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I. Hubeny, D. Mihalas, and K. Werner

Handling of Atomic Data

Thomas Rauch

Dr. Remeis-Sternwarte Bamberg, Sternwartstraße 7, 96049 Bamberg, Germany; Institut für Astronomie und Astrophysik, Sand 1, 72076 Tübingen, Germany

Jochen L. Deetjen

Institut für Astronomie und Astrophysik, Sand 1, 72076 Tübingen, Germany

Abstract. State-of-the-art NLTE model-atmosphere codes have arrived at a high level of numerical sophistication and are now useful tools to analyze high-quality spectra from the infrared to the X-ray wavelength range. The capacity of current computers permit calculations which include line spectra from all elements from hydrogen up to the iron group. The lack of reliable atomic data has become a critical problem for further progress.

We summarize available sources of atomic data, and discuss how these are implemented in the Tübingen Model-Atmosphere Package TMAP. We describe our Iron Opacity Interface IrOnIc which is used to calculate opacities of iron-group elements from Kurucz's and the Opacity Project's data.

We propose general use of the Tübingen Model-Atom Database TMAD, which would allow an easy exchange of ready-to-use model atoms between all model-atmosphere groups. The comparison of model-atmosphere calculations would then be much easier, and would save a great deal of manpower that is presently consumed preparing suitable model atoms for spectral analyses.

1. Introduction

In the early 80's of the last century, the implementation of approximate lambda-operators (ALO, leading to "accelerated lambda iteration", ALI) in the NLTE model-atmosphere codes at Kiel by Werner & Husfeld (1985) and Werner (1986) provided an efficient method to calculate synthetic stellar spectra of hot stars. Together with the access to the fourth CRAY computer (a CRAY-1 M) in Germany (at the Konrad-Zuse-Zentrum für Informationstechnik Berlin), which was installed in February 1984, powerful tools for spectral analysis of hot star spectra were developed. At the end of 1987, the Rechenzentrum der Universität Kiel installed a CRAY X-MP. Access to this machine (in the framework of the Norddeutscher Vektorrechner-Verbund) and the following, even more powerful, CRAY computers, made all our efforts possible.

The first of our NLTE codes, HYMOC (HYDrogen MOdel-atmosphere Code) (Werner 1986), was able to calculate only pure-hydrogen model atmospheres. However, inasmuch as the atomic data for hydrogen are well known, it was an ideal tool to investigate the numerical approximations, and limitations to the size of model atoms, used in earlier calculations, which were necessary before the ALI method was developed (Rauch & Werner 1988).

The next code PRO2 (PROgram no. 2) (Werner 1988; Werner & Dreizler 1999) is much more flexible, and is able to take into account all elements up to the iron group (Dreizler & Werner 1993; Rauch 1997). It has been used successfully for the analysis of hot stars (e.g. Rauch & Werner 1991; Rauch 1993; Rauch 2000). Our NLTE group moved from Bamberg (1993) and Potsdam (1995) to Tübingen (since 1996) where TMAP, the state-of-the-art Tübingen Model Atmosphere Package was created. With the newly developed IrOnIc code (§4), it was possible to calculate an extended grid of realistic stellar fluxes from models which take into account the opacities from H – Ni (Rauch & Deetjen 2001). These models are plane-parallel, in hydrostatic and radiative equilibrium, have 350 atomic levels which are treated in NLTE, about 1,000 individual lines from H - Ca, and millions of lines from the iron-group elements.

The state of the field of spectral-analysis of hot stars has completely changed within the last two decades. At the beginning of the 80's, the main obstacles were insufficient numerical methods and computational capacities. Rauch & Werner (1991) have shown the enormous progress which came with the ALI method, with examples of very detailed H + He + C + N models in contrast to "classical" H + He models. At present, the lack of reliable atomic data for metals, line-broadening tables, etc. set undesirable limits to highly-developed NLTE codes. This lack often hampers an adequate analysis e.g. of high-resolution UV spectra provided by the STIS (Space Telescope Imaging Spectrograph) aboard the Hubble Space Telescope (HST) or by the Far Ultraviolet Spectroscopic Explorer (FUSE).

2. Sources of Atomic Data

For the elements H, He, C, N, and O, we use standard sources such as Bashkin & Stoner (1975, 1978) and Moore (1959, 1971), for energy levels, Wiese et al. (1966, 1969) for transition probabilities, and input-data (mainly for C, N, and O) compiled for the program DETAIL (K. Butler, Munich, private communication). Most of the data can also be found e.g.

in the National Institute of Standards and Technology (NIST) Atomic Spectra Database
at `http://physics.nist.gov/cgi-bin/AtData/main_asd`,

in the Vienna Atomic Line Database (VALD) database
at `http://www.astro.uu.se/~vald`,

in The Atomic Line List of Peter van Hoof
at `http://www.pa.uky.edu/~peter/atomic/`,

or in the Kurucz Atomic Line Database
at `http://cfa-www.harvard.edu/amdata/ampdata/kurucz23/sekur.html`.

We wish to call attention to the compilation of Wiese, Fuhr, & Deters (1996) who show the difficulties in judging the quality of atomic data for C, N, and O.

For the elements F – Ca we use mainly data provided by the Opacity Project (§2.1). For the iron-group elements, we use both the Kurucz's lists (1993) and OP data. A. K. Pradhan provides atomic data, and links to related data and some review papers, e.g. Pradhan & Peng (1995)

at `http://www.astronomy.ohio-state.edu/~pradhan`.

2.1. Opacity Project Data

In the framework of the OP (Seaton 1987), opacities for stellar envelopes were calculated during 1987 – 1994. The OP work is documented in about 50 publications (`http://heasarc.gsfc.nasa.gov/topbase/publi.html`), e.g. 20 alone in J. Phys. B. A "final report" was given by Seaton et al. (1994). The aim of the OP was to provide *access to a complete and accurate dataset*, consisting of energies, photoionization cross-sections, and oscillator strengths.

TOPBASE (`http://heasarc.gsfc.nasa.gov/topbase/topbase.html`), the OP on-line atomic database, provides data for elements with $Z \in \{1-14, 16, 18, 20, 26\}$, and ions with $N_\mathrm{e} \in \{1-26\}$. Energy levels, hence transitions are complete for orbital quantum numbers $l \in \{\mathrm{s, p, d, f}\}$. Because the level energies calculated by the OP are slightly different from laboratory measurements (e.g. Werner & Rauch 1994), we replace them by Bashkin & Stoner (1975, 1978) values, if available.

A detailed investigation of OP photoionization cross-sections ($\sigma_\mathrm{bf}^\mathrm{OP}$) was made by Rauch (1997). The impact of $\sigma_\mathrm{bf}^\mathrm{OP}$ is significant, and I recommend use of the OP data. In our application, the OP data is interpolated by PRO2 to the frequency grid used. It is not necessary to use a very fine grid in the model-atmosphere calculation (see §5) in order to resolve the resonances in $\sigma_\mathrm{bf}^\mathrm{OP}$ – because of the energy-level uncertainty (see above), these are not at the correct wavelengths anyway. However, they contribute to the transition rates $R_{ij} \sim \int_0^\infty (J_\nu \sigma_{ij}/h\nu) d\nu$ and one has to be aware that they are then neglected there. In the event we have replaced the threshold energy, $\sigma_\mathrm{bf}^\mathrm{OP}$ is shifted accordingly.

Because an extrapolation of OP bound-free data into the high-energy range may result in negative cross-sections, PRO2 estimates the slope of the cross-section and, if necessary, replaces it by an approximation based on Seaton's formula (1962)

$$\sigma_\nu = \sigma_0 \left(\frac{\nu_\mathrm{th}}{\nu}\right)^s \left[\alpha + (1-\alpha)\frac{\nu_\mathrm{th}}{\nu}\right] \tag{1}$$

using $\alpha = 1$, and $s = 3$. σ_0 is then estimated from the last available OP data points. Setting negative cross-sections to zero might result in an arbitrary emission bump in what possibly has become an "opacity-poor" high-energy range of the synthetic spectrum.

2.2. Iron Project data

The Iron Project (IP, Nahar, these proceedings) has the goal of computing, on a large scale, electron-excitation cross-sections and rates of astrophysical and technological importance, using the most reliable procedures currently available (`http://www.usm.uni-muenchen.de/people/ip/iron-project.html`). The IP data will be available in TIPTOPBASE in the near future. The energy levels are much more accurate than those of the OP data. Thus we plan to use these data as soon as possible.

3. Hydrogen and Helium

Because of the limits of the accuracy of the numerical methods and computers presently available, the number of levels which can be treated simultaneously in NLTE by PRO2 is limited ($\lesssim$ 350). Thus, for every ion some (lower) NLTE and some (higher) LTE levels must be selected. For example, in the case of hydrogen a "classical" cutoff at a total number of 16 levels was used by Auer & Mihalas (1969). Rauch & Werner (1988) found that in the case of H I, eight NLTE levels yield an accuracy better than 1% in the emergent flux. A more accurate approach which eliminates the necessity of this cutoff has been presented by Hubeny et al. (1994). They generalized the occupation-probability formalism (HMF) of Hummer & Mihalas (1988) to NLTE conditions. Using exact partition functions, they have shown that the number of levels is not an indicator of the accuracy of a model. We generally use the HMF for hydrogen and helium (Werner 1996). For other species it is used in an approximate way as well.

A crucial point in model-atmosphere calculation are the collisional rates — even in the case of H I and He II, where atomic data are known much better compared to all other atoms/ions. For the collisional excitation rates of H I, we follow Sampson & Golden (1970, and references therein) and Mihalas (1972)

$$C_{ij} = 4\pi a_0^2 \sqrt{\frac{8k}{\pi m_e}}\, n_e\, T^{1/2} \left(\frac{E_H}{h\nu_{ij}}\right)^2 f_{ij}\, u_0 \left[E_1(u_0) + 0.148\, u_0 E_5(u_0) \right] \gamma \qquad (2)$$

Here f_{ij} is the optical oscillator strength of the transition $i \rightarrow j$, E_H is the ionization energy of hydrogen, $u_0 \equiv h\nu_{ij}/kT, \gamma \equiv \beta + 2(\alpha - \beta)/\Delta n$ where $\beta = 3 - 1.2/n_i, \quad \alpha = 1.8 - 0.4/n_i^2$ if $\Delta n > 1$, and $\gamma = 1$ otherwise. Mihalas (1967) remarked "Clearly the cross-sections we have chosen are very approximate, and we eagerly await better values from theory and experiment." for this formula. A detailed comparison with more recent data (e.g. Jones, Madison, & Srivastava 1991) remains to be done. The collisional excitation rates of helium are calculated by formulae of Mihalas & Stone (1968). The He I formulae that are used by PRO2 are summarized in Werner, Rauch, & Dreizler (2001). For He II we use

$$C_{ij} = \pi a_0^2 \sqrt{\frac{8k}{\pi m_e}}\, n_e\, T^{1/2} \left(\frac{E_H}{h\nu_{ij}}\right)^2 f_{ij}\, u_0\, e \left[\ln 2\, e^{-u_0} + E_1(u_0) \right] \gamma \qquad (3)$$

with $\gamma = \min(n_i, 1.1) \times \min[\,\Delta n, n_i - (n_i - 1)/\Delta n\,]$ (Mihalas 1972). Mihalas & Stone (1968) stated that "Naturally these expressions are only first approximations, but certainly they are right to order of magnitude.". As in the case of hydrogen, Jones, Madison, & Srivastava (1991) have published new data.

To summarize, model-atmosphere calculations are lacking reliable collisional data. While for hydrogen and helium at least approximate formulae are available, the situation for most metals is worse. If the optical oscillator strength of a transition is known, we use the van Regemorter formula (§4.4). If it is unknown, we use a formula given by Butler (`http://ccp7.dur.ac.uk/Docs/detail.ps`).

$$C_{ij} = \pi a_0^2 \sqrt{\frac{8k}{\pi m_e}}\, n_e\, T^{1/2}\,(1+u_0)e^{-u_0}. \tag{4}$$

4. IrOnIc

The Iron Opacity Interface IrOnIc allows one to create line cross-sections and model-atom files for iron-group elements, i.e. Ca to Zn. The aim of IrOnIc is to prepare radiative bound-bound (RBB), radiative bound-free (RBF), collisional bound-bound (CBB), and collisional bound-free (RBF) cross-sections (CS) as input for pro2.

A detailed consideration of all atomic line transitions, known from experiment or theoretical calculations would be impossible. The large number of levels would exceed both the computational power, and overwhelm the numerical methods for model-atmosphere calculations, available at the moment. Blanketing by millions of lines from the iron-group elements arising from transitions between some 10^5 levels can be attacked only with statistical methods.

4.1. The Basic Concept

The basic concept for achieving this goal is to combine all energy levels of one (model) ion into typically 6 – 20 energy bands (Haas 1997, Fig. 1). Whereby one can distinguish between levels with even and with odd parity. This reduces the number of levels dramatically, without losing too much information about the physics of the system (Anderson 1989; Anderson & Grigsby 1991). Each of these bands is then treated as a single NLTE level with a suitably averaged energy E_L and statistical weight G_L, which are computed from the individual levels within a particular band (Eq. 5–7). An atom whose level structure is simplified in this way is called a model atom.

$$E_L = \sum_{l \epsilon L} E_l\, g_l^* \Big/ \sum_{l\,\epsilon\, L} g_l^*\,, \tag{5}$$

$$G_L = e^{E_L/kT^*} \times \sum_{l\,\epsilon\, L} g_l^*, \tag{6}$$

$$g_l^* = a_s\, g_l\, e^{-E_l/kT^*}. \tag{7}$$

E_l and g_l are the energy and the statistical weight of a real atomic level l. L indicates a particular superlevel. T^* is a typical temperature, pre-chosen and fixed, given by the Saha ionization equilibrium, where the particular ionization stage dominates. The basic assumption here is that all individual levels within one band have the same NLTE departure coefficient.

Additionally, IrOnIc permits one to combine several chemical species into one generic model atom. A "generic model atom" means it appears to be one atom with several bands, but contains the co-added cross-sections of all species included in it. The contribution of the individual species to the total result is determined by their abundances a_s with respect to the dominant atom (e.g. Fe/Fe

= 1 and Ni/Fe = 0.5 etc.). Furthermore, IrOnIc allows one to generate a combined model atom. That means that one combines several model atoms for different elements. All calculations must be done on one common frequency grid.

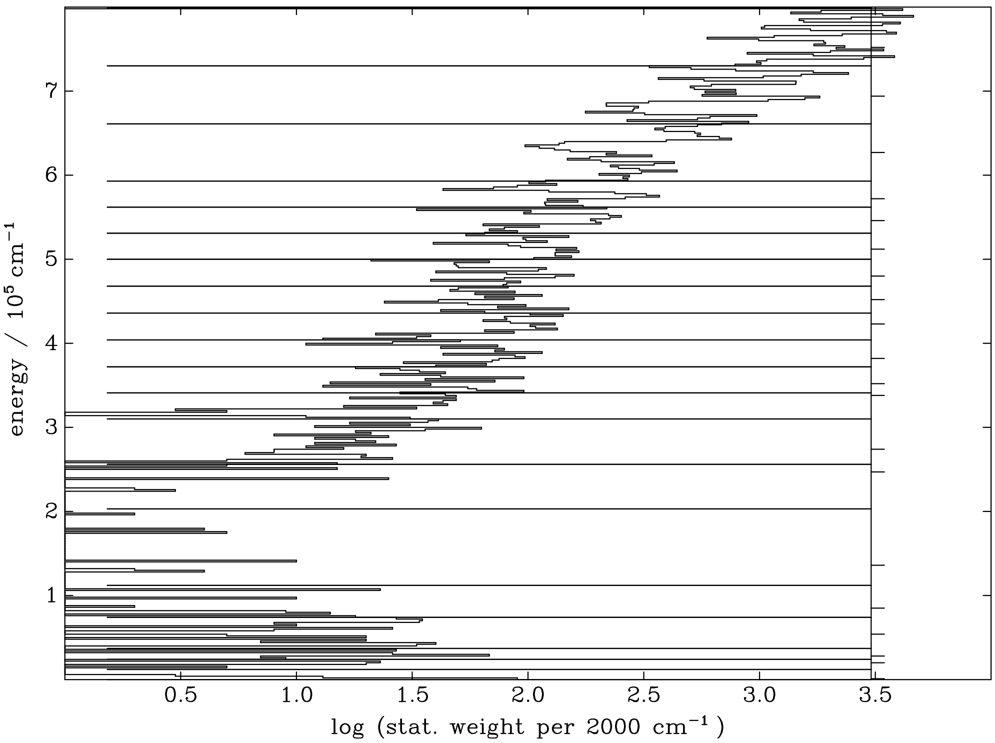

Figure 1. Energy distribution of statistical weights of the iron-group elements in ionization stage VI. Individual energy levels are grouped here into 20 bands (interval limits are indicated by horizontal lines) and merged into superlevels with an average energy (indicated by small tick marks at right hand side).

4.2. The Atomic data

Understanding the properties of model atoms and generic cross-sections requires knowledge about the basic properties of the individual atoms. The calculation of energy levels and transition probabilities by Kurucz (1993) and Seaton et al. (1994) are the most important sources of atomic data for our calculations. Nevertheless IrOnIc has a flexible interface, which, in principle, can handle all kinds of atomic data sources.

4.3. Calculation of the RBB cross-sections

The cross-section for a transition between two superlevels must be composed of the individual cross-sections between levels in the upper and in the lower band. This can't be done by co-adding all the individual oscillator-strengths f_{lu} into one "super-oscillator-strength", because this would result in only one unrealis-

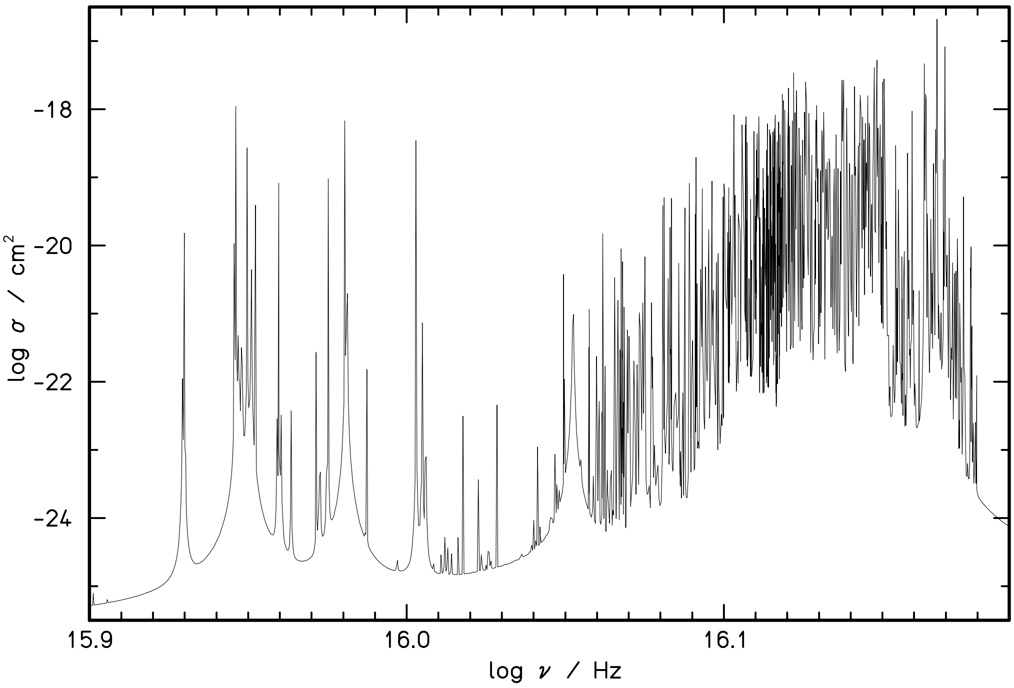

Figure 2. Example of the band-band cross-section of ionization stage VI in a generic model atom which includes all iron-group elements. 2,289 individual lines between two superlevels are co-added to form a complex photon cross-section which is sampled in 1,913 frequency points.

tically strong "superline". Therefore the frequency-dependent cross-sections of all individual lines are co-added in order to guarantee that each individual line core is considered at the correct frequency position:

$$\sigma_{LU} = \frac{\pi e^2}{m_e c} \sum_{(l\,\epsilon\, L;\, u\,\epsilon\, U)} g_l^* f_{lu}\, \phi(\nu_{lu} - \nu) \Bigg/ \sum_{l\,\epsilon\, L} g_l^* \,. \tag{8}$$

$\pi e^2/m_e c$ is the cross-section of a classical oscillator and ϕ is the normalized line-profile of the individual lines. The shape of the profile function is a Voigt profile with its width determined by various broadening mechanisms: natural line broadening, Doppler broadening, and Stark broadening. For the iron-lines the quadratic Stark effect is of importance. It describes the interaction between ions and electrons. According to Cowley (1971), the resulting broadening of the individual lines is approximately given by:

$$\gamma_{Stark} = 5.5 \times 10^{-5}\, \frac{n_e}{\sqrt{T}} \left[\frac{(n_{\rm eff}^{\rm up})^2}{z+1} \right]^2 . \tag{9}$$

Where $n_{\rm eff}^{\rm up}$ is the effective principal quantum number of the upper level, and z is the effective charge seen by the active electron. Because the iron-group cross-sections must be calculated in advance, the electron density and the temperature within the atmosphere cannot be used here. Therefore we calculate the broadening of the line, according to Rauch & Werner (1988), with a fixed temperature $T_{\rm line} = 3/4 \times T_{\rm eff}$. The variation of the electron density within an atmosphere is taken into account, by calculating γ_{Stark} for two different electron densities: namely 0 and 10^{16} electrons/cm^3. Because the Stark wings of the lines depend linearly on electron density, the values of γ_{Stark} for other electron densities can be interpolated linearly by Pro2.

In analogy to the inter-band cross-section σ_{LU} an intra-band cross-section σ_{LL} can be defined:

$$\sigma_{LL} = \frac{\pi e^2}{m_e c} \sum_{(l \,\epsilon\, L;\, l' \,\epsilon\, L} g_l^* f_{l\,l'} \phi(\nu_{l\,l'} - \nu) \Bigg/ \sum_{l \,\epsilon\, L} g_l^* \tag{10}$$

These cross-sections are used as additional background-opacities in the radiation-transport equation. This type of transition does not occur when the individual energy bands include levels of the same parity only.

The resulting RBB transitions σ_{LU} and σ_{LL} show a complex, frequency-dependent cross-section. An example of σ_{LU} is shown in Fig. 2.

4.4. The calculation of the CBB, RBF, and CBF cross-sections

The CBB cross-sections are calculated with the formula of van Regemorter (1962). For allowed dipole transitions we use

$$C_{ij} = \pi a_0^2 \sqrt{\frac{8k}{\pi m_e}}\, n_e \sqrt{T} \left[14.5 f_{ij} \left(\frac{E_H}{E_0} \right)^2 \right] u_0 e^{-u_0} \Gamma(u_0) \tag{11}$$

where $u_0 \equiv h\nu_{ij}/kT, E_0 = h\nu_{ij}, \Gamma(u_0) = \max\left[\bar{g},\, 0.276\, e^{u_0}\, E_1(u_0)\right]$, and $\bar{g} = 0.2$ for $n' \neq n$, otherwise $\bar{g} = 0.7$. $E_{\rm H}$ is the ionization energy of the hydrogen ground state. A generalized version of this formula in employed for collisions between bands of iron-group atoms (Werner & Dreizler 1999). Forbidden CBB transitions are calculated following Butler (`http://ccp7.dur.ac.uk/Docs/detail.ps`):

$$C_{ij} = \frac{8.631 \times 10^{-6}\, n_e\, e^{-u_0}\, \Omega}{g_i \sqrt{T}} \tag{12}$$

where

$$\Omega \equiv \sum_{i=1}^{\rm NFIT} a_i\, x^{i-1} \tag{13}$$

The fit parameters a_1, ..., $a_{\rm NFIT}$ for the *effective collision strength* are input parameters, $x = \log T - T_1$.

The RBF cross-section are treated in various manners. For iron and calcium detailed calculated data of the Opacity Project (The Opacity Project Team, 1995, 1997) are available. For the rest of the iron-group elements hydrogenic cross-sections are used. For the CBF cross-sections no calculated data exist for the iron group. Therefore they have to be estimated using the average RBF cross-section and the Seaton (1962) formula.

The number of frequency points can be reduced by a factor of 1,000 by using the statistical approach of the opacity sampling method. This method has been described by Peytremann (1974) for LTE atmospheres. Anderson (1991) and Dreizler & Werner (1992) then used this idea for the calculation of iron-group cross-sections. This Ansatz guarantees that the number of NLTE levels and frequency points required for model-atmosphere calculations is reduced by several orders of magnitude. For example a typical iron model atom (Fe IV – VI) is represented by 22 NLTE levels, which are calculated from 16,000 individual levels, and 83 superlines which are calculated from 2,200,000 individual lines.

For a direct comparison between observed and calculated spectra, however, a subsequent calculation of a formal solution with a sufficiently fine frequency grid is mandatory.

5. Model Atmospheres and Synthetic Spectra

The PRO2 NLTE model atmospheres are calculated in the most efficient way with very detailed model atoms (Rauch 1997), consideration of HMF, and Stark line broadening (Werner 1996; Rauch 2000). Moreover, it is sufficient to treat linear Stark effect by approximate formulae (Unsöld 1968; Werner, Heber, & Hunger 1991)

$$\kappa(\Delta\lambda) = \frac{\pi e^2}{mc^2}\lambda^2 f \frac{1}{s_n^* F_0} U\left(\frac{\Delta\lambda}{s_n^* F_0}\right) \tag{14}$$

with the microfield

$$F_0 = 2.61e\left[\sum_{\text{ions}} z_i^{3/2} n_i\right]^{2/3}. \tag{15}$$

$U(\beta)$ is given by van Dien (1949). $s_n = 0.0192\lambda^2[\,n_{\rm up}(n_{\rm up}-1)+n_{\rm low}(n_{\rm low}-1)\,]/Z$ is a measure of the width of the Stark pattern.

However, for the subsequent calculation of synthetic spectra even more detailed model atoms (including fine-structure splitting) and a finer frequency grid are necessary. Stark-broadening tables calculated for H I by Lemke (1997) and for He II by Schöning & Butler (1989), based upon VCS theory (Vidal, Cooper, & Smith 1973) need to be used. For some metal ions, broadening tables are published e.g. by Dimitrijević, Sahal-Bréchot, and others; check e.g. `http://adsabs.harvard.edu/abstract_service.html` for many references. For fine-structure splitting, we use the energies given by Bashkin & Stoner (1975, 1978). For the calculation of oscillator strengths for the respective transitions, we follow Kuhn (1969).

6. A Database of Ready-To-Use Model Atoms

When we started to work on this talk, we thought about the total time that we have spent since 1986 in the search, collection, and evaluation of atomic data, followed by the construction of model atoms and their extensive testing in model-atmosphere calculations. Because the observational techniques have improved tremendously in this time frame, and satellites such as FUSE and XMM-NEWTON provide spectra of superb quality in the high-energy range, the work on our model atoms continues steadily. We estimate that at least five man-years have been used for this purpose — in our group alone. Similar work has surely been done in all other model-atmosphere groups. Unfortunately, there is no standard format yet for the model atoms. This fact makes it difficult to compare results of model-atmosphere calculations from two different codes because the atomic data-file cannot be exchanged. Moreover, it appears to be both an enormous waste of man-power and a source of uncertainty. An attempt to concentrate on the construction of model atoms in a standard format, and collect these in a "database" which will be accessible via WWW (`http://astro.uni-tuebingen.de/~rauch/ModelAtoms_ready2use.html`) would be major progress in this field. Consequently, we propose such a database, henceforth called the Tübingen Model-Atom Database (TMAD), with a standard ASCII format which is adopted from our PRO2 format (§4.1). Creators of model atoms in the format required by the database may add their files. They must be accompanied by a description, which indicates the relevant parameter range (effective temperature, surface gravity), and references, where the model atoms have been used in spectral analyses.

6.1. Description of the pro2 Atomic Data Files

PRO2 expects an atomic-data file, which contains model atoms with atomic data, or file names of atomic data. It is first created by the user and then processed by an auxiliary program which partly checks the file for consistency. A few keywords (Table 1) are used to indicate different sections of the atomic data file (every section is closed by a single "`0`" in the first column of a line).

Table 1. Keywords in a PRO2 atomic data file

Keyword	Meaning	
`ATOM`	Introduces a new element. Its ions in increasing order follow. The subsequent line indicates the chemical abbreviation (`FORMAT A2`), the charge of the lowest ionization stage (in e^-) in the model atom, and the atomic weight (in AMU).	
`L`	NLTE levels	
`LTE`	LTE levels	
`RBB`	radiative	bound-bound transitions
`RBF`	radiative	bound-free transitions
`RDI`	radiative	di-electronic transitions
`RFF`	radiative	free-free transitions
`RLL`	"sample"	bound-bound (within one band)
`RLU`	"sample"	bound-bound (between two bands)
`CBB`	collisional	bound-bound transitions
`CBF`	collisional	bound-free transitions
`CBX`	collisional	bound-bound transitions (NLTE to LTE levels)

PRO2 level names are encoded in a 10-character string. This is a reminder of the early 80's when we had to punch FORTRAN cards and wanted to keep all information about one level on one card, i.e. we could use only 66 characters.

Table 2. Example of a hydrogen model atom. Note that level energies are given in frequency units and cross-sections in cm^2.

```
ATOM
H  0  1.008
L
H11       H21        3.2880912929E+15 2
H12       H21        8.2202193884E+14 8
0
LTE
H13       H21        3.6534150835E+14 18
0
RBB
H11       H12        1 1 4.1620E-01
0
RBF
H11       H21        1 3 7.91857E-18 1.  3.
H12       H21        1 3 1.58372E-17 1.  3.
0
RFF
H1                   2 0
CBB
H11       H21        1 0
0
CBF
H11       H21        1 0
H12       H21        1 0
0
CBX
H11       H13        3 0
H12       H13        3 0
0
L
H21       NONE       0.0000000000E+00 1
0
```

For "simple" elements this number was enough; but in the meantime we have realized that a 40-character string for the level-names would be much more convenient, for example:

`MG07␣1s22s2p2␣␣␣␣␣␣␣␣␣␣␣␣2DE␣3s␣1DO␣␣3/2`

allows one to identify unambiguously the element, ion, core- and valence-electron configuration, parity, and quantum numbers. Presently the rudimentary designation `MG73S'␣1D␣` is used.

A detailed description of this data format and of the formulae which are used for the transitions is given in the PRO2 User's Guide (Werner, Rauch, & Dreizler 2001). For all levels, the form for a general entry is:

`Level     Parent` E G

with the names of the level and its parent level (ground state of the next ionization stage), the ionization energy E (given in Hz), and the statistical weight G of the level. For all transitions, the form for a general entry is

$\mathtt{Level_l} \quad \mathtt{Level_u} \quad n_{\mathtt{form}}\ n_{\mathtt{dat}}\ \mathtt{P_1}\ \ldots\ \mathtt{P_{n_{dat}}}$

with the names of the lower ($\mathrm{Level}_{\mathtt{l}}$) and upper ($\mathrm{Level}_{\mathtt{u}}$) level, the number $n_{\mathtt{form}}$ of the formula which is used to calculate the cross-section, the number $n_{\mathtt{dat}}$ of input parameters that follow, and the input parameters, respectively. In the case of "sample" cross-sections, these are read in from data files which have been produced by IrOnIc (§4). A very simple model atom for hydrogen which can be used to calculate a (not very realistic) model atmosphere is shown in Table 2.

7. Conclusions

Present NLTE model-atmosphere codes have reached a very high level of sophistication. Now, strong efforts to achieve adequate atomic data must be continued in order to be able to analyze reliably the high-quality spectra which are already available from the infrared to the X-ray range. *Everyone who is calculating stellar atmospheres should be aware of the important role that atomic data plays, because one thing is for sure – even if you use a perfect code, if you put rubbish in, you will get rubbish out.*

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