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Implementing TOPbase/Iron Project: continuous absorption from Fe II

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ABSTRACT

We discuss implementation of TOPbase and Iron Project opacities for stellar spectral codes. We use a technique employed by Peach, where a Boltzmann-averaged cross-section is calculated for selected temperatures, and the opacity obtained from double interpolation in temperature and wavelength. It is straightforward to include *all* levels for which cross-sections have been calculated. Boltzmann-averaged cross-sections for Fe II show a local maximum between 1700 and 2000 Å. We suggest this feature arises from $3d^5 4s nl \rightarrow 3d^5 4p nl$ transitions within Fe II. *IUE* spectra of iron-rich CP stars show local minima in this region. Theoretical calculations of a representative stellar continuum demonstrate that Fe II photoionization contributes significantly to the observed minima.

Key words: atomic data – atomic processes – stars: atmospheres – stars: chemically peculiar.

1 INTRODUCTION AND RATIONALE

State of the art photoionization cross-sections have been available from The Opacity Project (Seaton 1994; The Opacity Project Team 1995) for more than a decade. Nevertheless, stellar atmospheres codes have been slow to incorporate these results fully. Surely, one reason for the delay in adopting these calculations is that metal opacities are not particularly important for many stellar atmospheres. The well-known opacities from hydrogen, bound–free and H^- usually dominate other sources.

But it is also tedious to incorporate the detailed TOPbase results into workable subroutines with typical algorithms, which treat levels individually or in groups. This technique is difficult for complex atoms, where no simple parametrization can describe all of the cross-sections adequately. In this paper, we propose adoption of the method used by Peach (1967), which provides a practical solution to this problem. We then discuss an example of stellar continuum calculations that uses TOPbase/Iron Project cross-sections along with her algorithm. We first outline the general problem of dealing with the TOPbase/Iron Project material.

Photoionization cross-sections in The Opacity Project Data Base (TOPbase) are given for typically hundreds of levels. For each level, the cross-sections may be given for several hundred to a thousand photon energies. The cross-sections include large deviations from the smooth hydrogenic functions, which are possible in multi-electron systems. The resulting features may be quite sharp, being essentially spectral lines, or they can be broader, when there is strong interaction between bound and continuum states. Not only do Fano profiles appear, but also broad, deep absorption minima (Cooper minima), which result from nodes in the radial wavefunctions. These are especially apparent in transitions involving *s* electrons, as in Na I. Broad absorption maxima can result from photoexcitation of core electrons (PEC), essentially bound–bound transitions of inner electrons. These maxima can appear in the cross-sections of numerous levels.

A consensus has emerged that it is permissable to smooth over the resonances of photoionization cross-sections (cf. Bautista, Romano & Pradhan 1998; Prieto et al. 2002). This smoothing affects the sharp features which we shall call *high-frequency components*, but leaves broader ones, such as Cooper minima or PEC. Prieto has published a number of resonance-smoothed photoionization cross-sections (RSP) on his web site (http://hebe.as.utexas.edu/at/at.cgi). Our current opacity routines use the Prieto RSPs for all atoms and ions with the exception of Fe I and II. Specifically, the following atoms and atomic ions are included: Li I, Be I and II, B I and II, C I, Na I, Mg I and II, Al I, Si I and II, S I, and Ca I and II.

For Fe I, we have sampled each 100 Å from material discussed by Bautista (1997). The Fe II cross-sections are from a web site of Dr Nahar (http://www-astronomy.mps.ohio-state.edu/nahar/), cf. Nahar & Pradhan (1994).

While the RSPs omit some of the higher TOPbase levels, they may still contain several hundred levels (e.g. Si I), with several hundred data points for each level. If all of this information were included in a standard FORTRAN data statement, the result would be thousands of records long. However, for practical calculations, the individual cross-sections are not necessary. We need only their appropriately weighted sums.

2 ALGORITHM AND CALCULATIONS

The continuous opacity resulting from a given atom or atomic ion is the weighted sum of the cross-sections over a number of levels.

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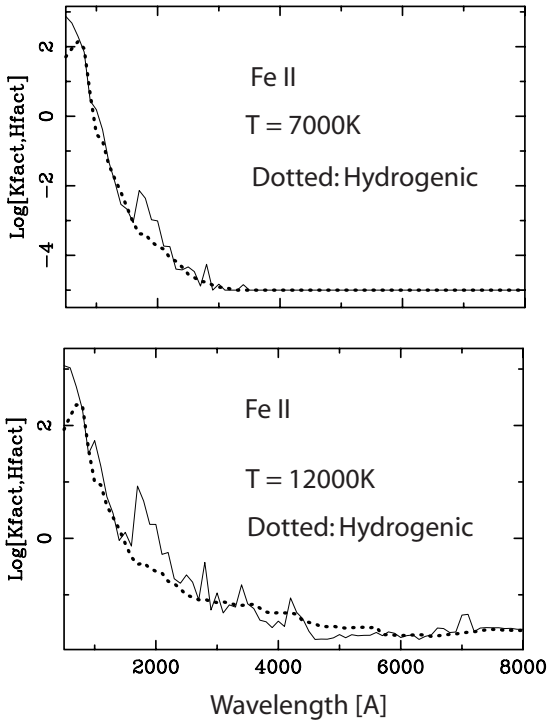

Figure 1. *K* factors for Fe II.

We define the *K* factor:

$$K\text{fact} = \sum_n g_n \exp\left[-(\chi_n/kT)\right]\sigma_n(\lambda). \quad (1)$$

Here, g_n is the statistical weight of the level n, χ_n/kT the appropriate Boltzmann factor, and $\sigma_n(\lambda)$ is the photoionization cross-section.

Consider the opacity resulting from photoionizations from level n of an atom or atomic ion in the ith ionization stage. Write the corresponding number density as $N_{n,i}$. Puting $N_{t,i}$ for the sum of the $N_{n,i}$ values in the ith stage of ionization, we have

$$N_{n,i} = N_{t,i}\frac{g_n}{u_i(T)}\exp(-\chi_n/kT), \quad (2)$$

where $u_i(T)$ is the partition function for the ith ionization stage. The opacity arising at all levels *from this ion* is thus

$$\kappa_i(\lambda) = N_{i,t}\frac{1}{u_i(T)}K\text{fact}. \quad (3)$$

In LTE, this *K* factor is a function only of the temperature and wavelength. Since it is a sum over cross-sections, some of the high-frequency structure for individual levels will be smoothed. One sees primarily the absorption edges and the most pronounced structure, for example the PEC. The algorithm consists of computing this *K* factor over the wavelengths likely to be or relevance, say from 500 to 8000 Å, for a relatively small number of temperatures. It is straightforward to include *all* of the levels in TOPbase, or the RSPs.

The opacities for any given atom or atomic ion are then found from bilinear interpolations in this temperature–wavelength grid.

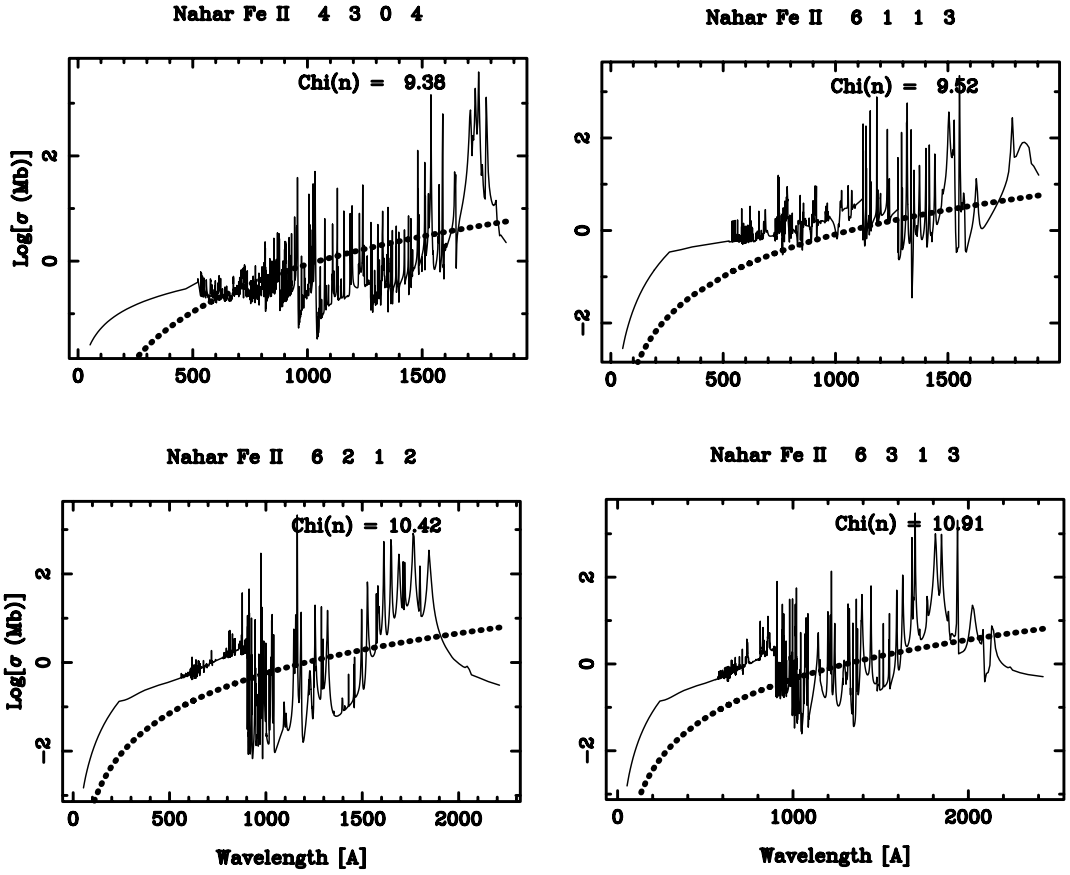

Figure 2. Fe II cross-sections (Nahar & Pradhan 1994) for levels with wide maxima in the region 1700–2000 Å. Hydrogenic cross-sections are shown by the dotted curves. The first three digits at the top of each plot identify the level or term by multiplicity, *L* value, parity (0 = even, 1 = odd). The fourth digit is a sequential number, from low to high excitation, of the term described by the first three digits. For example, 4 3 0 4 describes an even ^{4} F term, that is the fourth such term in order of excitation. In TOPbase, the first three digits are called ISLP and the fourth ILV. Chi(n) is he excitation energy of the level in eV.

We have calculated the K factor at 20-Å intervals, for all species except for Fe I.

With 20-Å sampling, K factors were first obtained for 376 points [(8000-500)/20 + 1]. Then unnecessary points were eliminated wherever 'interior' data could be fitted by linear interpolations from bounding points to within 2 per cent. For example, if the data at λ4020 could be fitted by interpolation between the points at λλ4000 and 4040, the point at λ4020 was dropped. This technique resulted in considerable shortening of the data statements, especially for lower temperatures.

The current routines for Fe I and II are considered provisional, because they have not been resonance-smoothed. The Nahar Fe II photoionization file is some 33 megabytes in size, and contains cross-sections for 745 states (or '*LS* multiplets'). We computed K factors every 20 Å (λλ500–8000) for 8 temperatures (2000–16 000 K). The adopted cross-section at each of the grid wavelengths is an average of the nearest four TOPbase points. We have postponed improving this algorithm until smoothed cross-sections are available. The current Fe II subroutine is some 360 FORTRAN statements, including data statements, comments and commented diagnostics. Comparisons between the K factors for smoothed and unsmoothed cross-sections for lighter species show differences in detail, but not major trends, extending over tens of Å. The feature discussed below is relatively broad.

Fig. 1 shows plots of the K factors for Fe II at 7000 and 12 000 K, based on the Nahar data file. The dotted line shows the resulting 'H factors', that is where the photoionization cross-sections are all assumed hydrogenic (Cowan 1981, equation 18.47). The feature between about 1700 and 2000 Å is notable. We suggest that it arises from core photoexcitations $3d^5 4snl \rightarrow 3d^5 4pnl$ within Fe II. It is important to notice that in these sorts of transitions the outer nl electron acts as spectator and has only little effect on the wavelengths and radiative rates of the core transitions. The related $3d^5 4s \rightarrow 3d^5 4p$ transitions in Fe III give rise to the strong lines in UV multiplets 34, 50, 51, and 52. We have made a further investigation of the nature of the $3d^5 4snl \rightarrow 3d^5 4pnl$ transitions in Fe II using the atomic structure code AUTOSTRUCTURE (Badnell 1986, 1997; Badnell & Pindzol 1989). This code is an extension of the atomic structure program SUPERSTRUCTURE by Eissner, Jones & Nussbaumer (1974). It allows for the calculation of level energies, and radiative and Auger rates within a statistical Thomas–Fermi–Dirac model potential (Eissner & Nussbaumer 1969). Thus, we compute the total of 8988 *LS*-coupling dipole allowed transitions $3d^5 4snl \rightarrow 3d^5 4pnl$ for $5 \leqslant n \leqslant 10$ and $0 \leqslant l \leqslant 3$, with the majority of the $3d^5 4pnl$ states lying above the the first ionization threshold. A little less than half of these transitions, 4090, end up in upper states that can autoionize to Fe III target states. Such transitions manifest themselves as PEC resonances in the close coupling photoionization cross-sections of Nahar & Pradhan (1994). Several of the cross-sections that contribute to the local peak in the 1700–2000 Å region are shown in Fig. 2. The remaining 4898 transitions go to levels that do not autoionize and must be treated as bound–bound transitions. We show a subset of the former lines in Fig. 3. The concentration of transitions in the region 1700–2000 Å is clear.

3 OBSERVATIONS

IUE spectra of iron-rich stars show significant depressions in the wavelength range from roughly 1700–1800 Å, as is shown in the top four panels of Fig. 4. These spectra were downloaded from the url http://archive.stsci.edu/iue/. Because of the high noise level

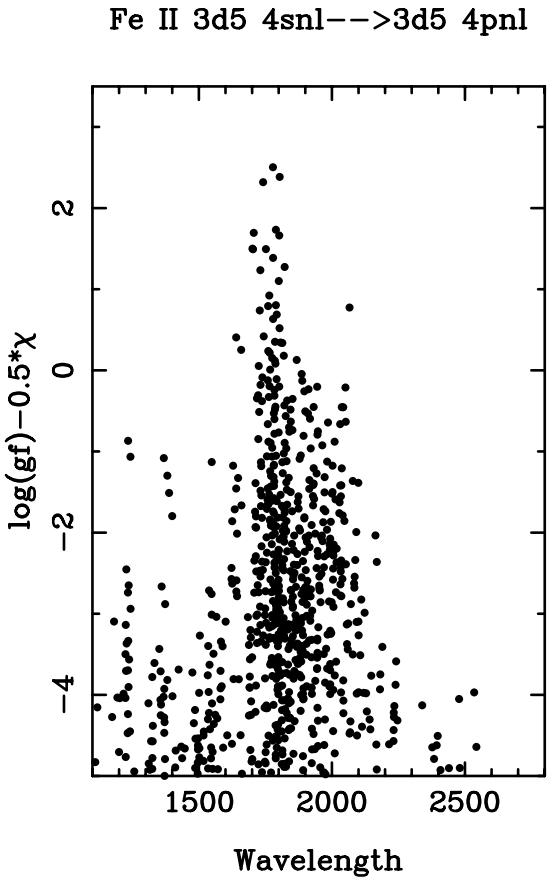

Figure 3. Intensity factors for Fe II lines subject to autoionization. The ordinate, $\log(gf) - 0.5\chi$, is roughly proportional to the logarithm of the strength of an absorption line if saturation did not occur. The logarithmic Boltzmann factor corresponds to $\theta = 5040/T = 0.5$ or 1080 K.

of the spectra, we have chosen to plot only the maxima within 10-Å regions. Complete spectra may be seen at the url cited in the figure. Smith & Dworetsky (1993) report high iron abundances in 112 Her and HR 6000. The magnetic Ap star α^2CVn has long been known to be iron-rich (cf. Cohen 1970), while Muthsam & Cowley (1984) showed HR 6870 (HD 168733) to be quite iron-rich. The stars 87 Psc and 53 Tau are iron-poor (see Smith & Dworetsky 1993), and their spectra lack the strong minima seen in the other four stars.

Lanz et al. (1996) discuss the region on the short-wavelength side of 1600 Å. The interpretation is not straightforward, though the figures shown here are clearly relevant for any interpretation. Note that HR 6000, notorious for its lack of strong Si II lines in ground-based photographic spectra, also lacks the depression short of λ1600 (cf. Andersen, Jaschek & Cowley 1984).

4 APPLICATION TO FE II

Fig. 5 shows calculated spectra in the wavelength region under consideration. The model was based on the adopted parameters of Kochukhov et al. (2002), an effective temperature of 11 600 K and $\log(g) = 3.0$. We also followed these authors in using crude abundances to set the model. We took abundances 0.1 Standard Abundance Distribution (SAD) (Grevesse & Sauval 1998) for elements helium through neon, and 10 SAD for all heavier elements. This was only for the determination of the temperature–pressure structure. A

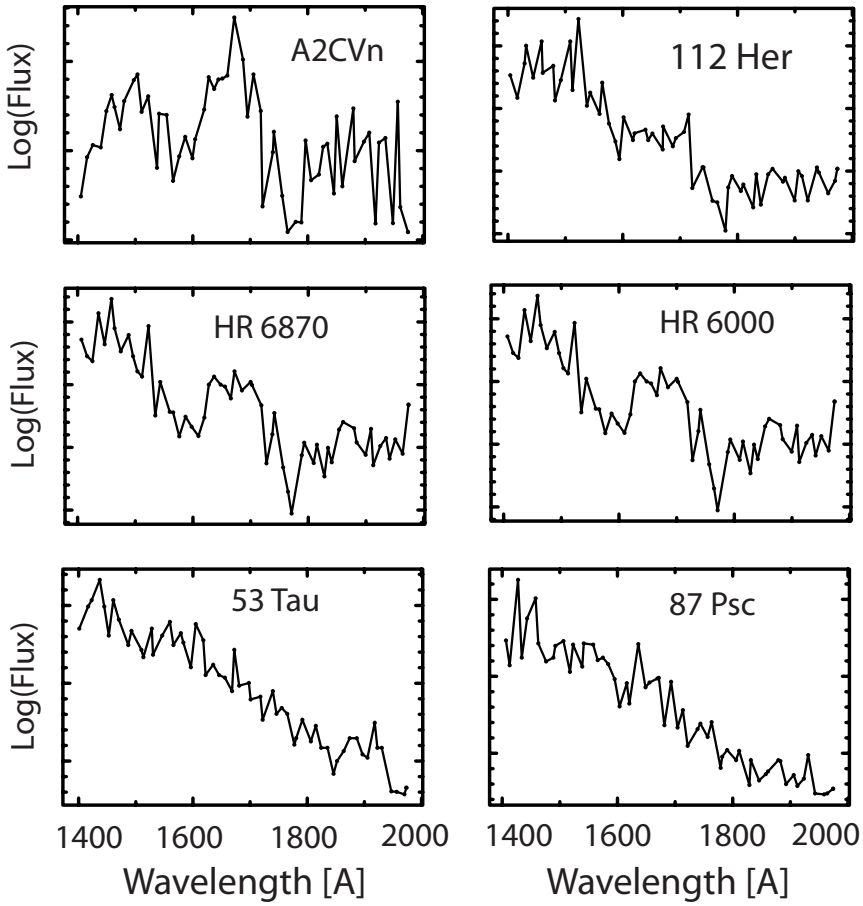

Figure 4. The top four panels are *IUE* spectra of iron-rich stars. The lower two panels show stars with iron deficiencies. Only the highest points within 10-Å intervals are plotted. The original spectra are available on line at http://archive.stsci.edu/iue/.

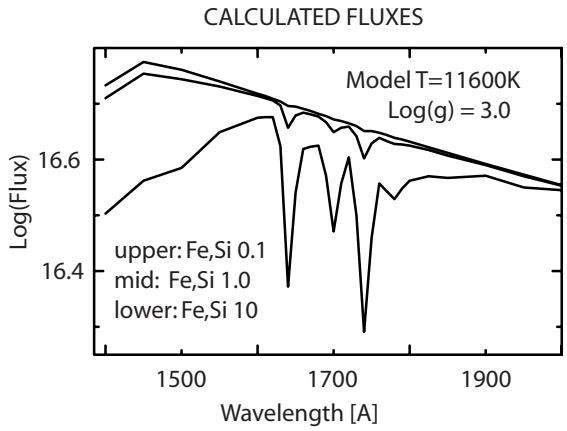

Figure 5. Calculated continuum fluxes for $T_e = 11\,600$ K, and $\log(g) = 3$. The plots, from upper to lower show results for iron and silicon 0.1, 1.0 and 10.0 times solar abundances.

flux-constant model was derived from an Atlas 9 model (Kurucz 1993), but the depth dependence was recalculated using Michigan routines as described in earlier papers (cf. Cowley 1996), except that our opacity routines now incorporate TOPbase data for the species enumerated above.

The three curves were all based on the same $T(\tau)$, though a new pressure structure was calculated based on the different iron and silicon abundances. Thus, the flux is not strictly constant in the models without the enhanced abundances. We do not consider this significant in the present exploratory calculations. The three curves shown are for iron and silicon enhanced by a factor of 10 (lower), solar (middle), and depleted by a factor of 10 (upper). All elements other than iron and silicon were assumed to have the same abundances used in the Atlas9 model.

The calculations show clearly that the Fe II continuum is significant in this region. Of the three calculated minima, the one at the shortest wavelength (about λ1640) is not well matched to the observations. It is certainly Fe II and not Si, as a separate calculation (not shown) has revealed. There is a possibly corresponding feature to be seen in the spectra of α^2CVn and HR 6000, though much weaker than in the calculations. This region deserves further study.

The two longer-wavelength minima, at approximately λλ1700 and 1740, fit the observations of the iron-rich spectra reasonably well. There is a small discrepancy in the wavelengths; the calculated minima are some 20 to 30 Å short of the stellar minima. However, these discrepancies are 2 per cent or less, well within the accuracy with which energy levels in Fe II were calculated (cf. Nahar & Pradhan, op. cit. Table 1).

5 CONCLUSIONS

Some of the absorption in the region λλ1700–2000 of the spectra shown in Fig. 4 will result from the strong transitions

in Fe II as well as the multiplets mentioned above in Fe III. However, we show here that a measurable contribution to the depression must result from the specific shapes of the Fe II photoionization cross-sections. Note that the lowest of the levels shown in Fig. 2, at 9.38 eV, is the 76th level above ground. Any attempt to treat higher levels in Fe II by a hydrogenic approximation or simple parametrization would miss the relevant structure.

A number of loose ends need to be tidied before our metal opacity routines can be considered satisfactory. We need smoothed cross-sections for Fe I and II, as well as other heavy species, such as Mn I and II or Co I and II that can be relevant for special stars. It is also necessary to make sure that the partition functions used with the TOPbase/Iron Project cross-sections are compatible with those levels. Provisional spot checks for a few spectra show that this is not likely to be a serious problem, as the calculated levels are usually within a few per cent of the laboratory values. Line opacity was not relevant for the current calculations. Eventually, we must consider the overlap between the TOPbase 'resonances' and predicted lines in the Kurucz data base.

These are matters for future contributions.

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