0.0099
22	$(2p_{3/2}3d_{5/2})_1$	812.88	0.6333	813.15	0.6095
26	$(2p_{1/2}3d_{3/2})_1$	827.32	2.6120	827.69	2.5514
30	$(2s_{1/2}3p_{1/2})_1$	894.81	0.0338	894.83	0.0358
32	$(2s_{1/2}3p_{3/2})_1$	899.18	0.2767	899.18	0.2868

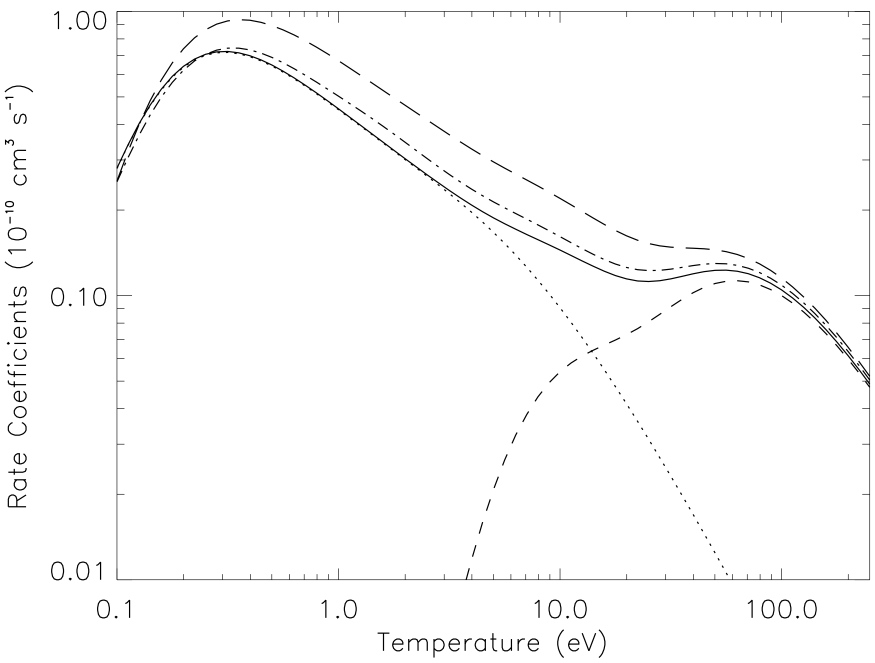

Figure 2: Comparison of the $\Delta n = 0$ DR rate coefficients of F-like iron. The dotted line is the present result for $P_{3/2} \rightarrow P_{1/2}$ channel, the dashed line is the present result for $P_{3/2} \rightarrow S_{1/2}$ channel, the solid line is the present total rate coefficients, the dash-dotted and long-dashed lines are the MCDF calculations and experimental results of Savin et al. (1999 ApJ Suppl. 123, 687).

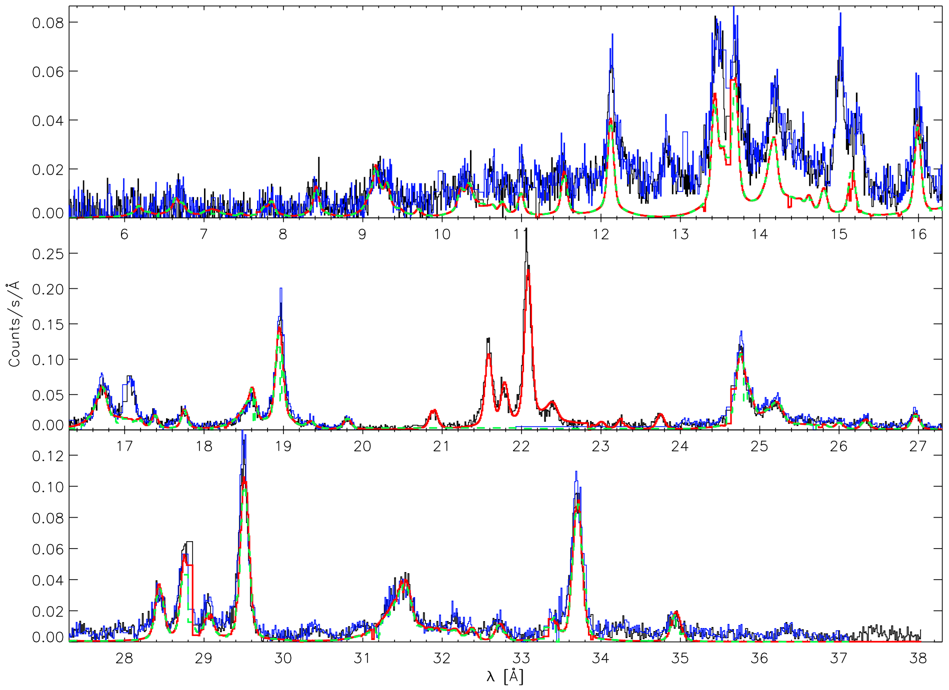

Figure 3: FAC model fitted to the XMM-RGS spectrum of NGC 1068. Red and green lines are the recombination spectrum calculated with FAC data for RGS1 and RGS2 responses. Only H-like and He-like ions are included in the model. Black and blue lines are the RGS1 and RGS2 spectra of NGC 1068 (Ali Kinkhabwala).

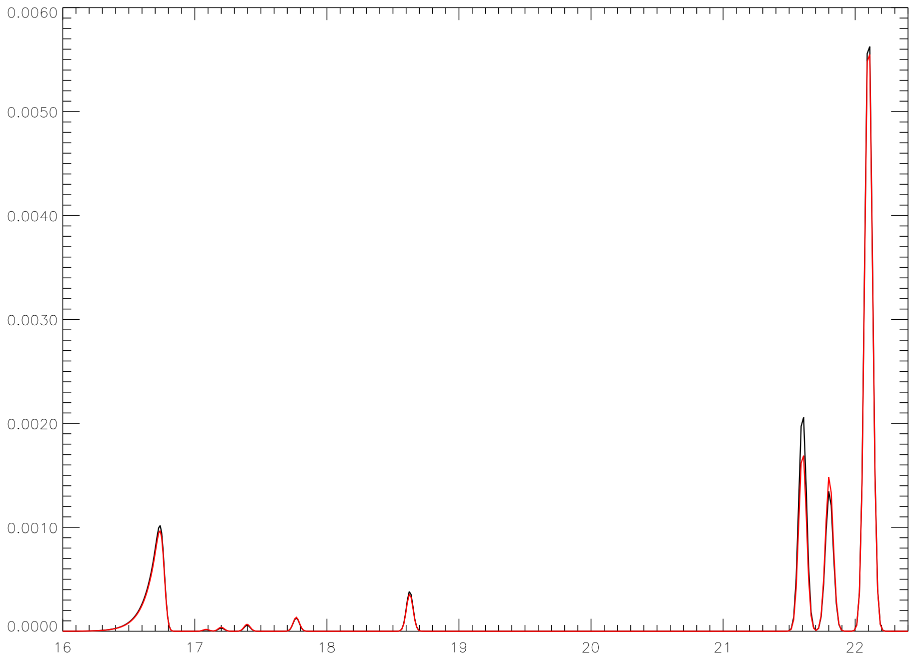

Figure 4: Recombination spectrum of He-like O with FAC and HULLAC. Red line is the FAC spectrum. Black line is the HULLAC spectrum (Ali Kinkhabwala).

Check out FAC and give it a try

Anonymous FTP.

space.mit.edu/pub/mfgu/fac/