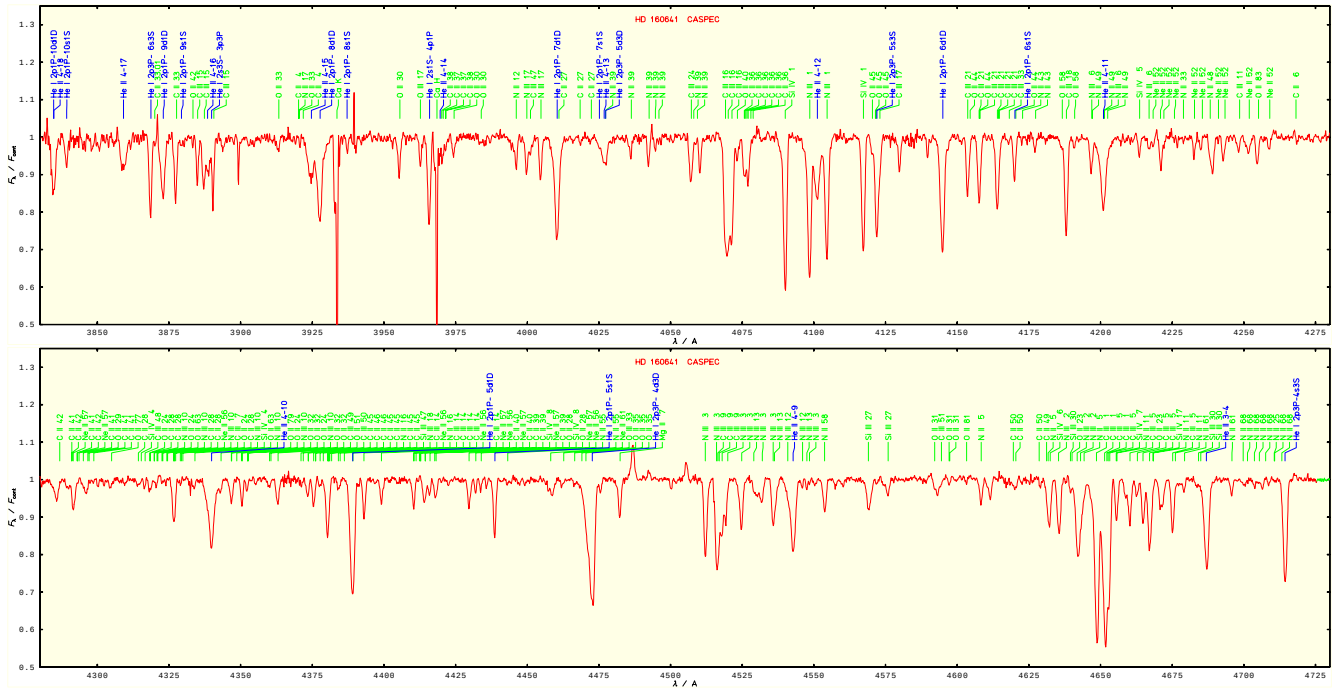

A User's Guide to the

Tübingen NLTE Model-Atmosphere Package

TMAP

ATOMS2

SETF2

LTE2

PRO2

LINE1

LINE1_PROF

and some Auxiliaries

T. Rauch, K. Werner, et al.

A User's Guide to the Tübingen NLTE Model-Atmosphere Package

TMAP

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Contents

List of Tables

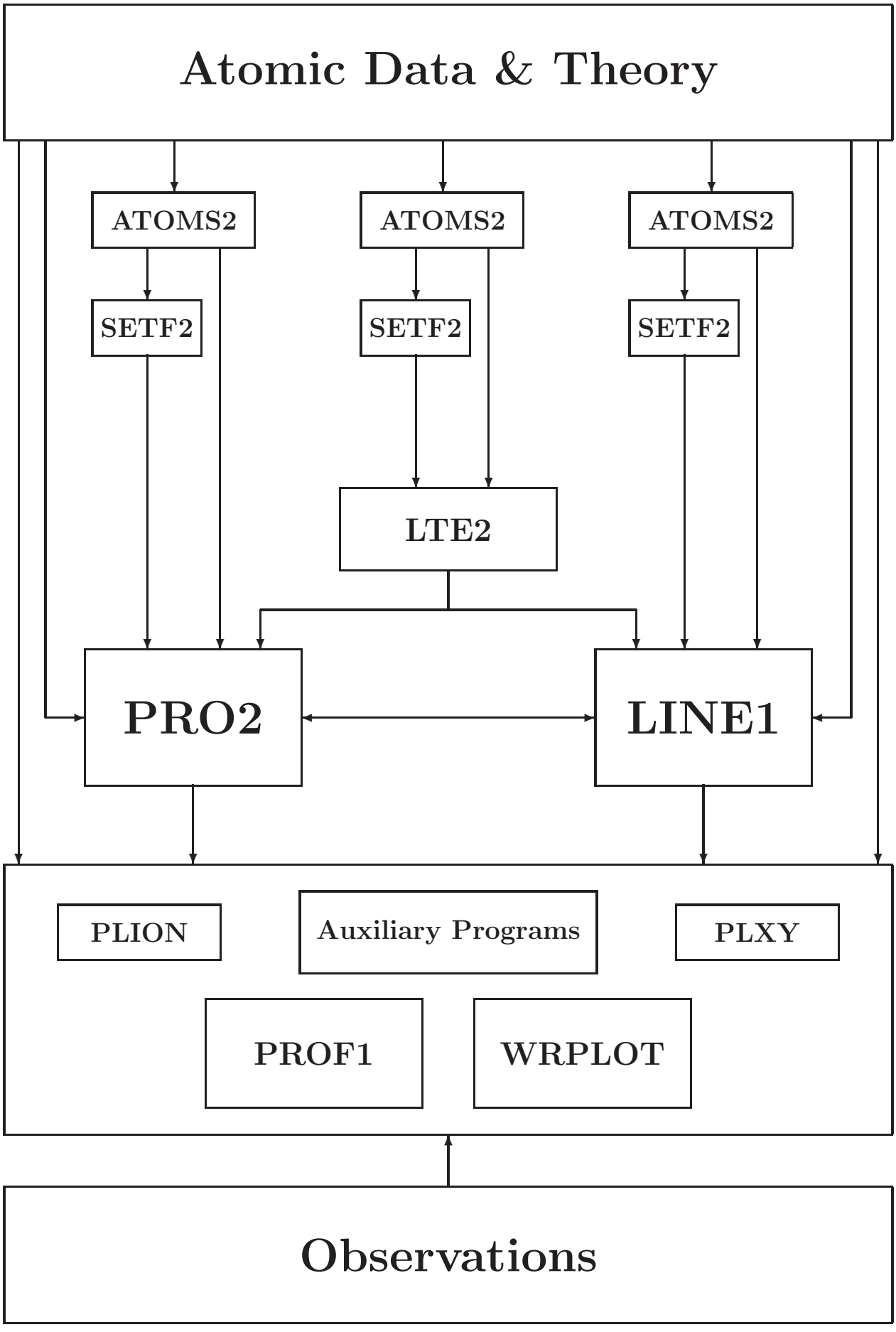
All Users of the Tübingen NLTE Model-Atmosphere Package are reminded to be careful at the creation and / or modification of the atomic data files.

Although *ATOMS2*, *SETF2*, *PRO2*, and *LINE1* check these files partly for consistency, small errors here can have large influence on the resulting model atmospheres.

All programs terminate in the case of fatal errors but can give only warnings when the input is ambiguous. The neglection of these warnings may be fatal!

For *PRO2* and *LINE1* output options are existing to print the model atoms and atomic data read by these programs. They should be used for checks — not only at the first time when the program is running with new or modified data!

Data flow


Atomic Data & Theory
ATOMS2
ATOMS2
ATOMS2
SETF2
SETF2
SETF2
LTE2
PRO2
LINE1
PLION
Auxiliary Programs
PLXY
PROF1
WRPLOT
Observations

0 Overview

In the following the Tübingen NLTE Model-Atmosphere Package (*TMAP*)is described, which is based on the approximated lambda iteration (ALI) method. It consists mainly out of a "LTE" model atmosphere program (*LTE2*) for the calculation of start models, a NLTE program (*PRO2*), a NLTE line formation program (*LINE1*) and a plot program (*PROF1*). To start the programs you need the following:

1. an executable *program* of the most recent program version. Details can be found in Sect. 1.
2. a *model atom file* with all model atoms and atomic data. This file is created by the user and partly checked and automatically filled up by the program *ATOMS2* (Sect. 2).
3. a *frequency grid file,* which contains the frequency points, the respective quadrature weights, and informations about every frequency point. It is created by the program *SETF2*. Details can be found in Section 3.
4. a *start model*. It can be either a "LTE" start model or a model which has been created by *PRO2* or *LINE1*. Further informations are summarized in Section 4.
5. *commands* for the program control (Sect. 5.4) and *print commands* (Sect. 5.5).

1 Creation of the Executables

All programs of the Tübingen NLTE Model-Atmosphere Package (*TMAP*) were developed on CRAY computers. They can generally be installed on all other computers. For the substitution of CRAY specific parts or system library routines, there exists a collection of own subroutines.

For the use of a new atomic data or frequency grid files it might be necessary to change the `PARAMETER` statements for the `DIMENSION` of various arrays. Subsequently the program has to be compiled and loaded. Shell scripts for compilation are available. *Please contact rauch@astro.uni-tuebingen.de for further instructions.*

All `PARAMETER` statements are collected in input files which are named `PARAND, PARA, PARA1`, and `PARA3`. All `PARAMETER` signed with "*" are used by *PRO2* only, all with "*" by *LINE1* only, the rest is valid for both programs.

PARANA

`NA` quadrature points for angular integration (default 3).
PRO2 allows NA $\in [3, 5]$.
LINE1_PROF allows NA $\in [3, 4, 5, 6, 7, 8, 9, 10, 12, 16, 20, 24, 32]$.

PARAND

`ND` depth points (default 90)

An investigation on the necessary number of depth points has shown that the computational time decreases (of course) for ND < 90 but the resulting line profiles are more narrow and the line cores are less deep. The line profiles converge at ND $\gtrsim$ 70. An 1% error is reached at ND $\geq$ 90. For much higher ND, the computational time increases tremendously and the models a less numerical stable.

PARA

`LTEMAX` LTE levels

`NATOMAX` elements

`NFMAX` frequency points

`NIONMAX` ionization stages

`NLATOMS` non-LTE levels (of one element)

`NLMAX` non-LTE levels (total of all elements)

PARA1

`NRBBMAX` transitions **r**adiative **b**ound-**b**ound

`NRBFMAX` transitions **r**adiative **b**ound-**f**ree

`NRFFMAX` transitions **r**adiative **f**ree-**f**ree

`NRLLMAX` transitions **rbb** for "sample" cross-sections within one level band (complex ions) (Sect. 2.2)

`NRLUMAX` transitions **rbb** for "sample" cross-sections (Sect. 2.2)

`NCBBMAX` transitions **c**ollisional **b**ound-**b**ound, (only electron collisions)

`NCBFMAX` transitions **c**ollisional **b**ound-**f**ree, (only electron collisions)

`NCBXMAX` transitions **c**ollisional **b**ound-e**x**tra, (only electron collisions)

as well as the same `PARAMETER` with a `D` instead of `X` at the end (`NXXXMAD`): maximum number of input values in the atomic data file for the transition `XXX` (e.g. `NCBBMAD`)

Exception: `NRBBMAD`, either like above or – if larger – maximum number of frequency points in a line transition

`NRBFMAW`* `DIMENSION` of the array `SIGBF`

`NRBLMAX`* for the selected line, the number blends within its line profile

`NRLFMAX`* lines to select in a single job for the calculation of their profile

PARA3

`NRDIMAX` transitions **r**adiative **di**electronic bound-free

`NRDIMAD` (analogous `PARA1`)

`NSIG`* `DIMENSION` of the array `SIGBF` (value NRBFMAW (= NSIG) is given by *SETF2* and *LINE1_PROF*)

In the case that the `PARAMETER` limit is exceeded, e.g. the number of NLTE-levels in the atomic-data file is higher than `NLMAX`, the programs stop with an error message, partly only in the log file (`STOP '.......'`). Working with model atoms much below the `PARAMETER` limits is a waste of core memory and I/O time. Take care that the PARAMETER values do not create bank conflicts, i.e. avoid 2^n values!

2 Creation of Atomic Data Files

All programs expect an atomic data file, which contains model atoms and atomic data. It is firstly created by the user (Sect. 2.7) and then processed by the program *ATOMS2*.

The model ions of one element have to be inserted in increasing order while any order of elements is accepted.

The processing of the atomic data file is directed by *keywords* which meanings are explained in the following. All **keywords** as well as all **strings** have to be inserted flush left (e.g. level names, Sect. 2.1). All **numerical data** can be written format free. *Attention: all input lines have a maximum length of 80 characters!*

2.1 Level Names (*TMAP* Code)

The levels are named using an A10 string. The element code is at the beginning (e.g. `HE`) and the following (one or two) numbers indicate the ionization stage (e.g. `HE2`). This is mandatory. The next numbers indicate the principal quantum number of the level (e.g. `HE26`). For levels with a complicate configuration, the electron system and the magnetic quantum number may be added (e.g. `O42P 2PO`). Singly excited levels are marked by a " ' ", doubly excited by a " ' ' " directly before the electron system indication (e.g. `N33S' 2PO`). In the case of explicitly considered multiplet splitting the angular momentum is added at the end (e.g. `C452D5/2`).

2.2 List of Keywords for the Atomic Data File

```
.
0
ATOM
L
LTE
RBB
RBF
RDI
RLL
RLU
CBB
CBF
CBX
TL
DB
```

2.3 Description of the Keywords

The expression "card" which is frequently used in the following is a relic from the PUNCH era and is used for historical reasons.

keyword .
comment, not written to atomic data file

keyword 0 (Null)
necessary to end the validity of some keywords (e.g. `L, LTE, ...`)

keyword ATOM

introduces a new element. The following card indicates:

1. the chemical abbreviation (`FORMAT A2`),
2. charge of the lowest ionization stage (in e^-) in model atom,
3. atomic weight (in AMU).

Example:

```
ATOM
HE 0 4.0026
```

means: all following cards describe an helium model atom, starting with neutral helium He I, the atomic weight is 4.0026 AMU.

keyword L
introduces non-LTE levels. All cards following this keyword indicate:

1. level name (`FORMAT A10`, Sect. 2.1),
2. name of ground state of the following ionization stage (`FORMAT A10`, Sect. 2.1), if **no** parent exists: `NONE`,
3. energy to the ionization limit in Hz,
4. statistical weight, if **no** parent exists: 1.0.

Example:

```
L
HE26␣␣␣␣␣␣HE31␣␣␣␣␣␣3.6548882425E+14    72
0
```

levels of an ionization stage are expected **in increasing energetic order** (from the ground state). The keyword `0` completes the list of NLTE levels for this ionization stage.

keyword LTE
introduces LTE levels analogously to the keyword **L**. Do not forget to complete the list with the keyword `0`. Important: some formulae for the free-free opacity (Sect. A) expect at least one LTE level in the respective ion. Attention: this is **not checked** by the program.

Radiative and collisional transitions are introduced by:

RBB radiative bb

RBF radiative bf

RDI radiative dielectronic bf

RLL radiative bb for "sample" cross-section within one level band (complex ions)

RLU radiative bb for "sample" cross-section

CBB collisional bb

CBF collisional bf

CBX collisional from NLTE to LTE levels

All lists following these keywords have to be completed by the keyword `0`. A card which follows one of the keywords (except `RDI`) indicates

1. lower level (A10),
2. upper level (A10),
3. formula number for the calculation of the cross-section (Sect. A),
4. number n of following input data,
5. n input data for the calculation of the cross-section.

Example:

```
RBB
H11␣␣␣␣␣␣␣H13␣␣␣␣␣␣␣1    1  0.0791
0
```

This is the line transition Ly_β, cross-section calculation with formula No. `1`, one input number (`0.0791`).

For `RDI` transitions a third level is introduced between lower and upper level which is the upper level of the stabilizing transition and **has to be** introduced before as a LTE level.

For `RLU` and `RLL` transitions the level names are followed by the name of the file which contains the "sample" cross-section.

Example:

```
RLU
FE31␣␣␣␣␣␣FE33␣␣␣␣␣␣26_02_01_03
0
```

keyword RFF
introduces radiative free-free transitions. The following card indicates:

1. the ionization stage (A10, chemical element abbreviation + ionization stage, e.g. `HE2`),
2. formula number for the calculation of the cross-section (Attention: Def. `LTE`!)
3. number n of the following input data,
4. n input data.

keyword TL
The card which follows this keyword indicates the "line temperature" T_{line} for all following `RBB` transitions. This is necessary to change the temperature used for the calculation of the Doppler width (default $T_{\mathrm{line}} = \frac{3}{4}T_{\mathrm{eff}}$) in the creation of the frequency grid (Sect. 3). The default is again valid after

```
TL
0
```

keyword DB
introduces an explicit frequency grid for all following `RBB` transitions. The following card indicate:

1. number n of frequency points of the line,
2. n frequency points (**distance from line center in Doppler widths!**).

Example:

```
DB
7
-3 -2 -1 0 1 2 3
```

If the first frequency point is 0.0, only "half" lines are created.

This grid is valid until the next keyword `DB` appears. The default is valid after

```
DB
0
```

Note: In the Tübingen Model-Atom Database (Sect. 2.4), standard DB values are given that are about the maximum needed at low effective temperatures and high surface gravities. These values have to be altered at least for lower surface gravities. A test calculation with *PRO2* will show the line widths. Use, e.g., H I λ 1215 Å, and reduce the maximum DB values. In case that they are too low, "steps" in the flux level are prominent in the line wings. (The Doppler width of a specific line can be calculated by /home/rauch/bimod/doppler.Linux_x64.)

The DB adjustment results in a lower number of frequency points and, thus, faster model calculation.

A good compromise may also be to replace

```
DB
33
-2048.0  -1024.0   -512.0   -256.0
 -128.0    -64.0    -32.0    -16.0
   -8.0     -4.0     -2.0     -1.0
   -0.5     -0.3     -0.2     -0.1
0.0
    0.1      0.2      0.3      0.5
    1.0      2.0      4.0      8.0
   16.0     32.0     64.0    128.0
  256.0    512.0   1024.0   2048.0
```

by the insertion of a grid of additional frequency points using, e.g.,

```
/home/rauch/bimod/prep\_conts\_man.Linux\_x64 > F\_BASE << eos
1175  1255  0.5
eos
```

and a reduced DB that represents the line core much finer than the base grid (for F_BASE see Sect. 3)

```
DB
15
-2048.0
                    -2.0     -1.0
   -0.5     -0.3     -0.2     -0.1
0.0
    0.1      0.2      0.3      0.5
```

```
1.0      2.0
                    2048.0
```

2.4 TMAD

The Tübingen model-atom database *TMAD* (`http://astro.uni-tuebingen.de/~TMAD`) provides ready-to-use model atoms in *TMAP* format.

2.4.1 Model calculations (PRO2)

TMAD provides, in general, model atoms at maximum size, i.e. using all data from standard atomic-data resources. For model calculations, model ions can be reduced typically to 15 to 20 NLTE levels (Sect. 2.5, cf. Jahn et al. 2007) to avoid unreasonable computation times. In addition, the input for the DB keyword (Sect. 2.5) has to be adjusted to avoid calculations of line profile very far off the line centers where the line absorption is negligible. *TMAD* uses a standard of 2400 Doppler widths which may be necessary only for models with very high surface gravities.

2.4.2 Line-formation calculations (PRO2)

Models from Sect. 2.4.1 may not include all levels, e.g. for C IV lines in the optical wavelength range around 4660 Å. Thus, a subsequent line-formation calculation has to be performed with fixed atmospheric structure, i.e. only NLTE occupation numbers for the atomic levels are calculated. It may not be useful to extend all ions and to consider all levels given in *TMAD*. The *cookbook* says, "for all ions for which lines are identified, include five more levels than the highest from which strategic lines are arising".

In case of the C IV $\lambda\lambda$4660 Å / He II λ4685 Å absorption trough in PG 1159 stars, it is sufficient to extend C IV only for a line-formation calculation, even in models that consider all species from H to Ni.

LINE1 and *LINE1_PROF* provide the possibility to collect occupations numbers of newly considered levels from different models Sect. 8.3, e.g. if five line-formation calculations were performed (based on the same model) with individually extended C IV, O V, O VI, Ne VI, and Ar VI. This saves an enormous amount of CPU time.

2.4.3 Spectra calculations (LINE1_PROF)

To calculate the emergent synthetic spectrum, a formal solution is performed with *LINE1_PROF*. *TMAD* provides model atoms that account for fine-structure splitting of the atomic levels. These have to be the same like the unsplitted levels used for the line-formation calculations. (Sect.2.4.2).

2.5 ATOMS2

The interactively created atomic data file is — if designed following the instructions in Sect. 2 — ready, i.e. it can be used for the creation of a frequency grid as well as for model atmosphere calculations. However, *it is highly recommended to process it with the program* ATOMS2, which is able to detect a lot of errors and gives warnings. In case of fatal errors it even terminates. There exist options which make *ATOMS2* create automatically model ions or fill up them.

The program *ATOMS2* is available at Tübingen's PC/Workstation cluster in its latest version: **/home/rauch/bimod/atoms2.Linux_x64**.

An atomic data file (*ATOMS*) created by *ATOMS2* is unambiguously defined by:

- the input file (here: *OPTIONEN*)
- the interactively created atomic data file (here: *ATOMIN*)

In the input file *OPTIONEN* one can write directives for *ATOMS2*. *ATOMS2* expects *OPTIONEN* and *ATOMIN* subsequently as input, *OPTIONEN* has to be finished in any case with `END␣OPTIONS`,
even if none of the following options is given:

`AUTO␣ION␣H␣␣␣␣I in il ir`

This option creates a complete H model atom. *in* is the principal quantum number of the highest H I NLTE level, *il* is the principal quantum number of the highest H I LTE level, *ir* is the principal quantum number of the highest H I NLTE levels up to which all RBB transitions are considered. (The conditions $il > in$ and $ir \leq in$ are fulfilled.) In case that *ir* is negative, only transitions from *ATOMIN* up to the NLTE level *ir* are used. (This is necessary if *ATOMIN* contains information about line broadening, default is Doppler line broadening). In the case that *ir* is positive, *ATOMIN* does not need to contain any H model atom.

`AUTO␣ION␣HE␣␣II in il ir`

same like `AUTO␣ION␣H␣␣␣␣I` (see above) but mandatory; in the case that *ATOMIN* contains a He I model ion, *ATOMS2* creates He II and He III model ions, otherwise a complete He model atom.

`CBB-AUTO-FILL`

If this option is given, missing CBB transitions are automatically inserted and possible errors in *ATOMIN* corrected — as far as *ATOMS2* is able to detect them. The output of *ATOMS2* has to be checked for respective error messages or warnings.

`CBB-AUTO-FILL␣␣(IGNORE)`

same like `CBB-AUTO-FILL`; possible errors are only reported in the output but not corrected.

`CBB-AUTO-FILL␣␣(␣␣NONE)`

If this option is given, all CBB transitions are disregarded. This `...-AUTO-FILL` option is only useful for the detailed calculation line profiles. This option is automatically set, if the option `LINEFORMATION` ... is given (see below).

Analogously to the `CBB-AUTO-FILL` ... options, the following options are valid:

`CBF-AUTO-FILL`
(for unknown cross-sections, hydrogen-like values are automatically inserted)

`CBF-AUTO-FILL␣␣(␣␣NONE)`

`CBF-AUTO-FILL␣␣(␣␣NOOP)`

(for OpacityProject cross-sections, hydrogen-like values are automatically inserted)

`CBX-AUTO-FILL`

`CBX-AUTO-FILL␣␣(IGNORE)`

`CBX-AUTO-FILL␣␣(␣␣NONE)`

`RBB-AUTO-FILL␣␣(␣␣NONE)`

`RBB-AUTO-FILL␣␣(␣␣H1␣␣)`

`RBB-AUTO-FILL␣␣(␣␣HE2␣)`

`RBF-AUTO-FILL`
`RBF-AUTO-FILL␣␣(␣␣NOOP)`

(for OpacityProject cross-sections, hydrogen-like values are automatically inserted)

(set `CBF-AUTO-FILL␣␣(␣␣NOOP)` also)

`RDI-AUTO-FILL␣␣(␣␣NONE)`

`RLL-AUTO-FILL␣␣(␣␣NONE)`

`RLU-AUTO-FILL␣␣(␣␣NONE)`

`LINEFORMATION␣-␣RBB-INTERVALL=[␣␣1000,␣␣7000],␣ION=H1`

This option can be set for line-profile calculations in order to restrict number of line transitions in the atomic data file *ATOMS* to a selected interval (here: [1000, 7000] Å). If this shall be valid for all (line profiles), `ION=NON` has to be inserted. To insert all line transitions — i.e. even outside the given interval — of a selected ion in *ATOMS* (line formation), the *TMAP* code (Sect. 2.1, here: `H1`) has to be given.

If this option is given, all
`C..  -AUTO-ION␣␣(␣␣NONE)`
options and the
`RDI␣-AUTO-ION␣␣(␣␣NONE)`
option are automatically set.

`LIST␣OF␣ALL␣RBB,␣ION:␣␣␣`

This option creates a table of all line transitions of the selected ion under consideration of a possible `LINEFORMATION ...` option with its interval restriction.

`END␣OPTIONS`

This option finishes the file *OPTIONEN* and is necessary if one of the other options has been given.

The program *ATOMS2* creates a large informative output which includes generally the atomic data file as created by *ATOMS2*, informations about wavelengths of levels, thresholds, line transitions, and some statistics. Excited levels are marked in the output with "**", all transitions which were inserted following the ...`AUTO-FILL ...` options are marked with "`AF`".

All parameters which are valid for the created atomic data file *ATOMS* (Sect. 1), are summarized in a table at the end of the output. Under unix a

grep para ¡output filename¿

extracts them from the output file.

2.6 TIRO

The Tübingen Iron-Group Opacity (*TIRO*) service creates atomic data files and cross-section data for radiative bound-bound and bound-free transitions of iron-group elements (calcium, scandium, titanium, vanadium, chromium, manganese, iron, cobalt, and nickel). It is based on the program

IrOnIc that was developed at Tübingen. *TIRO* enables the *VO* user to consider iron-group elements in model-atmosphere calculations easily, in various ways, and without spending own calculation time for the creation of the necessary input data. It is controlled via web interface (`http://astro.uni-tuebingen.de/~TIRO`) in which the following inputs have to be given.

- The name, institute, and email address of the user have to be given to inform the user about the status of the process and the location of the results.
- The resulting line profiles depend on the line temperature $T_{\rm L}$. $T_{\rm L}$ is 3/4 $T_{\rm eff}$ and corresponds to the mean temperature in the lineforming region.
- A frequency grid can be uploaded. The corresponding file has to be written in plain text with monotonically increasing frequency points and must be in *TMAP* (`http://astro.uni-tuebingen.de/~TMAP`) format. Alternatively, a start and end wavelength as well as a spacing or maximum number of points can be chosen. The frequency grid is then created automatically by *TIRO*. The calculations are performed on this frequency grid or already calculated cross-sections from the database are interpolated to this frequency grid.
- It is possible to retrieve data for all ionization stages up to IX. The requested ionization stages can be chosen.
- Cross-sections for the iron-group elements can be created considering all or some of them individually or generically. When the individual option is chosen, an easy adjustment of the abundances in the model atmosphere calculation is possible. A generic model atom consists of selected iron-group elements. In this case, the given abundance ratios are fixed in the resulting model atom. For both cases the line type of the underlaying atomic data can be selected. They are taken from Kurucz' line lists and can be chosen between lines with measured wavelengths (POS) or measured and calculated wavelengths in addition (LIN).

After submitting the data, the given parameters are stored in a request file. *TIRO* checks regularly if requests are waiting and processes them one after the other. The user is informed via email when the handling of the data starts. The resulting files are stored in a compressed tar archive that is accessible via a wget command. The user is informed via email about its location. The files for bound-bound transitions contain a table with frequencies in the first column, cross-sections in the second (calculated for electron density 0) and in the third column (calculated for electron density $10^{16}/\mathrm{cm}^3$). The corresponding files for bound-free transitions include a table with frequencies in the first and cross-sections in the second column.

2.7 Auxiliary Programs

Some programs are currently available which help to design model atoms etc. All these programs work interactive and are (more or less :-(...) self-explaining.

2.7.1 FORMEL4

The programs *PRO2* and *LINE1* can consider – besides pure Doppler line broadening – the quadratic ("formula 3") and the linear ("formula 4" — this gives the name of the program ...) Stark effect for the line broadening. Both formulas need some input data which has to be includes in the atomic data file *ATOMS*. (Sect. 2).

The program *FORMEL4* (/home/rauch/bin/formel4) calculates these data (mainly the classical damping constant and the effective quantum number) from an existing atomic data file.

The calculated data is saved into the files *FORMEL4.DAT* and *FORMEL4.RBB*. *FORMEL4.RBB* can be used the replace the respective section of the atomic data file which was used to calculate the data.

FORMEL4 inserts also the vacuum wavelengths, starting with the keyword WAVELENGTH: in columns 81-91. The wavelength values may be the replaced by measured wavelengths in order to shift those lines which arise from levels with uncertain energies to the correct wavelengths. A subsequent run (necessary!) of *SETF2* on the modified *ATOMS* yield a frequency grid with these lines at the correct wavelengths.

2.7.2 LEVEL

The level energies in literature are commonly given in cm^{-1}, measured from the ground state of their ionization state. In the Tübingen NLTE Model-Atmosphere Package (*TMAP*), the level energies given are the difference to the next ionization limit, i.e. the energy which is necessary to ionize into the ground state of the next ionization stage. The program *LEVEL* simply transforms these energies.
The program *LEVEL* (/home/rauch/bin/level) runs interactively. It is possible to calculate

- energies of single levels
- energies of combined levels

Furthermore it is possible to combine

- levels from an existing atomic data file

The data is saved into *LEVEL.DAT* and (for the combination of levels) into *XX.ENTARTET* (XX is the principal quantum number of the combined levels).

2.7.3 MKIDENT_FROM_KURUCZ

Due to our statistical approach to create atomic data files from Kurucz's data (Kurucz 1991, 2009, 2011) of elements with atomic numbers $Z \geq 20$, the wavelengths of individual lines can only be read from Kurucz's data files. The two procedures
/home/rauch/tools/lineidentification_LIN.bat and
/home/rauch/tools/lineidentification_POS.bat
for Kurucz's data files with theoretical and laboratory measured lines (.LIN) and with positively identified lines (.POS), respectively) may be used to create

```
\IDENT <wavlength> <ion>
```

cards that can be used by WRPLOT (Sect. 11). An explanation how to use these procedures is found in their headers.

2.7.4 MULTIPLET

During the calculation of the model atmospheres, multiplets are considered with a combined level. For the subsequent detailed line profile calculation, it is necessary to split these multiplets into single components. While (in most cases) the level energies can be taken from literature, there are only rudimentary informations about the oscillator strengths of the single components. The program *MULTIPLET* (/home/rauch/bin/multiplet) splits up oscillator strengths of doublets, triplets, and quartets under the assumption of LS coupling.

The calculated data is saved into *MULTIPLET.DAT*.

2.7.5 SEATON

For some RBF cross-sections of levels of the ions He I, C I – C IV, N I – N V, O I – O III, Ne I – Ne II, Mg I – Mg II, Si I – Si IV etc., tables have been calculated by Hofs"a"s. These can be evaluated with

the program *SEATON* (). One gets input parameter for the Seaton formula(Sect. A.4). For those levels which are not included in the tables, *SEATON* can calculate a hydrogen-like cross-section.

2.7.6 SGF

To reduce the pixel-to-pixel variation (or the noise) of observations, a low-pass filter may be used. The program *SGF* (/home/rauch/bin/sgf) processes data following Savitzky & Golay (1964). Two parameters, *np* and *m* have to be given. *np* is the number of a subset of the data which is used for a fit. *m* is the degree of the polynomial used in the least-squares fit method. *m* has to be carefully chosen - a too-high value smoothes out real spectral features.

3 Creation of Frequency Grids

The program *SETF2* creates the binary file *FGRID* which contains the frequency grid used by *LTE2*, *PRO2*, and *LINE1*.

SETF2 processes data from the atomic data file *ATOMS*. *Attention:* SETF2 *has not the capabilities to detect errors like* ATOMS2*!* For the creation of a frequency grid *SETF2* uses only data which belongs to the keywords *L*, *RBF* und *RBB* (Sect. 2.2) and checks these for errors.

Thus, it is indispensable to transform every new or modified, interactively created atomic data file with the program ATOMS2 *in order to check for errors and inner consistency.*

The program *SETF2* is available for all users at Tübingen's PC cluster in its latest version: **/home/rauch/bimod/setf2.Linux_x64**.

A frequency grid is unambiguously defined by its input files *ATOMS*, *DATEN*, *CONTS_MAN*, *F_BASE*, and *POS_LIST*. All frequency points are clearly named (*TYP*) in the frequency grid (see below.).

ATOMS
is the atomic data file (Sect. 2).

DATEN
This file contains:
- the effective temperature $T_{\rm eff}$,
- the *output parameter*,
- the *weight parameter* $\nu_{\rm W}$,
- the *line parameter*,
- the *EUV parameters EUVmax* und *EUVnumber*,
- *f-value limit*.

The *effective temperature* $T_{\rm eff}$ is necessary for the calculation of the frequency discretization within a line transition (central frequency ν_0). The position of the frequency points is depending on the Doppler width $\Delta\nu_{\rm Doppler} = \frac{\nu_0}{c}\sqrt{\frac{2kT}{m_{\rm ATOM}}}$. This default value can individually be substituted by the keywords `TL` in *ATOMS*.

If the "RBB" record in *ATOMS* contains the keyword WAVELENGTH: in columns 81-91, *SETF2* uses the value directly following this keyword for the central wavelength of the respective line transition. The program *FORMEL4* can preset this value which may be replaced or inserted (with the keyword!) manually in order to shift the line to the specified wavelength.

Two edge frequency points are inserted for every bound-free transition in *ATOMS* (keyword `RBF`): this is necessary because the ionization into excited levels is considered in detail by *PRO2* und *LINE1*. These frequency points are set at the ionization energy ν_0 of the respective level and at $\nu_0 + 10^{-12} \cdot \nu_0$. These points are used to split up the complete frequency grid in single integration intervals.

For all line transitions in *ATOMS* a particular number of frequency points is inserted. Their order is controlled by the *line parameter*. If nothing else is defined in *ATOMS* (keyword `DB`), the following arrangements are automatically set:

In the case that the frequency points which are inserted for a line transition overlap with those of another line or with edge frequency points, the overlapping lines have to have a symmetric arrangement of their frequency points ("full lines" — like inserted if the *line parameter* is set to 1, Tab.1)

The choice of *line parameter* 0 is generally possible for all other line transitions under the

Table 1: The *line parameter* and default frequency point arrangements for line transitions

line parameter	frequency points	$(\nu - \nu_0)/\Delta\nu_{\rm Doppler}$	comment
0	5	$0, \frac{2}{3}, \frac{4}{3}, 2, \frac{8}{3}$	universal
1	9	$-\frac{8}{3}, -2, -\frac{4}{3}, -\frac{2}{3}, 0, \frac{2}{3}, \frac{4}{3}, 2, \frac{8}{3}$	universal
-1	5	like 0, in case of line overlaps like 1	universal
-3	3	$0, \frac{4}{3}, \frac{8}{3}$	pre-iteration

premise that the flux gradient is almost constant over the full width of the line. This kind of frequency discretization within a line transition is named "half line".

An automatical differentiation is made if the *line parameter* is set to -1. This has the great advantage that fewer frequency points are inserted in the grid, compared to *line parameter* 1.

The *line parameter* -3 is equivalent to *line parameter* -1 but inserts only three points (five in case of overlap) for a line. This saves memory and computational time but is somewhat unrealistic because the line profile is not well represented by this frequency point arrangement. At least a subsequent iteration with a more detailed frequency grid (e.g. created by *SETF2* from the same atomic data file *ATOMS* but with the *line parameter* -1) is necessary.

The *f-value limit* can be chosen to represent lines with f-values smaller equal than the *f-value limit* analogously to *line parameter* -3, independent from DB values in *ATOMS*. This reduces slightly the number of frequency points in *FGRID*.

The frequency grid contains by default the interval $1.0{\cdot}10^{12}{-}2.99792458{\cdot}10^{17}$Hz (= 1 Å, Tab.3). The optional parameter *EUVmax* allows to change the maximum: in the case that *EUVmax* is larger than $2.99792458 \cdot 10^{17}$Hz, *EUVnumber* indicates the number of frequency points which are inserted by *SETF2* in the range $1.0 \cdot 10^{17} - EUVmax$ Hz; in the case that *EUVmax* is smaller that $2.99792458 \cdot 10^{17}$Hz, *EUVnumber* is disregarded.

CONTS_MAN
This optional file contains additional frequency points (given in Å or Hz)

In this input file frequency points can be requested to insert which are important for the evaluation of the models, e.g. in the case of the emergent flux and the calculation of specific colors. Doubly requested points are disregarded ...

CONTS_MAN can be created using

```
/home/rauch/bimod/prep_contsman.Linux_x64 > CONTS_MAN << eos
min max <step / resolving power>
eos
```

for wavelength or frequency points. In case that the third argument is ≥ 100, prep_contsman assumes it to be the resolving power. prep_contsman accepts more than one input line.

F_BASE
This optional file contains additional frequency points (given in Å or Hz)

If the file *F_BASE* exists and contains valid input data, all requested points are created as base grid in the interval $\nu_{\rm min}^{\rm base} - \nu_{\rm max}^{\rm base}$. The largest base grid can actually contain 200 000 frequency points. Subsequently, *SETF2* creates (like described above) the "normal" frequency grid based on *ATOMS* and *DATEN*. The *line parameter* is automatically set to 1.

In contrast to frequency points requested in *CONTS_MAN* which are definitely present in the created *FGRID*, all base grid points are eliminated if "normal" frequency points (including points

requested in *CONTS_MAN*) are found in the interval $\left[\frac{1}{2}\left(\nu_{i-1}^{base}+\nu_{i}^{base}\right),\frac{1}{2}\left(\nu_{i}^{base}+\nu_{i+1}^{base}\right)\right]$ Hz.

F_BASE can be created using prep_contsman, see above.

POS_LIST
This optional file contains additional frequency points (given in Å or Hz)

It should be created by **/home/rauch/tools/line_identification_POS.job** (edited for the required elements and ionic species) for Kurucz POS lines only.

SETF2 reads the line centers from **POS_LIST** and creates for each line nine frequency points ($\Delta\lambda/\mathring{A} = -0.005, -0.003, -0.002, -0.001, 0.000, 0.001, 0.002, 0.003, 0.005$). This is necessary to avoid artificial "fading" of iron-group lines by a later convolution of the synthetic spectrum with a rotational of instrumental profile.

Wavelengths > 2000 Å are given by Kurucz as air wavelengths and are converted into vacuum wavelengths to match the line positions during the model-atmosphere calculations.

After the creation of the frequency grid in accordance with *ATOMS*, *DATEN*, *CONTS_MAN*, *F_BASE*, *POS_LIST* the IR, UV, and EUV range and the intervals between the lines and edge are automatically completed.

Every frequency point is unambiguously named in the frequency grid with a CHARACTER∗50 string: In detail the fields have the following meaning:

`1␣␣␣2␣␣␣␣␣3␣␣␣␣4␣␣␣␣␣␣␣␣␣5␣␣␣␣␣␣␣␣␣6␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣`

field 1:

- `CONT` for all continuum points, which were set in accordance to *ATOMS*, *DATEN*, *CONTS_MAN*, and *F_BASE*
- `C/ED` for all continuum points, which were automatically created, e.g. in order to separate integration intervals
- `EDGE` for all continuum points, which were inserted to represent the bound-free transitions in *ATOMS* (see above)
- `LINE` for all line transition points

field 2:

- `(HALF)` for all line transition points, "half lines" (see above)
- `(FULL)` for all line transition points, "full lines" (see above)
- `␣RED␣␣` for all continuum points at the end of integration intervals (in general from one bound-free transition to another)
- `␣BLUE␣` — `␣RED␣␣` (RED and BLUE indicate the location of the point relatively to the threshold / edge: BLUE is set exactly at the threshold frequency, RED is set at longer wavelength, i.e. "redwards")

field 3:

- ␣␣␣** for threshold frequency points for levels ionizing into excited levels

field 4:

- AUTO_ADD␣␣ for all automatically inserted continuum frequency points (to fill-up too-large intervals)
- AUTO_IR␣␣␣ for all automatically inserted continuum frequency points (to fill-up to the IR limit of $1.0 \cdot 10^{12}$Hz)
- AUTO_UV␣␣␣ for all automatically inserted continuum frequency points (to fill-up to the EUV limit of $2.99792458 \cdot 10^{17}$Hz)
- BASE␣␣␣␣␣␣ for all inserted (and not eliminated — see above) continuum frequency points optionally requested in *F_BASE*
- MANUELL␣␣␣ for all inserted continuum frequency points optionally requested in *CONTS_MAN*
- HE26␣␣␣␣␣␣ for all edge and line transition frequency points lower level in the *TMAP* code (Sect. 2.1, here: He II, level with principal quantum number 6.

field 5:

- HE27␣␣␣␣␣␣ for all edge and line transition frequency points upper level in the *TMAP* code (Sect. 2.1, here: He II, level with principal quantum number 7

field 6:
For all line transition points the position of the point in the line is indicated:

- CONT/RED␣␣␣␣␣␣␣
- CENTER␣␣␣␣␣␣␣␣␣
- CONT/BLUE␣␣␣␣␣␣

For every frequency point a quadrature weight is calculated corresponding to the weight and the *line parameter*. The following points are considered:
• integration intervals do not include a complete edge, i.e. EDGE/RED and EDGE/BLUE of the same threshold
• the quadrature weights are calculated following the trapezoidal law for $\nu < \nu_W$ (*weight parameter*, see above) and following the Simpson law for $\nu_W < \nu$. The Simpson law is necessary because the flux is exponentially decreasing for $\nu > \nu_W$ and the trapezoid law is not sufficient. In principle, all weights can be calculated following the Simpson law — *SETF2* will then insert a few more frequency points.
• "half lines" have corrected weights
• In the case of line overlaps "full lines" have to be considered (automatically: *line parameter* 1 or — better — -1, or keyword DB in *ATOMS*)

The output of *SETF2* should be controlled in detail. *SETF2* comments all operations and gives warnings in case of ambiguity. In the case of fatal errors, *SETF2* terminates.

The quadrature weights require special attention: the check sums of all single intervals as well as of the complete frequency grid have to be *exactly* 1. If this is not the case, it is possible that negative quadrature weights appear ("half lines" in cases were "full lines" are necessary). In order to correct for this, the atomic data file *ATOMS* has to be modified (keyword `DB`) or the *line parameter* has to be set to -1 (this automatically corrects these cases).
Attention: A frequency grid with wrong quadrature weights will cause an abort in programs like PRO2 or LINE1.

The size of the output is controlled by the *output parameter*:
• `PRINT CHECK` reduces the output to a minimum, only warnings, fatal errors, and information about the quadrature weights are displayed.
• `PRINT` gives a complete output, incl. the complete frequency grid.
In both cases the parameter *NFMAX, NRBBMAX, NRBBMAD*, and *NRBFMAW* (Sect. 1) are printed, which are valid for *ATOMS* and *FGRID*. Under unix a

grep para ¡output filename¿

extracts them from the output file.

• `PRINT ASCII` *FGRID* is created formatted.

In case that the input atomic-data file was created by *ATOMS2* for line-profile calculations (Sect. 2), *SETF2* creates two files, *ION_USER* and *LINIEN_USER*, that may be used as input files (*ION* and *LINIEN*) for *LINE1_PROF* (Sect. 9). *LINIEN_USER* contains a line closest to the center of the RBB interval (*ATOMS2*, Sect. 2) and a respective BLENDRANGE to cover the complete RBB interval. *ION_USER* contains the proper ion according to *LINIEN_USER*.

4 Start Models

Start models are necessary for the programs *PRO2* and *LINE1*. They can come from different sources. Within the Tübingen NLTE Model-Atmosphere Package (*TMAP*)all models can be used as start models. It is distinguished between two types of start models.

4.1 PRO2 and LINE1 Models

A model which is calculated by *PRO2* or *LINE1* can be used as start model. The convergent models (with the same parameters, same *ATOMS* and *FGRID*) from both programs should be identical.

New NLTE-levels, i.e. levels that are not found in the start model, are set to LTE occupation numbers. This is valid especially for completely new elements and can be a problem in the case of higher elemental abundances due to the inconsistency in the conservation of particles ...

For the detailed calculation of line profiles, automatic multiplet splitting is optional in *LINE1* for all C IV, N V, O VI levels and a wide variety of C III, N IV, and O V levels. The list of multiplets is permanently updated.

4.2 "LTE" Models

The program *LTE2* produces "LTE" models (without any consideration of line blanketing) within a large range of photospheric parameters. The created model has *PRO2* format and is a start model for *PRO2* or *LINE1*.

4.3 Calculation of a LTE2 Model

The program *LTE2* calculates models in gray approximation. It uses the same atomic data (*ATOMS*, Sect. 2) and frequency grid files (*FGRID*, Sect. 3) like *PRO2* and *LINE1*. No line blanketing is considered. *LTE2* is controlled via the input file *DATEN* with a number of options (Sect. 4.3.2).

4.3.1 The Method

The program *LTE2* calculates a model atmosphere based on the requested effective temperature $T_{\rm eff}$, surface gravity g, chemical composition, and the files *ATOMS* and *FGRID*.

An equidistant $\log\tau$ scale (τ is the Rosseland optical depth) with *ND* depth points (Sect. 1) is created on which start values for the temperature stratification are calculated. This $\log\tau$ scale can be manipulated by some options (see below).

With the basic assumption of LTE,

$$\boldsymbol{S_\nu \equiv B_\nu(T),}$$

the mean intensity of the radiation field is

$$\boldsymbol{J(\tau) = S(\tau) = B\left[T(\tau)\right] = \frac{\pi}{\sigma_R}\cdot T^4}$$

i.e. the flux is constant ($\frac{dH}{d\tau} = J - S \equiv 0$). Thus, also the 1st moment of the radiation field $\frac{dK}{d\tau} = H$ is constant and yields the exact integral

$$\boldsymbol{K(\tau) = H\cdot\tau + c = \frac{1}{4}F\cdot\tau + c}$$

From this, we get $K(\tau) \to \frac{1}{4}F \cdot \tau$ for $\tau \gg 1$. $K(\tau) = \frac{1}{3}J(\tau)$ for $\tau \gg 1$ is the general solution for the intensity

$$\boldsymbol{J(\tau) = \frac{3}{4}F\,[\tau + q(\tau)]}$$

The temperature at the depth point l is

$$\boldsymbol{T_l = \sqrt[4]{\frac{3}{4} \cdot {T_{\rm eff}}^4 \cdot [\tau_l + q(\tau)]}}$$

$q(\tau)$ is called Hopf function.

The hydrostatic equation is solved in inside direction. The first four (outer) depth points are treated following the Runge-Kutta method. Then, the other points are calculated with a predictor-corrector method of Ham. In detail, the electron density at each depth point is calculated for the actual temperature and the given photospheric composition. The iteration method is based on Mihalas, Stellar Atmospheres, Second Edition, 5-2. Subsequently, *LTE2* calculates LTE occupation numbers for all levels of all elements using the Saha-Boltzmann equation. From these values, the Rosseland mean opacity $\bar{\kappa}_R$ is determined.

$$\boldsymbol{\frac{1}{\bar{\kappa}_{\rm R}} \equiv \frac{\pi}{4\sigma_{\rm R}T^3}\int_0^\infty \kappa_\nu^{-1} \cdot \frac{\partial B_\nu}{\partial T}d\nu}$$

LTE2 gives as result the electron density as well as the total particle density for the whole atmosphere. The original $\log\tau$ scale is transformed into a $\log m$ scale (m is the mass column density, measured from the outer limit of the atmosphere).

In practice, the temperature stratification of the inner atmosphere differs evidently from a "real" LTE or NLTE stratification, even for pure continuum models without consideration of line blanketing. Thus, with these start models, *PRO2* or *LINE1* need a relatively large number of iterations to calculate the right temperature structure. In order to reduce this number of iterations, an Unsöld-Lucy temperature correction can be carried out until the temperature structure is stable. Some option can be given to control the temperature correction method. (Sect. 4.3.2).

4.3.2 The Options

With some directives in the input file *DATEN*, *LTE2* can be controlled. Especially, the photospheric parameters line effective temperature $T_{\rm eff}$, surface gravity g, and photospheric abundances (which are necessary in any case) are selected.

The input file *DATEN* for the program *LTE2* has the following structure (Sect. 5.4):

DATEN
`T␣EFF␣T`
`LOG␣G␣g`
`ABUNDANCE␣xx hh`

T has to be given in Kelvin; g in cgs; xx element in *TMAP* code (Sect.2.1), hh abundance fraction by particle numbers.

Please note that $\sum_{\rm i=1}^{\rm NATOMS} hh_i = 1$! *LTE2* will check this. In the case that $\sum = 1$, *LTE2* will adopt the given abundances unchanged; if not, *LTE2* will re-normalize the given values! Please check STDOUT for respective information!

`TAU␣SCALE␣MINIMUM␣-8.0`*

This option sets the limit ($\log \tau_1$) of the outer atmosphere. This limit can be varied under the premise that the atmosphere has to be optically thin over the complete frequency grid at least at the first depth point. (This is one of the basic assumptions of *PRO2* and *LINE1*. *Attention: the requested value is only a start value which can be different from that of the finally calculated "LTE" model.*

`TAU␣SCALE␣MAXIMUM␣2.6`*

This option sets the limit ($\log \tau_{\mathrm{ND}}$) of the inner atmosphere. This limit can be varied under the premise that the atmosphere has to be optically thick over the complete frequency grid at least at the inner depth point. (This is one of the basic assumptions of *PRO2* and *LINE1*. *Attention: the requested value is only a start value which can be differ from that of the finally calculated "LTE" model.*

`TAU␣SCALE␣x y z`

This option defines the arrangement of the inner depth points.

- $z = 0.0$: depth points are logarithmically equidistant, $\Delta\tau = \frac{\tau_{\max} - \tau_{\min}}{ND}$ (start values)
- $z > 0.0$: like $z = 0.0$, but the distance (start value) of the innermost depth points (89-90) is z (default is $z = 1.0\mathrm{E} - 05$)
- $z < 0.0$: like $z = 0.0$, but the distance of the depth points (x $\rightarrow$ y) decreases logarithmically by the factor z

`ITMAX=100`*

maximum number of iterations of the Unsöld-Lucy temperature correction method
In the case that a negative temperature is detected, *LTE2* will stop immediately. The output model contains then the atmospheric structure of the iteration before.

`DAMP=0.5`*

start value of an artificially introduced damping factor within the Unsöld-Lucy temperature correction method. This factor is partly necessary because the method appears to be unstable in most cases. In the course of the iterations, this value is automatically reduced to increase the stability — this might seem to be convergence ...

`EPS=1.0E-6`*

"convergence" (see above) limit (to stop the Unsöld-Lucy temperature correction)

`LTE2␣START␣MODEL`

This option is only valid if the file *TIN* is available which is the original file *TOUT* of a former *LTE2* run and contains the temperature stratification of the previously calculated "LTE" model.

This option is helpful if a model has not reached the "convergence" limit (see above) in the first run and shall be brought to a better "convergence". Moreover, the "fake convergence" due to the automatically reduced damping factor can be checked.

`OUTPUT␣MODEL␣FORMATTED`

The output model is saved formatted.

`PRO2␣START␣MODEL`

This option is only valid if a *PRO2* or *LINE1* model is supplied as start model *MIN*. This is helpful to introduce new elements or to vary their abundance ratios. The temperature stratification of a convergent NLTE model is used here to calculate LTE occupation numbers (particle conservation) for all levels of *all elements*. With this option, `ITMAX=0` is set automatically, to preserve the temperature structure. A follow-up line formation calculation (i.e. at fixed temperature) with *PRO2* or *LINE1* supplies a start model with NLTE occupation numbers and a — hopefully — good approximation of the final temperature stratification.

The following options can be given to control the output of *LTE2*. Their meaning should be clear ... `XXXX` can be substituted by `EACH` or `LAST`.

`PRINT␣ABUNDANCES`

`PRINT␣EMERGENT␣FLUX`

`PRINT␣INTEGRATED␣EDDINGTON␣FLUX,ITERATION,XXXX`

`PRINT␣OPTIONS`

`PRINT␣MODEL␣ATOMS␣(OVERVIEW)`

`PRINT␣LEVELS`

`PRINT␣LTE␣MODEL`

`PRINT␣TEMPERATURE␣CORRECTIONS,ITERATION,XXXX,ALL␣DEPTHS`

`PRINT␣TEMPERATURE␣CORRECTIONS,ITERATION,XXXX,MAX.`

`PRINT␣WARNINGS`

The final model is saved by *LTE2* into the file *MODELL*. The last record in *MODELL* is:

MODPRG,DATE,TIME

(CHARACTER MODPRG∗5,DATE∗8,TIME∗8 with MODPRG='LTE2 ', DATE and TIME with actual creation time) is added in order to identify the model. The temperature structure of the model is saved in the file *TOUT* (see above).

The program *LTE2* is available at Tübingen's PC/Workstation cluster in its latest version: **/home/rauch/bimod/lte2.Linux_x64**.

The actual PARAMETERs are:

- `NATOMAX =  3`
- `NIONMAX =  9`
- `NLMAX   = 139`
- `LTEMAX  = 109`
- `NFMAX   = 1299`

Other executables of *LTE2* with different PARAMETERs have to be created (Sect. 1).

5 NLTE Models: PRO2

5.1 The Method

The program *PRO2* (Werner 1986; Werner et al. 2003; Rauch & Deetjen 2003; Werner et al. 2012) calculates plane parallel NLTE model atmospheres in radiative and hydrostatic equilibrium. It is based on the "**A**ccelerated **L**ambda **I**teration (ALI) method (Werner & Husfeld 1985). It consists mainly out of two iteration cycles. The "outer" cycle is called "Scharmer iteration" (this name is taken from Scharmer 1981 who worked on solutions of radiative transfer problems using approximate lambda operators) and iterates the radiation field according to

$$\boldsymbol{J}_\nu^n = \boldsymbol{\Lambda}^* \boldsymbol{S}_\nu^n + (\boldsymbol{\Lambda} - \boldsymbol{\Lambda}^*) \cdot \boldsymbol{S}_\nu^{n-1}$$

The source function S_ν of the actual iteration n is depending on the radiation field J_ν which is to be calculated. To calculate S_ν, the non-linear statistical equations have to be solved under consideration of the radiative and hydrostatic equilibrium. This is done in the "inner" iteration cycle by a [quasi-] Newton-Raphson iteration. In the following this procedure is called "linearizations".

5.2 The PARAMETERs

For the compilation of *PRO2* the files *PARA.INC*, *PARA1.INC*, and *PARA3.INC* have to be adjusted to the used atomic data file *ATOMS* (Sect. 2) and the frequency grid *FGRID*.

Example parameter files look like:

PARA.INC
```
     PARAMETER(  NLMAX= 229,  NIONMAX= 79,  NATOMAX= 17,
 >               NFMAX=7999,  LTEMAX =931,  NLATOM =229   )
```

PARA1.INC
```
     PARAMETER(  NRBBMAX=249,  NRBFMAX= 229,  NCBBMAX=599,  NCBFMAX=229,
 >               NRFFMAX= 61,  NCBXMAX=4999,  NRLLMAX=  1,  NRLUMAX=  1,
 >               NRBBMAD=999,  NRBFMAD=   6,  NCBBMAD=  6,  NCBFMAD=  2,
 >               NRFFMAD=  2,  NCBXMAD=   8,  NRLLMAD=  1,  NRLUMAD=  1   )
```

PARA3.INC
```
   PARAMETER(  NRDIMAX=1,  NRDIMAD=1,  NSIG=599999  )
```

The PARAMETER denote maximum numbers of e.g. elements etc. (see below) which can be treated with *PRO2* if the files are used for its compilation, respectively.

parameter	maximum numbers of
NLMAX	NLTE levels
NIONMAX	ions
NATOMAX	elements
NFMAX	frequency points
LTEMAX	LTE levels
NLATOM	NLTE levels (block-matrix method, for one element, set value equal to NLMAX)
NRBBMAX	radiative bound-bound transitions
NRBFMAX	radiative bound-free transitions
NCBBMAX	collisional bound-bound transitions
NCBFMAX	collisional bound-free transitions
NRFFMAX	radiative free-free transitions
NCBXMAX	collisional bound-bound transitions (to LTE levels)
NRLLMAX	radiative transitions within a band of a complex ion
NRLUMAX	radiative transitions low→up of complex ions
NRBBMAD	data points in formula used for RBB
NRBFMAD	data points in formula used for RBF
NCBBMAD	data points in formula used for CBB
NCBFMAD	data points in formula used for CBF
NRFFMAD	data points in formula used for RFF
NCBXMAD	data points in formula used for CBX
NRLLMAD	data points in formula used for RLL
NRLUMAD	data points in formula used for RLU
NRDIMAX	radiative di-electronic transitions
NRDIMAD	data points in formula used for RDI
NSIG	size of array SIGBF (NRBF× frequency points)

NSIG uses the number of frequency points between the thresholds and the maximum energy. This reduces the size of he array SIGBF and saves core memory.

These PARAMETERS are given in the output of *ATOMS2* and *SETF2* (please use e.g. `grep para` to extract them for this output). The PARAMETER NSIG is named there NRBFMAW. In the PARAMETER files used for the compilation of *LINE1*, NSIG has to be eliminated from *PARA3.INC* and NRBFMAW has to be added in *PARA1.INC* accordingly.

5.3 Input and Output Files

The program *PRO2* expects the following input files (only those which are marked with "*" are necessary):

ATOMS*
atomic-data file (Sect. 2)

DATEN*
contains all input cards, used as a here document for STDIN (file name can be freely chosen)

FGRID*
frequency grid (Sect. 3)

MODIN*
start model (Sect. 4)

RBF_CUTOFF

optional input file, that can be used to set specific bound-free absorption cross-section equal to 0, starting at a given frequency.

Example:

```
cat > RBF_CUTOFF << eos
LOW␣␣␣␣␣␣␣UP␣␣␣␣␣␣␣␣CUTOFF-FREQUENCY
C432S␣␣␣␣C522S␣␣␣␣1.0E16
HE28␣␣␣␣␣HE31␣␣␣␣␣1.2E17
```

The first record in *RBF_CUTOFF* (in the above example !) is optional.

The program *PRO2* creates the following output files:

MODOUT
(output model)

NEGDENS
Indicates that negative density values exist in *MODOUT*. *MODOUT* can be read by *LINE1* and transformed into a formatted version. This model may be edited then.

STOP
Indicates that a model converged. *PRO2* will stop immediately in case that this file exists in the working directory because it assumes convergence then (cf. Sect. 10). This can be used to stop *PRO2* calculations (e.g. to restart the jobs with a changed input file *DATEN*.

5.4 Input Options

The program *PRO2* can be controlled by a number of input options. Some of them are initialized with a *default* value (indicated by *) and can be omitted if no other values shall be requested. Indispensable blanks are indicated by ␣. Numerical data can be inserted *format free*.

```
.  whatever
```

commented by "." in the first column, disregarded by *PRO2*

```
ABUNDANCE␣AA x
```

introduces the abundance of the element `AA` (flushed to the left). The input x is the number ratio relative to hydrogen. If the start model contains already the element AA, this card is disregarded.

```
ABUNDANCE␣AA␣x␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣MASS␣FRACTION
```

introduces the abundance of the element `AA` (flushed to the left). The input x is the *mass fraction*. If the start model contains already the element AA, this card is disregarded.

```
ACCELERATION␣OF␣CONVERGENCE␣FROM␣ITERATION 999*
```

the Ng method for acceleration of convergence is used, starting from iteration 999. After every 4th iteration, all photospheric parameters are extrapolated from the previous iterations.

`BROYDEN=0*,␣␣␣SWITCH-LIMITS␣␣0-->1,␣1-->2,␣2-->1␣:  1.E-33* 1.E-33* 1.E+33*`

This option invokes a quasi-Newton method ("Broyden method") instead of the Newton-Raphson iteration of the linearized equations.

=0 Newton-Raphson iteration

=1 Broyden method, at the beginning of each Scharmer iteration started by a normal Newton-Raphson iteration step. This is only suitable for diagonal operators ($\Lambda = 3$).

=2 Broyden method, at the beginning of each Scharmer iteration started with the updated matrix of the last Scharmer iteration. This is only suitable for diagonal operators ($\Lambda = 3$).

=3 like `BROYDEN`=1, but suitable for tridiagonal operators ($\Lambda = 4$).

=4 like `BROYDEN`=2, but suitable for tridiagonal operators ($\Lambda = 4$).

The three switch-limits ϵ_1, ϵ_2, ϵ_3 indicate

ϵ_1 switch from `BROYDEN=0` $\rightarrow$ `1`, if the relative corrections of the Scharmer iteration are smaller than ϵ_1. Is ($\epsilon_1 \geq$1.E33) required, the 1st Scharmer iteration immediately starts with the Broyden method.

ϵ_2 switch from `BROYDEN=1` $\rightarrow$ `2`, if the relative corrections of the Scharmer iteration are smaller than ϵ_2.

ϵ_3 switch back to the next lower `BROYDEN` stage, if the relative corrections for the temperature or the electron density a higher than ϵ_3. This shall avoid divergent iterations.

While in the case of diagonal operator the switches occur locally following local criteria, the tridiagonal operators require global judgement and used the highest relative correction found in the whole atmosphere. Informations about the switches can be printed to STDOUT (see below).

`CHANGE␣EFFECTIVE TEMPERATURE␣x`

generally, *PRO2* takes the information about $T_{\rm eff}$ from the start model (Sect. 4). With this card, the another $T_{\rm eff}$ can be chosen. This works in small steps and takes much less time than the calculation of a new model with almost the same parameters.

`CHANGE␣LOGG␣x`

like `CHANGE EFFECTIVE TEMPERATURE`, but for a new value of the surface gravity g

`CHANGE␣ABUNDANCE␣AA␣x␣␣␣␣␣␣␣␣MASS␣FRACTION`

like `CHANGE EFFECTIVE TEMPERATURE`, see `ABUNDANCE` for `MASS FRACTION`.

`COMMENT:`

With this card any comment can be printed at the beginning of the output.

`DEPTH␣DEPENDENT␣LINE␣PROFILES,␣LINEARIZATION:␣XXXXX`

This option `XXXXX` = `FIRST` or `EACH␣` is indispensable if depth dependent line profiles shall be calculated. `FIRST` saves a lot of computational time.

`ERRNEW=1.E-10`*

limit for the relative corrections to stop the linearizations

`ERRSCH=1.E-04`*

limit for the relative corrections to stop the Scharmer iteration

`FORMAL␣SOLUTION`

PRO2 carries out two formal solutions (with/without line opacities) and saves the line profile in the file `LINES`.

`FREQUENCY␣GRID␣FORMATTED`

The frequency grid *FGRID* (input) is formatted.

`STEP␣UP␣F-VALUES:␣*****-START:␣IIII␣`x_1 x_2 x_3

The oscillator strengths of all lines of a selected ion IIII are reduced by a factor of x_1 at the beginning of the iterations and stepped up by a factor of x_2 every x_3 Scharmer iterations.

For ***** the two possibilities `INPUT` or `MODEL` can be requested. With `INPUT`, *PRO2* uses the values of x_1, x_2, and x_3 as requested in the card; with `MODEL`, *PRO2* reads these values from the start model (Sect. 4) if a previous *PRO2* has not reached unity for all step-up values and thus, written them to the output model.

`STEP␣UP␣F-VALUES:␣NO␣KANTOROVICH␣RESET␣AFTER␣STEP␣UP`

In general, after each increase of f-values, the Broyden/Kantorovich method is reset. This card suppresses this reset.

`STEP␣UP␣F-VALUES:␣LIMIT␣FOR␣ABS.␣REL.␣NG␣CORRECTION␣x`

In case that the absolute relative total density correction exceeds x (default value: 0.1), the next step up is skipped.

`GAMMA=1`*

The value defines the optical depth $\tau_\nu = \gamma$ which separates the region of the line wing for which the *core* and the *wing* approximations shall be used.

`IGNORE␣CPU␣TIME␣LIMIT`

set the security time (necessary to complete the job) equal 0. This can only be used if it is sure that the requested number of iterations can be completed within the jobs run time limit.

`INCREASE␣COLLISIONAL␣RATES␣BY␣FACTOR␣x`

The collisional rates can be increased in order to simulate a LTE model atmosphere. The factor x has to be $> 10^{+30}$, in order to guarantee that collisions dominate the photosphere ...

`INNER␣BOUNDARY:␣LAMBDA-ITERATION`

`INPUT-MODEL␣FORMATTED`

`ITMAX=1`*

maximum number of Scharmer iterations

`JACOBI␣FRESH-UP,INTERVAL 5`*

calculation of the Jacobian every 5^{th} Scharmer iteration. Only valid in case of Broyden or Kantorovich method.

`KANTOROVICH=2,␣␣␣␣SWITCH LIMITS␣␣␣0-->1,␣1-->2,␣2-->1␣:  1.E33`* `0.1`* `1.0`*

like the `BROYDEN` card.

=0 Newton-Raphson iteration

=1 Jacobian is calculated at the beginning of every Scharmer iteration but then kept constant.

=2 Jacobian is calculated at the beginning of the 1st Scharmer iteration but then kept constant. A new calculation of the Jacobian is done following the JACOBI␣FRESH-UP card (see above)

`LINEARIZE␣HYDROSTATIC␣EQUATION`

With this option the hydrostatic equation is solved simultaneously with the statistical equation and not (default) solved subsequently.

`NO␣RENORMALIZATION␣OF␣COMPLEX␣LINE␣CROSS␣SECTIONS`

undoes a previously made re-normalization of the *sample* cross-sections for iron group elements

`NO␣TEMPERATURE␣CORRECTION`

the radiative equilibrium is omitted from the linearization

`T-CORRECTION␣ONLY␣IN␣LOG␣M␣INTERVAL:␣`m_{min} m_{max}

the temperature correction is restricted to the selected $\log m$ interval.

`T-CORRECTION␣PROFILE:␣X`

the temperature correction is damped by simple functions (ND = total number of depth points)

X	
1	depth point / ND
2	(depth point / ND)^2
3	$\sqrt{depthpoint/ND}$

`LAMBDA=3`*

selects the Λ operator

$\Lambda = 3$ diagonal operator by Olson & Kunasz

$\Lambda = 4$ tridiagonal operator by Olson & Kunasz

Both operators are generally parameter-free. In practice, it is less time consuming to do a Λ iteration in the optical thin case. This can be done by requesting a special `GAMMA` parameter (see above).
In order to accelerate the convergence, both operator switch to *core saturation* if $\tau_\nu > 100$.

`LINEARIZATION␣MODE:␣BLOCK-MATRIX-ITERATION,␣XX YY ZZ`

with this option, only the occupation numbers of the given elements (here XX YY ZZ) are iterated. In combination with the card `SOLVE STATISTICAL EQUATIONS ONLY`, a "classical" *line formation* iteration is done. In all depth points, XX is Newton-Raphson iterated (inclusive constraint equations) first, then YY, and at least ZZ. *Attention: this option alone does not switch off the constraint equations!*

`LINEARIZATION␣MODE:␣BLOCK-MATRIX-ITERATION,␣ALL`

like `LINEARIZATION MODE: BLOCK-MATRIX-ITERATION, XX YY ZZ`. All elements are iterated in order of their appearance in the atomic data file *ATOMS*.

`MICROTURBULENCE␣[KM/S] 0.0`*

with this option, the microturbulence pressure is considered in the hydrostatic equation but **not** in the calculation of the line profiles!

`NEWMAX=1`*

maximum number of linearizations

`OCCUPATION␣PROBABILITY␣FORMALISM␣FOR␣AA`

The Hummer-Mihalas (HM) formalism is used to calculate the level dissolution for AA = H1 or AA = <ion>.

`OPACITY␣PROJECT␣RBF␣DATA␣:  START␣AT␣EDGE`

PRO2 can calculate bound-free cross-section using data from the Opacity Project (OP). Here the OP data set is used and the cross-sections start at the threshold energy of the respective level.

`OPACITY␣PROJECT␣RBF␣DATA:␣FULL␣DATA␣SET`

see above, the complete OP data set is used (which may start at lower energy the the level energy in order to simulate the transition from the line absorption to the continuous absorption at the series limit.

`OPACITY␣PROJECT␣RBF␣DATA:␣ONLY␣EDGE␣VALUE`

see above, a mean value of the OP data at the threshold energy is calculated, then the absorption cross-sections are calculated using the Seaton formula in hydrogenic approximation.

`OPACITY␣PROJECT␣RBF␣DATA:␣MISSING␣HYDROGENIC`

see above, for those levels which are not found in the OP data set hydrogen-like threshold cross-sections are calculated. Then, the Seaton formula is used.

`OPACITY␣PROJECT␣RBF␣DATA:␣HYDROGENIC`

see above, all bound-free transitions, which are found in the atomic data file *ATOMS* and request explicitly the use of OP data are calculated with hydrogen-like threshold cross-sections and the Seaton formula.

`OUTPUT-MODEL␣FORMATTED`

`RADIATIVE␣EQUILIBRIUM:␣DIFFERENTIAL/INTEGRAL␣FORM`

The radiative equilibrium is calculated using a combination of the differential and the integral method.

`READ␣NEW␣TEMPERATURE␣STRUCTURE`

A temperature structure is read in from file *TEMPERATURE.IN*. This temperature may be interpolated from other models in order to speed up the calculation of "in-between" models. *TEMPERATURE.IN* is an ASCII table with $\log m$ and T, however, the $\log m$ values are ignored.

`REDUCE␣LOG␣CVEC␣x`

This options scales the inhomogeneity vector of the linearized equations. This is useful to overcome numerical instabilities and to avoid too-large corrections in the beginning of the iterations. This card has to be inactivated to get a finally converged model.

`SAVING␣MODEL:␣EACH␣ITERATION`

a temporary model (MODTMP) is saved in the working directory $TMPDIR. An example how to save this temporary model automatically in case of a failed model calculation is given in Sect. D.8.5.
An
ln -sf MODTMP ${name}
before the start of the model calculation, where ${name} is the assigned name of the output model helps to identify the model.

`SET␣TEMPERATURE t` $\log m_1$ $\log m_2$ `[scaling factor]`

within $\log m_1 \leq \log m \leq \log m_2$, the model temperature is set to

$t > 0$: t

$t = -1$: cubic-spline interpolation of t

$t = -2$: linear interpolation of t

$t = -3$: t read from model TIN

$t = -4$: t is temperature value of next depth point with $\log m > \log m_2$.

$t = -5$: like $t = -3$, but an additional third argument (scaling factor) has to be given that is multiplied to the TIN temperature

`SHIFT␣EDGE␣BBBBBBBBBBFFFFFFFFFF x`

The absorption threshold of the level `BBBBBBBBBBFFFFFFFFFF` given in the *TMAP* code (Sect. 2.1) is artificially shifted to the frequency point x. *Attention: The given frequency x has to fit exactly a point within the frequency grid* FGRID*!* All shifts are printed to STDOUT.

`SKIP␣ATOM␣AA␣BELOW x`

the element AA (flushed to the left) with occupation numbers less than x are eliminated from the statistical equations

`SKIP␣ION␣III␣BELOW x`

ion III (flushed to the left) with occupation numbers less than x are eliminated from the statistical equations

`SKIP␣LEVELS␣BELOW x`

levels with occupation numbers less than x are eliminated from the statistical equations

`SKIP␣OCCDRVF␣AFTER␣1ST␣LINEARIZATION`

The derivations of the source functions are only calculated once (in the 1st linearization) and are then kept fixed. *Attention: This saves an enormous amount of computational time in case of many NLTE levels and many frequency points but it works well only in the case of almost converged models.*

`SOLVE␣STATISTICAL␣EQUATIONS␣ONLY`

switches off the constraint equations for n_e, n_H, n_g, T

`SOLVE␣STATISTICAL␣EQUATIONS␣ONLY␣␣␣RE-SOLVE PARTICLE CONSERVATION`

switches off the constraint equations for n_e, n_H, n_g, T within the Newton-Raphson iteration. The hydrostatic and particle conservation equations are then solved subsequently.

`SWITCH␣OFF␣LINES`

All line transitions are ignored. *Attention: sample lines of iron-group elements can not be switched off.*

`TIME␣LIMIT 2000`*

cpu time for the job to calculate. Only valid on non-CRAY machines

`TRANSITION␣IN␣DETAILED␣RADIATIVE␣BALANCE␣XXXXXXXXXXYYYYYYYYYY`

With this option, the radiative transition `XXXXXXXXXXYYYYYYYYYY` given in the *TMAP* code (Sect. 2.1) is calculated in detailed radiative equilibrium. Thus, this transition is eliminated from the statistical equations but not from the calculation of the opacities and emissivities.

`UNSOELD-LUCY␣TEMPERATURE␣CORRECTION␣DAMP= x`

With this option, the radiative equilibrium is eliminated from the linearization. The temperature structure is calculated after the linearizations with the Unsöld-Lucy temperature correction method. The damping factor x is used to avoid over-corrections and numerical instabilities.

`UPPER␣AND␣LOWER␣LIMITS␣FOR␣RELATIVE␣T-CORRECTION␣`t_1 t_2

The relative temperature corrections (iteration i) are limited to the range $T_i \cdot t_1 \leq T_{i+1} \leq T_i \cdot t_2$ at

all depth points.

5.5 Output Options

The following `PRINT` and `PLOT` cards create output on STDOUTt and plot data files, respectively. The plot files are written in *WRPLOT* readable format. The option should be easily understandable ... Generally, for `XXXX EACH` or `LAST` can be inserted. ii indicates an I2 format specifier (FORTRAN).

5.5.1 Output to STDOUT

`PRINT␣ABUNDANCES`

`PRINT␣BROYDEN␣INFORMATIONS`

`PRINT␣CORRECTIONS␣OF␣LAST␣LINEARIZATION,ITERATION:LAST,DEPTH␣INCREMENT: i`

`PRINT␣CORRECTIONS␣OF␣TOTAL␣DENSITIES,ITERATION:LAST,DEPTH␣INCREMENT: i`
in the case of non-linearization of the hydrostatic equation (default, see above)

`PRINT␣CP-TIME/ITERATION,XXXX`

`PRINT␣DATA␣FOR␣DIELECTRONIC␣RECOMBINATIONS`
prints especially the frequencies which are selected by *PRO2*.

`PRINT␣DEPARTURE␣COEFFICIENTS,ITERATION:XXXX,DEPTH␣INCREMENT:15`

`PRINT␣EMERGENT␣FLUX,ITERATION:XXXX`
prints also $T_{\rm eff}$, which is an sensitive control parameter

`PRINT␣FREQUENCY␣GRID`

`PRINT␣INFORMATION␣ABOUT␣INPUT␣SAMPLE␣CROSS␣SECTIONS`

`PRINT␣INPUT␣MODEL,DEPTH␣INCREMENT:ii`

`PRINT␣INPUT␣MODEL,DEPTH␣INCREMENT:ii␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣(STRUCTURE␣ONLY)`

`PRINT␣INTEGRATED␣SURFACE␣FLUX,ITERATION:XXXX`

`PRINT␣KANTOROVICH␣INFORMATIONS`

`PRINT␣LEVELS`
prints level names, energies, and statistical weights of all LTE / NLTE levels

`PRINT␣LEVEL␣SKIP␣INFORMATION`

`PRINT␣MAX.␣REL.␣CORRECTIONS␣EVERY␣ii␣ITERATIONS`

`PRINT␣OCCUPATION␣PROBABILITIES,ITERATION:XXXX,DEPTH␣INCREMENT:ii`

`PRINT␣OPACITY␣PROJECT␣INFORMATION`

`PRINT␣OUTPUT␣MODEL,ITERATION:XXXX,DEPTH␣INCREMENT:ii`
prints temperature and density structure, **and** all occupation numbers of the NLTE levels

`PRINT␣OUTPUT␣MODEL,ITERATION:XXXX,DEPTH␣INCREMENT:ii␣␣␣(STRUCTURE␣ONLY)`
prints temperature and density structure

`PRINT␣MODEL␣ATOMS␣(OVERVIEW)`

`PRINT␣NUMBER␣OF␣FUV␣PHOTONS`

`PRINT␣OPTIONS`
prints the most important input parameters

`PRINT␣PARAMETER␣NSIG`
for the optimization of the PARAMETER NSIG, NRLUMAD, and NRLLMAD

`PRINT␣RADIATION␣FIELD,ITERATION:XXXX,DEPTH␣INCREMENT:ii`

`PRINT␣RBF␣CUTOFF␣FREQUENCIES`
prints the frequency where the RBF cross-section of a level is set equal 0

`PRINT␣ROSS,ITERATION:LAST`
print the value of ROSS for the inner boundary condition

`PRINT␣TAUSCALES,ITERATION:XXX,DEPTH␣INCREMENT:ii`

`PRINT␣WARNINGS`

`LP-PLOT␣OPTICALLY␣THICK/THIN,ITERATION:XXXX`

A plot of the $\tau = 1$ limit in the atmosphere is printed and saved in a file (*PLLP*).

5.5.2 Output into Plot Data Files

`PLOT␣CORRECTIONS`
Plot data is written into file *PLOTCORR*.

`PLOT␣DEPARTURES xmin xmax ymin ymax`
Plot data is written into file *PRFLUX*.

`PLOT␣␣EMERGENT␣FLUX,ITERATION:XXXX`
Same like PRINT card, output is written into file *PRFLUX*.

`PLOT␣FLUX xmin xmax ymin ymax`
Plot data is written into file *PRFLUX*.

`PLOT␣IONIZATION␣FRACTIONS AA xmin xmax ymin ymax`
Plot data is written into file *IONPLOT*.

`LP-PLOT␣OPTICALLY␣THICK/THIN,ITERATION:XXXX,FILE␣ONLY`
A plot of the $\tau = 1$ limit in the atmosphere is saved in the file *PLLP* only.

`PLOT␣RBF␣CROSS␣SECTIONS XXXXXXXXXXYYYYYYYYYY 0 0 0 0`
The RBF cross section of level XXXXXXXXXXYYYYYYYYYY is saved in the file *PLRBF*.

`PLOT␣TEMPERATURE␣STRATIFICATION`
Plot data is written into file *STRUCTURE*.

6 Adjust the log m Intervals of Existing Models: CUTM and NDSCALE

6.1 Adjust log m Intervals of Models

One boundary condition of *TMAP* is that at least the outer two depth points have to be optically thin and at least the inner two depth points have to be optically thick.

For the calculation of model grids, it is an advantage to use approximately the same $\log m$ interval for all models as well as the frequency grids (see above).

In case of numerical instabilities it may be helpful to adjust the $\log m$ interval of existing models. This is done by *CUTM* (to reduce the $\log m$ interval, both minimum and maximum) and *EXTEND* (to reduce the minimum $\log m$).

Since the number of depth points will deviate from the standard of 90, *NDSCALE* can interpolate models with any number of depth points to a new models with a chosen number of depth points.

6.1.1 Reduce the Depth Interval: CUTM

First copy a binary TMAP model (90 depth points) to the file MODIN, and start e.g. /home-/rauch/bimod/cutm.Linux_x64. *CUTM* asks for the $\log m$ interval and writes the reduced model to the file MODOUT. The following displays an example batch-job file for *CUTM*:

```
#!/bin/sh
set +x;.  ${HOME}/.jobstart
# do not edit the beginning of this file
########################
## own job following ##
########################
cp <binary input model> MODIN
/home/rauch/bimod/cutm${sys} << eos
-7.50
+2.00
eos
mv MODOUT <binary output model>
#
# do not edit the rest of this file
######################
set +x; ${HOME}/.jobend ${TMPDIR}
```

6.1.2 Extend a Model Atmosphere to the Outside: EXTEND

Start with the creation of a formatted TMAP model and copy it to the file *MODIN*. Write the number ND of depth points of this models into the file *MODIN_ND*. and start e.g. /home-/rauch/bimod/extend.Linux_x64. *EXTEND* asks for the $\log m$ minimum and writes the extended model to the file *MODOUT*. The following displays an example batch-job file for *EXTEND*:

```
#!/bin/sh
   set +x;.  ${HOME}/.jobstart
   # do not edit the beginning of this file
   ########################
   ## own job following ##
   ########################
   echo ‘‘90’’ > MODIN_ND
   cp <formatted input model> MODIN
   /home/rauch/bimod/extend${sys} << eos
   -8.00
   eos
   mv MODOUT <binary output model>
   #
   # do not edit the rest of this file
   ####################
   set +x; ${HOME}/.jobend ${TMPDIR}
```

6.1.3 Interpolate Models for a New Depth-Point Number: NDSCALE

NDSCALE can interpolate a model to a new number of depth points. The may be necessary in case that the $\log m$ interval of a model was adjusted (Sect. 6.1).

Copy a binary TMAP model to the file MODIN, and start e.g. /home/rauch/bimod/ndscale.Linux_x64. *NDSCALE* asks for the old and new number of depth points and writes the interpolated model to the file MODOUT. The following displays an example batch-job file for *NDSCALE*:

```
   #!/bin/sh
   set +x;.  ${HOME}/.jobstart
   # do not edit the beginning of this file
   ########################
   ## own job following ##
   ########################
   cp <binary input model> MODIN
   /home/rauch/bimod/ndscale${sys} << eos
   75
   90
   eos
   mv MODOUT <binary output model>
   #
   # do not edit the rest of this file
   ####################
   set +x; ${HOME}/.jobend ${TMPDIR}
```

7 Interpolate between Existing Models: INTER

7.1 Interpolate between Existing Models

/home/rauch/bimod/inter.Linux_x64. *INTER* read two models, *MOD.1* and *MOD.2*, that have been calculated with the same *ATOMS* and same number of depth points, and linearly interpolates them to *MOD.I*. This model can be used ideally as a start model for PRO2.

8 NLTE Line Formation and Models: LINE1

The program *LINE1* calculates — based on a suitable start model (Sect. 3) — model atmospheres like *PRO2*, NLTE occupation numbers at fixed temperature and (optional) density stratification (e.g. for new levels in the case of extended model ions), and theoretical line profiles of selected lines under consideration of the most recent line broadening theories.
The input and output options are generally the same like those of *PRO2* (Sect. 5.4 and 5.5).

8.1 Input Files

The program *LINE1* expects the following input files (only those which are marked with "*" are necessary):

ABUNDi
It is possible to read occupation numbers for newly implemented levels from 14 additional, already existing models (→ *MODINi*). *i* (from *ABUNDi*) is a number from 1 to 9 (model 1 is *MODIN*, with abundance file **ABUND**, model 2 is *MODIN2*, with abundance file **ABUND2**, etc.) and 0, A, B, C, D, E for 10, 11, 12, 13, 14, and 15, respectively. . Abundance ratios are taken from the first model that includes the element, i.e., with ascending priority from 1^{st}, 2^{nd}, ..., 15^{th} model. If the elemental abundances of the input model (→ *MODIN*) and of the models *MODINi* differ, scaling factors can be given in the files *ABUNDi* which are applied to the occupation numbers of the model *MODINi*, respectively.

Example:

```
C␣2
N␣1.3
```

It is recommended to add the complete set of occupations numbers to a model that does not include the respective species. Otherwise the lower levels may artificially be underoccupied.

ADJUST
In practice NLTE model atmosphere calculations have shown that is is not possible in all cases to consider all line transitions simultaneously from the beginning. One method to overcome this problem is to reduce the oscillator strengths at the beginning with reduction factors which increase to unity in the course of the iteration.

The input file *ADJUST* contains the reduction factors and the factors with which the reduction factors are increased every iteration until the original oscillator strengths are reached.

Example:

```
C4_______C4_______ 1.0E-5 1
C422S␣␣␣␣␣C422P␣␣␣␣␣ 0.01 1.05
C452S␣␣␣␣␣C452P␣␣␣␣␣ 1.0E+5 1.0E+00
```

means:

the oscillator strengths of all C IV line transitions are reduced by a factor of 10^{-5}. This factor is constant over the whole calculation. Additionally, the C IV 2s-2p line is individually reduced by the factor of 0.01 (→ total of 10^{-7}) but this factor (0.01) is increased by 5% every iteration. The C IV 5s-5p line is considered with its correct oscillator strength ($10^{-5} \cdot 10^{+5} = 1$). *In the case that the temperature correction yields negative temperatures, the oscillator strengths are kept at their last value.*

ATOMS*
atomic data file (Sect. 2), like for the start model or extended ...

DATEN

input and output options (Sect. 5.4, 5.5, and 8.3)
this files has to be copied to stdin because *LINE1* reads the options from there (e.g. `/home/rauch/bimod/line1 < DATEN`).

DISTA
The frequency grid for the detailed calculation of line profiles is created by *LINE1* itself. The discretization of the frequency points within the line transitions can be split in intervals with different distances from point to point in order to represent the line centers or possible forbidden components (e.g. → He I λ4471Å) with a sufficient number of (narrowly spaced) frequency points. *DISTA* contains informations how many points at which distance ($\Delta\lambda$ in Å) shall symmetrically (to the line center) be inserted in these intervals.
Example:

```
5 0.1
10 0.3
15 0.5
```

results in points at ($\Delta\lambda$ in Å, only the "red" wing given):
0.0, 0.1, 0.2, 0.3, 0.4, 0.7, 1.0, 1.3, 1.6, 1.9, 2.4, 2.9, 3.4, 3.9, 4.4

In case of many lines and a high resolution, the parameter NRBBMAD (Sect. 1) may become very high. Due to compiler limitations in the size of arrays, no executable may be created then. To avoid this, the use of a respective *F_BASE* file (Sect. 3) and an adjusted *DISTA* is recommended.
Example:

F_BASE creates an equidistant frequency grid from 3000 Å to 7000 Å ($\Delta\lambda = 0.1$ Å), then a *DISTA*

```
2 0.01
4 0.02
6 0.03
8 0.05
9 100.00
10 0.01
```

is sufficient (narrow points only until the *F_BASE* resolution is reached, then just an end point of the line and a CONT/(BLUE/RED) point (Sect. 3). In addition, a dynamical use of *DISTA* in *LINE1_PROF* is helpful and is described in Sect. 9.

FGRID*
frequency grid (Sect. 3), not necessary in the case of line profile calculations (see above)

ION
contains the code for the selected ion (line profile calculations). It differs from the *TMAP* code (Sect. 2.1): the element is given in CHARACTER∗2 format (flushed to the left) and the ionization stage is indicated in the third (and fourth) column.

Examples:

```
HE2
C␣2
CA10
```

SETF2 creates this file for a given atomic-data file (Sect. 3).

LINIEN this file contains information about the range which has to be considered in the calculation of the line profiles and the selected line to calculate:

`BLENDRANGE␣␣␣␣␣40.0`*

This card is of special importance and has to be the **first record** in *LINIEN*.
• *LINE1* searches in the interval $[\lambda_o - \lambda_{Blendrange}, \lambda_o + \lambda_{Blendrange}]$ for line frequency points (Sect. 3) of other line transitions. All line transitions with points between CONT RED and CONT BLUE of the selected line (see below), are regarded as a blend and included in the calculation in detail. All other line transitions in the input file *ATOMS* (see above) are disregarded in the creation of the internal atomic data and frequency grid files by *LINE1*. This minimizes both, core memory and computational time requirements.
• *LINE1* considers in the creation of the internal atomic data and frequency grid files only those radiative bound-free (RBF) transitions with an ionization energy smaller than $c/(\lambda_o - \lambda_{Blendrange})$ because RBF transitions with a higher ionization energy do not contribute to the opacity within the blendrange. This minimizes also the core memory and computational time requirements.

`XXXXXXXXXXYYYYYYYYYY`

TMAP code (Sect. 2.1) of selected lines for which theoretical line profiles shall be calculated
SETF2 creates this file for a given atomic-data file (Sect. 3).

MODIN*
start model (Sect. 4)

MODINi
see **ABUNDi**

OP_RBF_XXXX
bound-free cross-sections from the Opacity Project for levels of the ion XXXX

STARK_H1
VCS-like Stark broadening tables for H I
H I line-broadening has changed in since 2008. The reason is that an error (for high members of the spectral series only) in the H I line-broadening tables by Lemke (1997) that were used before. Tremblay & Bergeron (2009) and Tremblay & Bergeron (2015, priv. comm.) provide, parameter-free Stark line-broadening tables for H I considering non-ideal effects. These replaced Lemke's data for the lowest members of the Lyman ($n - n' = 1 - [2 - 21]$), Balmer ($n - n' = 2 - [3 - 22]$), Paschen ($n - n' = 3 - [4 - 22]$), and Brackett ($n - n' = 4 - [5 - 14]$) series. These profiles can only consistently used with the Hummer & Mihalas (1988) equation-of-state (cf.,

`OCCUPATION␣PROBABILITY␣FORMALISM␣FOR␣H1`

in Sect. 5.4). For higher series members, we use the Holtsmark approximation.

STARK_ALIII
tables for Al III (Dimitrijević & Sahal-Bréchot 1993a)

STARK_HE1
tables of Barnard et al. (1969) and Griem (1974) for He I

STARK_HE2
VCS-like tables for He II (Schöning & Butler 1989a,b)

STARK_C4
tables for C IV (Schöning 1993)

STARK_N5
tables for N V (Schöning 1995)

STARK_HEI

tables for He I (Dimitrijević & Sahal-Bréchot 1990)

STARK_CIV
tables for C IV (Dimitrijević et al. 1991b; Dimitrijević & Sahal-Bréchot 1992c)

STARK_CV
tables for C V (Dimitrijević & Sahal-Bréchot 1996)

STARK_NV
tables for N V (Dimitrijević & Sahal-Bréchot 1992b)

STARK_OIV
tables for O IV (Dimitrijević & Sahal-Bréchot 1995)

STARK_OV
tables for O V (Dimitrijević & Sahal-Bréchot 1995)

STARK_OVI
tables for O VI (Dimitrijević & Sahal-Bréchot 1992a)

STARK_SIIV
tables for Si IV (Dimitrijević et al. 1991a)

STARK_SVI
tables for S VI (Dimitrijević & Sahal-Bréchot 1993b)

Note: For H I, He I, He II, C IV (STARK_C4), and N V STARK_N5 the tables have only to be loaded. *LINE1* uses these data files if they are available. For the other ions an option has to be given (see below) in *DATEN* to use the broadening tables for all lines of the ion, or for selected line transitions by requesting formula 5 (keyword `RBB`) in *ATOMS* (Sect. 2).

8.2 Output Files

The program *LINE1* creates (besides STDOUT) the following plot data files (in accordance with the options given). Note that in general wavelengths ≤ 3000 Å are given as vacuum wavelengths and wavelengths > 3000 Å as air wavelengths.

ANGJ_C.DAT
specific intensity (continuum only) for different angles (see PARAMETER NA, Sect. 1)

ANGJ_L.DAT
specific intensity for different angles (see PARAMETER NA, Sect. 1)

PLDEP
departure coefficients for selected levels

PLDIFF
abundance profiles for all elements

PLEFL
emergent flux (complete frequency interval)

PLLP
limit $\tau = 1$ (complete frequency interval)

PLPRF
line profiles

PLRBF
bound-free cross-sections of selected levels

PLWF
emergent flux ($F_\lambda(\lambda)$ – WF denotes wavelength + flux.

PLWFP
emergent flux ($F_\lambda(\lambda)$ and relative flux F_λ / $F_{\rm cont}$ – WFP denotes wavelength + flux + normalized flux (profiles ...).

PLWFP_VACUUM
emergent flux ($F_\lambda(\lambda)$ and the relative flux F_λ / $F_{\rm cont}$ – WFP_VACUUM denotes wavelength + flux + normalized flux (profiles ...). *All wavelengths are vacuum wavelengths.*

PLWP
emergent flux ($F_\lambda(\lambda)$ – WP denotes wavelength + normalized flux (profiles ...).

STRUCTURE
temperature stratification

For the evaluation and visualization of the output and plot data files several auxiliary programs are available (Sect. 11).

8.3 Options

For *LINE1* most of the options described in Sect. 5.4 and 5.5 are valid. There are some further options. Their meaning should be clear ...

`ACCEPT␣CHANGED␣EFFECTIVE␣TEMPERATURE␣X`

LINE1 generally takes $T_{\rm eff}$from the start model (*MODIN*). For very large models the change of $T_{\rm eff}$ (in small steps) takes much less times than the complete new calculation with mainly the same (!) parameters. However, still some iterations are needed ...

`ACCEPT␣CHANGED␣ABUNDANCES`

LINE1 generally takes the chemical composition from the start model (*MODIN*) and ignores `ABUNDANCE` cards in the input file but for newly implemented elements. For very large models the change of the abundances (in small steps) takes much less times than the complete new calculation with mainly the same (!) parameters. However, also still some iterations are needed ...

`CPU-TIME␣TTTTT`

maximum CPU time for the job, TTTTT given in seconds

`CPU-TIME␣0.0`

This card transfers the total cpu time (then: stop) to *LINE1*. There are load dependent variations

of the system cpu time which accounts to the user cpu time. These variations can effect the security time needed by *LINE1* in order to complete the iteration, write the model, etc.

`DOPPLER␣PROFILES`

This option sets the line broadening of all line transitions in the atomic data file *ATOMS* generally to Doppler line broadening. This can be used for a quick overview about blends within a selected range.

`FORCE USE OF LINE BROADENING TABLES`

This option enables the use of line broadening tables instead of approximate formulae during the model atmosphere calculation.

`ITERATION␣IN␣DEPTHS ii jj kk`

The the first kk iterations are carried out only between depth points ii – jj.

`LINE␣TEMPERATURE␣FROM␣FORMATION␣DEPTH`

The line temperature $T_{\rm line}$ is by defaults set to $\frac{3}{4} \cdot T_{\rm eff}$ (Sect. 3). The different lines form in very different depths, i.e. at different temperatures. This card allows to select the temperature at the formation depth ($\tau = 1$) of the line core for every lines as line temperature, respectively.

`LINEARIZATION␣MODE:␣BLOCK-MATRIX␣ITERATION,␣ION`

analogously to `LINERIZATION␣MODE` ... in Sect. 5.4. This card allows to select one single ion to iterate.

`MATRIX␣INVERSION:␣MINV`

The matrix inversion for the solution of the statistical equations is carried out by the SCILIB routine MINV. *Attention: numerically instable for* $n > 200, \ldots, 220$.

`MATRIX␣INVERSION:␣INV`

The matrix inversion is done by an own routine.

`MATRIX␣INVERSION:␣GIRL`

The matrix inversion is done by routine GIRL (single precision). More stable than MINV in some cases!

`MATRIX␣INVERSION:␣GIRLDP`

The matrix inversion is done by routine GIRL (double precision).

`MATRIX␣INVERSION:␣SGETRF␣+␣SGETRI`

The matrix inversion is done by the LAPACK routines SGETRF and SGETRI.

`MISSING OCCUPATION NUMBERS FROM I MODELS`

The occupation numbers of newly considered levels are read from I models ($I = \max i$, see *ABUNDi* and *MODINi*, above) in increasing order. A consequence of NLTE modeling is the over-population of low-lying levels. A strong extension of models towards higher levels will not consider their de-population and may underestimate the population of the lowest. In this case, use the REPLACE␣OCCUPATION␣NUMBERS card (see below).

`MICROTURBULENCE␣[KM/S]␣0.0`

analogously to Sect. 5.4. *LINE1* considers the microturbulence also in the calculation of the line profiles.

`NEWMAXB= 20*`

maximum number of linearizations of the Broyden or Kantorovich iterations

`REPLACE␣OCCUPATION␣NUMBERS␣FOR␣AAAA␣FROM␣MODEL␣I`

Occupation numbers of model I will be used for all levels of ion AAAA.

`USE␣DIMITRIJEVIC␣BROADENING␣TABLES␣FOR␣C␣IV`

With this option, all C IV line transitions in the atomic data file *ATOMS* are calculated with the stark broadening tables by Dimitrijević (if found there).

If the Dimitrijević tables shall be used only for selected lines, in *ATOMS* formula 5 instead of formula 3 or 4 has to be requested.(Sect. 3).
— The tables (Sect. 8.1) have to be loaded in any case . . . —

`USE␣DIMITRIJEVIC␣BROADENING␣TABLES␣FOR␣AL␣III`

`USE␣DIMITRIJEVIC␣BROADENING␣TABLES␣FOR␣C␣V`

`USE␣DIMITRIJEVIC␣BROADENING␣TABLES␣FOR␣HE␣I`

`USE␣DIMITRIJEVIC␣BROADENING␣TABLES␣FOR␣N␣V`

`USE␣DIMITRIJEVIC␣BROADENING␣TABLES␣FOR␣O␣IV`

`USE␣DIMITRIJEVIC␣BROADENING␣TABLES␣FOR␣O␣V`

`USE␣DIMITRIJEVIC␣BROADENING␣TABLES␣FOR␣O␣VI`

`USE␣DIMITRIJEVIC␣BROADENING␣TABLES␣FOR␣P␣V`

`USE␣DIMITRIJEVIC␣BROADENING␣TABLES␣FOR␣SI␣IV`

`USE␣DIMITRIJEVIC␣BROADENING␣TABLES␣FOR␣S␣VI`

all these cards like `USE␣DIMITRIJEVIC␣BROADENING␣TABLES␣FOR␣C␣IV`.

`PRINT␣ATOMIC␣DATA␣FILE␣ATOMS_2`

print the internally created atomic data file (see above) for the line profile calculations

`PRINT␣EQUIVALENT␣WIDTH`

A small table with the equivalent widths of all selected lines is printed to STDOUT.
Attention: For the calculation of the equivalent widths of the selected lines, the interval [CONT RED,CONT BLUE] (Sect. 3) is used — with all included blends
In order to study the equivalent widths of selected lines in detail the blendrange has to be set to a small-enough value that includes only the components of the multiplet or the atomic data file *ATOMS* has to be created with only the requested line transition.

`PRINT␣EQUIVALENT␣WIDTH␣(LONG)`

like `PRINT␣EQUIVALENT␣WIDTH` but this table includes all frequency points in the interval [CONT RED,CONT BLUE] and gives additionally the accumulated equivalent widths.

`PRINT␣MULTIPLET␣SPLITTING`

LINE1 is able to split the NLTE occupation number of multiplets (see above). With this card all multiplet splittings are reported.

`PRINT␣VCS␣TABLE`

`PRINT␣FORMATION␣DEPTH␣OF␣LINES␣AND␣THRESHOLDS`

`PRINT␣FREQUENCY␣GRID␣FGRID_2`

print the internally created frequency grid (see above) for the line profile calculations

`PRINT␣LEVELS␣WITH␣LTE␣START␣VALUES`

`PRINT␣LINES␣AND␣BLENDS`

`PRINT␣PROFILE␣TYPES`

With this option, information about the used line-broadening theories for all calculated lines is printed to STDOUT. The same information is always included in the plot data file *PLPRF* as far as the necessary plot option (see below) is active to create it.

`PRINT␣STATISTICS␣OF␣FGRID_2`

`PRINT␣WARNINGS`

```
PLOT␣EMERGENT␣FLUX␣␣LOG␣FNUE␣/␣LOG␣NUE
PLOT␣EMERGENT␣FLUX␣␣FNUE␣/␣NUE
PLOT␣EMERGENT␣FLUX␣␣LOG␣FLAM␣/␣LOG␣LAM
PLOT␣EMERGENT␣FLUX␣␣FLAM␣/␣LAM
PLOT␣EMERGENT␣FLUX␣␣FLAM␣/␣LAM␣␣INTERVAL: LAMBDAMIN LAMBDAMAX
```

```
PLOT␣LIMIT␣TAU=1,ITERATION:EACH
```

With this option, a plot file *PLLP* is created which contains the geometrical depth (logarithmical) of the limit $\tau = 1$ for the complete frequency grid. It can be plotted with the program *PLXY* (Sect. 11).

```
PLOT␣LINES
PLOT␣TEMPERATURE␣STRATIFICATION,ITERATION:LAST
PLOT␣TEMPERATURE␣STRATIFICATION,ITERATION:EACH
```

9 Synthetic Spectra: LINE1_PROF

The program *LINE1_PROF* calculates — based on a suitable start model (Sect. 3) — a synthetic spectrum and/or line profiles of selected lines under consideration of the most recent line-broadening theories.
The input and output options are the same like those of *LINE1* (Sect. 8).

`DIFFUSION MODEL`

read a diffusion model calculated by *NGRT*.
In general, an atomic data file for a selected wavelength range (in order to limit the number of frequency points) should be created using *ATOMS2*, e.g. with the card:

`LINEFORMATION␣-␣RBB-INTERVALL=[␣␣␣1000,␣␣␣7000],␣ION=NON`

The use of IrOnIc data for iron-group elements requires to use the same frequency grid for the calculation of the synthetic spectrum. Thus,

`PRINT␣ENTSTEHUNGSTIEFEN␣DER␣LINIEN␣UND␣KANTEN`

LINE1_PROF prints the formation depths of line cores and ionization edges

`PLOT␣IONIZATION␣FRACTIONS`

LINE1_PROF writes ionizations fractions of all ionic species in *ATOMS* to the file PLION that may be saved to e.g.<name>. Using

ln -sf <name> ion2devide.dat
/home/rauch/bin/ion2devide.Linux_x64

yields a series of ionfrac.<II> (II is the ionic species). These files can be plotted together in one plot with the template

/home/rauch/tools/IonFrac.wr ,

that has to be edited properly for the individual star.

`SAVE␣FGRID_2`

allows to save the frequency grid created by *LINE1_PROF* is saved into the files *FGRID_2* (binary) and *FGRID_3* (ASCII). *FGRID_3* can be used by IrOnIc then. In order to check the respective *ATOMS* file, *SETF2* has to be used to create a "start" input *FGRID* file.

LINE1_PROF considers the same input files like *SETF2*, *CONTS_MAN*, *F_BASE*, and *POS_LIST*.

A difference is the content of *F_BASE*, where
λ_{min} λ_{max} $\Delta\lambda$
have to be given. There may be entries for different intervals.

LINE1_PROF uses an external frequency grid, if

`FGRID_2␣FROM␣INPUT`

is activated.

`DYNAMIC␣DISTA` λ_{min} λ_{max} `DYNFACTOR`

In general, spectral lines are more narrow in the X-ray or UV compared to the IR. To avoid excessively high NRBBMAD values, a dynamic adjustment of the blue and red line limits is necessary. The values given in the input file *DISTA* are inter/extrapolated to *DISTA* values $\times 1$ at λ_{min} and *DISTA* values $\times DYNFACTOR$ at λ_{max}.

The program *LINE1_PROF* creates (besides STDOUT and the files mentioned in Sect. 8) the following plot data files (in accordance with the options given).

IDENT
for each line within the BLENDRANGE (Sect. 8), an
`\IDENT <wavlength> <ion> <transition>`
card is created that can be used by WRPLOT (Sect. 11) for line identifications.

To combine subsequent IDENTs with identical ion name, use /home/rauch/tools/mkIDMULT.Linux_p64 with an input file id.in. The results will be in an output file id.out.

PLDIFF
element mass fractions in case of a diffusion input model

10 Clean Up

TMAP requires a controlled clean up from time to time.

10.1 Delete TMAP Working Directories

The general job structure of TMAP is

```
#!/bin/sh
set +x;.  ${HOME}/.jobstart
# do not edit the beginning of this file
########################
## own job following ##
########################



# do not edit the rest of this file
####################
set +x; ${HOME}/.jobend ${TMPDIR}
```

`${HOME}/.jobstart` creates a working directory of the form
/scratch/weekly/<username>/YYYY-MM-DD_hh:mm:ss
that is deleted at the end of a job by `${HOME}/.jobend`. In case of a user break (<CTRL C>), the working directory and all data therein remain on the scratch disk. These have to be deleted regularly by

~rauch/tools/clearTMAPscratch@all_linux_no_ask .

Be aware, that this command deletes all TMAP working directories. In case that TMAP jobs are still running, they will fail!

10.2 Kill TMAP Jobs

In case that TMAP jobs were started using the nohup command, they will continue even if the user logged out or if the console was rebooted. Then, these jobs can be killed individually on the respective machines (cf. user of the *S*TOP file, Sect.. 5), or with the procedure

~rauch/tools/kill@all_linux_no_ask .

Be aware, that this command kills all your jobs (not only TMAP jobs) on all linux machines but at your local machine!

11 Auxiliaries

Three plot programs, *PROF1*, and *PLXY*, are available on the computers at Tübingen. They are designed for the visualization of plot data files from the Tübingen NLTE Model-Atmosphere Package (*TMAP*). The program *PLXY* is able to plot any x-y table. The additional program WR-PLOT is a plot program which is not exclusively based on the Tübingen NLTE Model-Atmosphere Package (*TMAP*). The two auxiliary programs *RTFZ* and *PLADD* are designed to interactively rectify and co-add spectra.

The programs are to be used interactively and allow an individual design of the plot. Interactive labeling etc. is possible. All interactively inserted label can be saved in files *program.AUX* and can be re-loaded if the program is invoked again later.

The plot files are created in PostScript format, EPSF is optional for a later inclusion in LaTeX documents. The plot programs support color — *PROF1* uses the "pen" number as follows:
1 black
2 red
3 blue
4 green
5 yellow
6 cyan
7 magenta

A more detailed description follows in the next sections.

At Tübingen, the programs are found at
/home/rauch/tools/pladd
/home/rauch/tools/plxy
/home/rauch/tools/prof1
/home/rauch/tools/rtfz

All programs are self-explaining ...

In the following sections some general comment on the programs are summarized. For details, especially for one-purpose derivates of the programs, please contact the authors.

11.1 PLADD

The program *PLADD* may be used to interactively co-add spectra with individual weights. Parts of the spectra which are obviously corrupted, e.g. by cosmics, can be eliminated. The program expects input spectra data file with the convention ¡name¿.ii, where ii is a two digit integer (default is 01). In the case of echelle spectra, ii is the order number:
Example file names to be co-added:

- longslit

  star1_date1.01

  star1_date2.01

  star1_date3.01

  star1_date4.01

star1_date5.01

- echelle

  star1_date1.44
  star1_date1.45
  star1_date1.46
  star1_date1.47
  star1_date1.48
  star1_date1.49
  star1_date2.44
  star1_date2.45
  star1_date2.46
  star1_date2.47
  star1_date2.48
  star1_date2.49

With *PLADD*, normalized as well as absolute flux spectra can be co-added. The absolute fluxes can be pre-normalized (with a constant value) for the processing. A Savitzky-Golay filter Savitzky & Golay (1964) may be invoked to clarify in case of heavy over-sampling.

11.2 PROF1

For the direct evaluation and visualization of line profile plot data files which are created by *LINE1*, or are available in WRPLOT format, the program *PROF1* is available.

PROF1 can plot the data as well as process them in order to compare them to observations etc. A small "help" menu is available which can be invoked from the *PROF1* main menu. Several submenus can be accessed from this main menu (input "L" at the right row ...). It is worthwhile to note that there is a plot box menu which can be accessed from the first row of the main menu.

For all further questions and assistance the authors are available via email.

In the following, the format of the line profile and spectra files is briefly summarized:

11.2.1 Line Profile Data Files

The line profile data files consist out of a *LINE1* header and any number of plot data sets. The header has the following structure:

`A5` program code of the line profile calculation, e,g. `LINE1`
`A8` date of the line profile calculation
`A8` time the line profile calculation
`A5` program code of the model atmosphere calculation , e,g. `PRO2`
`A8` date of the model atmosphere calculation
`A8` time of the model atmosphere calculation
`I5` number of the following plot data sets

Every plot data set is devided in three parts, i.e. a header, the plot data, and information about blends and the line broadening theories used for the calculation of the theoretical line profiles.

The header has the following format:

`A80`	comment (free)
`A80`	comment (free)
`A80`	comment (free)
`A27,F11.3,A42`	both strings (free) **number field: central wavelength in Å**
`A80`	title
`A80`	abscissa label
`A80`	ordinate label
`I5`	number of following values in the data set

The central wavelength in the marked field is of special importance because PROF1 uses this value as origin of an internal coordinate system. The data of the line profiles is given relative to the line center. All following program steps refer to this wavelength.

It follows the number of x-y pairs as announced in the header. There is no special format necessary but the first four columns have to be blank.

At the end of every data set an information segment follows which is used by *PROF1* to find the position of blends in the calculated line profile and to get informations about the line broadening theories which were used to calculate the line profiles. This segment has the following form:

`I3`	total number of lines (incl. blends) in this data set
`A20,2F13.3`	type of lines in *TMAP* Code (Sect. 2.1), distance (Å) relative to the central wavelength (see above), central depression of the line
⋮	
`I3`	total number of lines
`A20,A10`	line broadening theory used to calculate the line (e.g. `VCS 88`)
⋮	

11.2.2 Spectra

The basic format of all spectra files which are accepted by *PROF1* is:

`A20`	name of spectrum
`I6`	number of x-y pairs
`6X,*`	x-y pairs
⋮	

The number of x-y pairs is currently limited to 18 000.

11.2.3 PROF1 Auxiliary Files

The program *PROF1* can create a variety of auxiliary files. These files are explained in the following. They can be recognized by their extension.

• **.AEQ**
This file is created if equivalent widths are measured with *PROF1*. It contains information about the measured interval, theoretical, and observed equivalent width (measure from the spectrum).

• **.AUX**
This file is created if labels are interactively inserted *and saved!* It can be easily edited and used for a following *PROF1* session.

• **.CMD**
While a *PROF1* session is active, all commands are recorded and can be saved at the end of the session. Thus, a batch job is created which can be run as a procedure and creates automatically plot files. If different plot data files are copied to the same path subsequently, this procedure can create "standard" plots of different plot files.

• **.DAT_REN**
This file is created if a spectrum is normalized by *PROF1* and saved (basic format, see above).

• **.LOAD**
In this file all spectra a listed which shall be automatically loaded by *PROF1* at the beginning of the session. It can be created from the "spectra menu" of *PROF1*.

• **.MRK**
In this file the base points for the rectification of spectra with natural splines can be saved.

• **.REN**
This file contains information about the normalization of a spectrum. Sometimes it appears necessary to correct the position of the local continuum. The following session can refer to this file, and thus, uses the same base points for normalization.

• **.REN_DAT**
This file contains a re-normalized spectrum.

• **.SET**
In the file information (defaults) about the size of the plot box etc. are saved. It is read by *PROF1* at the beginning of the session.

11.3 PLXY

The program *PLXY* is an universal plot program for VMS and UNIX. The UNIX version is based on the *PGPLOT* graphics subroutine library which is provided by the California Institute of Technology (in the www, a documentation about this library is found under `http://astro.caltech.edu/~tjp/pgplot/#documentation`). It expects in the plot data file only a x-y table. Optional, commands can be given either by keywords (see below) in the plot data file or interactively.

11.3.1 Keywords for Commands in Plot Data Files

The program *PLXY* accepts some commands given in the plot data file which can be inserted at every position but flushed to the left. Valid are the last commands given before the end of a data set. Strings, e.g. for a comment, start directly after the ":" — without any "␣".

- `O:` origin of the plot (X_0,Y_0 in cm), new plot box
- `A:` abscissa label, OFF: no label
- `B:` width of plot box given in cm
- `C:` color index, 16 colors are predefined (Fig. 2), they can be changed interactively
- `D:` line style
  `1` full line
  `2` dashed
  `3` dot-dash-dot-dash
  `4` dotted
  `5` dash-dot-dot-dot
- `E:` distance of tick marks
- `H:` height of plot box given in cm
- `K:` comment
- `M:` star position for sky map, Example:
- `M: 1 0 03 44.0 -44 04 12.0`
  `Longmore 4`
- `N:` new data set
- `O:` ordinate label, OFF: no label
- `P:` thickness of line
- `S:` plot symbols, numbers taken from the *PGPLOT* symbols, a small selection is summarized in Tab.2
- `T:` title

Table 2: Selection of plot symbols available for the use in *PLXY*

#	symbol
840	○
841	□
842	△
843	♢
844	⋆
845	+
846	×
847	∗

- `X:` $X_{\min}$ $X_{\max}$
- `Y:` $Y_{\min}$ $Y_{\max}$

11.3.2 Output devices

Three output devices can be requested:

0 /dev/null, i.e. no output

3 PostScript file *plxy_xxxx.eps*, *xxxx* is a running counter

5 screen

11.4 RTFZ

RTFZ may be used to normalized spectra individually. *RTFZ* expects a xy table with the original spectrum. Continuum points can be set manually and a cubic spline fit will be performed for selected parts of the spectrum. In order to achieve more clarity, it is possible to smooth the spectra during the rectifying process by a Savitzky-Golay filter.

11.5 TEUV

The Tübingen EUV Absorption (*TEUV*) tool was created to apply interstellar absorption to theoretical stellar spectra in the wavelength range $\lambda < 911\,\text{Å}$, where bound-free absorption by interstellar elements has a string influence on observed fluxes. This has to be considered when these observations are modeled. The hot and cool components of the interstellar medium are represented in the *TEUV* tool.

The program is intuitive to handle and controlled via a web interface (`http://astro.uni-tuebingen.de/~TEUV`) where all parameters of the interstellar components can be entered and the input model-flux table can be uploaded. For further assistance, the mouse can be hovered over the blue labels.

The following fields have to be selected or filled in:

- Contact data: The user has to enter name and email address. In case any error occurs, the administrator can contact the user for assistance.

- Upload model and observation: For a fast and easy adjustment of the parameters, the resulting model will be displayed. An observation that covers the wavelength range $\lambda < 911$ Å is necessary for comparison. Input model and observation must contain wavelength in Å and in increasing order in the first and flux in erg/cm^2/sec/A in the second column.

- Normalization: For the first overview of the observation, model, and corrected model, a normalization of the theoretical models is necessary to match the observation. Therefore, the observed flux at 928 Å or at a chosen wavelength (< 928 Å) has to be entered.

- Instrumental resolution: *TEUV* can also apply a correction with a Gaussian profile to the theoretical models to account for instrumental resolution. The FWHM of tha Gaussian has to be given in Å.

- The two components: For both components, temperature in K, radial and turbulent velocities in km/sec as well as the column densities in cm^{-2} of the single ions have to be entered.

After "Upload and Submit", the theoretical model is corrected according to the given parameters. Additionally, models with a ten times larger and smaller H I and He I column densities are created. To be able to display these models, the maximum number of output wavelength points is reduced. It may take some seconds until these corrections are applied. Then, the uploaded model, observation, and corrected model are displayed. For an easier adjustment of the parameters, the user can choose to display the models with varied H I and/or He I column densities.

If the user wants to download the resulting model, the "Download your ISM_choice" button can be used. This triggers the calculation of the corrected model without normalization, for all entered wavelength points with the instrumental resolution applied. If the *TEUV* tool is used to determine results that are published later, the quote to cite in the acknowledgement is given at the website. The user can store the resulting file via the "Get your results file" button.

11.6 WRPLOT

WRPLOT is a program by Wolf-Rainer Hamann et al. which can be used to manipulate and visualize data. A manual for the use of this program is available at `http://astro.uni-tuebingen.de/~TMAP`

A Formula Collection

In this formula collection, those formulae are summarized which are used in the programs of the Tübingen NLTE Model-Atmosphere Package (*TMAP*). The abbreviations for the different transitions (CBF- ...) refer to those of Sect. 1. The last numbers of the section titles are the formula numbers which have to be inserted in the atomic data file (*ATOMS*, Sect. 2, 2.2).

A.1 CBB Transitions

A.1.1 van-Regemorter Formula (Allowed Dipole Transitions)

$$C_{\mathrm{ij}} = \pi {a_0}^2 \sqrt{\frac{8k}{\pi m_{\mathrm{e}}}} n_{\mathrm{e}} \sqrt{T} \left[14.5 f_{\mathrm{ij}} \left(\frac{E_{\mathrm{H}}}{E_0} \right)^2 \right] u_0 e^{-u_0} \Gamma(u_0)$$

$$u_0 = h\nu_{\mathrm{ij}}/kT, \quad E_0 = h\nu_{\mathrm{ij}}, \quad \Gamma(u_0) = \max[\bar{g}, 0.276 e^{u_0} E_1(u_0)]$$

$\bar{g} = 0.2$ for n'≠n else $= 0.7$. E_{H} is the ionization energy of the hydrogen ground state.

$$\pi {a_0}^2 \sqrt{\frac{8k}{\pi m_{\mathrm{e}}}} = 5.465 \cdot 10^{-11}$$

2 input parameters: f_{ij}, $\bar{g}$

A.1.2 Forbidden Transitions

$$C_{\mathrm{ij}} = \frac{8.631 \cdot 10^{-6}}{g_{\mathrm{i}} \sqrt{T}} n_{\mathrm{e}} e^{-u_0} \Omega$$

$$\Omega = \sum_{\mathrm{i}=1}^{NFIT} a_{\mathrm{i}} \cdot x^{i-1}$$

`NFIT+1` input parameters: `NFIT`, a_1, ... , a_{NFIT}
for the *effective collision strength*. Is only one parameter supplied (explicitly: 1), then $\Omega = 1$ is set.

A.1.3 Hydrogen

following Mihalas

$$C_{\mathrm{ij}} = 4\pi {a_0}^2 \sqrt{\frac{8k}{\pi m_{\mathrm{e}}}} n_{\mathrm{e}} \sqrt{T} \left(\frac{E_{\mathrm{H}}}{h\nu_{\mathrm{ij}}} \right)^2 u_0 f_{\mathrm{ij}} \left(E_1(u_0) + 0.148 u_0 E_5(u_0) \right) \gamma$$

$\gamma = \beta + 2(\alpha - \beta)/\Delta n$ for $\Delta n > 1$, and $\gamma = 1$ else $\beta = 3 - 1.2/n_{\mathrm{i}}$, $\alpha = 1.8 - 0.4/n_{\mathrm{i}}^2$

no input parameter

A.1.4 He II

following Mihalas & Stone

$$C_{\mathrm{ij}} = \pi {a_0}^2 \sqrt{\frac{8k}{\pi m_{\mathrm{e}}}} n_{\mathrm{e}} \sqrt{T} \left(\frac{E_{\mathrm{H}}}{h\nu_{\mathrm{ij}}} \right)^2 u_0 f_{\mathrm{ij}} e \left(e^{-u_0} \ln 2 + E_1(u_0) \right) \gamma$$

$$\gamma = \min\left[n_{\mathrm{i}}, 1.1\right] \cdot \min\left[\Delta n_{\mathrm{i}}, n_{\mathrm{i}} - \frac{n-1}{\Delta n}\right]$$

no input parameter

A.1.5 He I: Allowed Transitions from its Ground State

following Mihalas & Stone

$$C_{1j} = 4\pi {a_0}^2 \sqrt{\frac{8k}{\pi m_e}} n_e \sqrt{T} f_{1j} \left(\frac{E_H}{h\nu_{1j}}\right)^2 u_0 E_1(u_0)$$

1 input parameter: f_{1j}

A.1.6 He I: Allowed Transitions but not from its Ground State

following Mihalas & Stone

$$C_{ij} = 4\pi {a_0}^2 \sqrt{\frac{8k}{\pi m_e}} n_e \sqrt{T} f_{ij} \left(\frac{E_H}{h\nu_{1j}}\right)^2 u_0 \left(E_1(u_0) - \frac{u_0}{u_1} e^{-0.2} (E_1(u_1)\right)$$

$$u_1 = u_0 + 0.2$$

1 input parameter: f_{ij}

A.1.7 He I: Forbidden Transitions from its Ground State

following Mihalas & Stone

$$C_{ij} = \pi {a_0}^2 \sqrt{\frac{8k}{\pi m_e}} n_e \sqrt{T} \frac{a}{{n_{eff}}^3} u_0 \frac{1}{\pi {a_0}^2} \left[a_0 E_1(u_0) + a_1 u_0 e^{-b_1 u_0} x_1 + a_2 u_0 e^{-b_2 u_0} x_2\right]$$

$$x_i = \frac{b_i \left(u_0 + \frac{1}{c_1}\right) + 2}{\left(u_0 + \frac{1}{c_i}\right)^3}$$

$$n_{eff} = Z \sqrt{\frac{E_H}{h\nu_{th}}} \quad (Z = 1)$$

8 input parameters: a, a_i, b_i, c_i (found in tabular form in M&S; Attention: their equation A16 is wrong!)

A.1.8 He I: Forbidden Transitions between its $n = 2$ Sublevels

following Mihalas & Stone

$$C_{ij} = \pi {a_0}^2 \sqrt{\frac{8k}{\pi m_e}} n_e \sqrt{T} e^{-E_0/kT} \Gamma_{ij}(T)$$

$$E_0 = h\nu_{ij}$$

$$\log \Gamma = c_0 + c_1 \log T + c_{-2} (\log T)^{-2}$$

3 input parameters: c_0, c_1, c_{-2} (in tabular form by M&S)

A.1.9 Unknown Collisional Cross-Sections

$$C_{\mathrm{ij}} = \pi {a_0}^2 \sqrt{\frac{8k}{\pi m_{\mathrm{e}}}} n_{\mathrm{e}} \sqrt{T} e^{-u_0} \left(1 + u_0\right)$$

no input parameter

A.1.10 Ω-Fit of 3rd Degree

like A.1.2, but:

$$\Omega = \sum_{\mathrm{i}=1}^{4} a_{\mathrm{i}} \left(\log T\right)^{i-1}$$

4 input parameters: a_1, a_2, a_3, a_4

A.1.11 Mg II: Allowed Transitions from its Ground State

following Mihalas (1972)

$$C_{\mathrm{ij}} = \pi {a_0}^2 \sqrt{\frac{8k}{\pi m_{\mathrm{e}}}} n_{\mathrm{e}} \sqrt{T} 4 f_{\mathrm{ij}} \frac{{E_{\mathrm{H}}}^2}{E_0} u_0 \left(a E_1(u_0) + b e^{-u_0}\right)$$

2 input parameters: a, b

A.1.12 van-Regemorter: Combined Levels of Complex Ions

$$C_{\mathrm{ij}} = \pi {a_0}^2 \sqrt{\frac{8k}{\pi m_{\mathrm{e}}}} n_{\mathrm{e}} \sqrt{T} e^{-u_0} \Gamma_{\mathrm{ij}}(T)$$

$$\log \Gamma_{\mathrm{ij}}(T) = a_0 + a_1 x + a_2 x^2 + a_3 x^3, \quad x = \log kT \quad \text{[in eV]}$$

4 input parameters: a_0, a_1, a_2, a_3

A.1.21 He I: Transition between its Levels with $s \leq 4$

D. Hummer, priv. comm.
no input parameter

A.1.25 Ω-Fit in Temperature, General Case

equal to `DETAIL` Formula No. 25,
8 input parameters

A.1.26 Ω-Fit in $\log T$, General Case

equal to `DETAIL` Formula No. 26,

$$\Omega = \sum_{\mathrm{i}=1}^{NFIT} a_{\mathrm{i}} \left(\log T - T_1\right)^{i-1}$$

`NFIT+2` input parameters: T1, `NFIT`, a_1, ..., a_{NFIT}

A.2 CBF Transitions

A.2.1 Hydrogen, $n = 1, \ldots, 10$

following Mihalas

$$C_{\rm ik} = \pi {a_0}^2 \sqrt{\frac{8k}{\pi m_{\rm e}}} n_{\rm e} \sqrt{T} e^{-h\nu_{\rm th}/kT} \Gamma_{\rm i}(T)$$

own fit formulae for Γ, because Mihalas is restricted in temperature,
no input parameter

A.2.2 He II, $n = 1, \ldots, 10$

following Mihalas, like `CBF1`, own fit formulae for Γ, because Mihalas is restricted in temperature, no input parameter

A.2.3 He I, $n \leq 15$

$$C_{\rm ik} = \pi {a_0}^2 \sqrt{\frac{8k}{\pi m_{\rm e}}} n_{\rm e} \sqrt{T} \sigma_0 \left\{ u_0 E_1(u_0) - \frac{0.728 {u_0}^2}{u_1} E_1(u_1) - 0.189 {u_0}^2 e^{-u_0} \left(\frac{2.0 + u_2}{{u_2}^3} \right) \right\}$$

$$u_0 = h\nu_{\rm th}/kT,\ u_1 = u_0 + 0.27,\ u_2 = u_0 + 1.43$$

1 input parameter: σ_0 (in tabular form by Mihalas & Stone)

A.2.4 Seaton Formula

$$C_{\rm ik} = 1.55 \cdot 10^{13} \bar{g} \sigma_0 n_{\rm e} \frac{1}{\sqrt{T}} e^{-u_0} {u_0}^{-1} \quad \bar{g} = [0.1, 0.2, 0.3] \quad \text{for } Z = [1, 2, \geq 3]$$

Z = charge of the ion σ_0 = threshold photoionization cross-section
2 input parameters: σ_0, $\bar{g}$

In case that formula 4 is requested and a cross-section of 0.0 inserted, a mean cross-section (at the threshold energy) of the Opacity Project data is calculated and used as threshold cross-section (Sect. A.4).

A.2.5 Lotz Formula

$$C_{\rm ik} = \pi {a_0}^2 \sqrt{\frac{8k}{\pi m_{\rm e}}} n_{\rm e} \sqrt{T} P \left(\frac{E_{\rm H}}{E_0} \right)^2 u_0 \left\{ E_1(u_0) - \frac{\alpha u_0}{u_1} E_1(u_1) \right\}$$

3 input parameters: P, α, c
$u_1 = u_0 + c$

A.2.6 Mg II $3s \rightarrow$ Mg III $2p^6 + \epsilon$

following Mihalas (1972)

$$C_{\rm ik} = \pi {a_0}^2 \sqrt{\frac{8k}{\pi m_{\rm e}}} n_{\rm e} \sqrt{T} \left(\frac{E_{\rm H}}{E_0} \right)^2 \left\{ a u_0 E_1(u_0) + b (u_0/u_1)^2 [E_1(u_1) + e^{-u_1}] \right\}$$

$$u_1 = u_0 + c$$

3 input parameters: a, b, c

A.3 RBB Transitions

A.3.1 Doppler Profiles

$$\boldsymbol{\sigma_{\mathrm{ij}} = \frac{\sqrt{\pi} e^2}{m_{\mathrm{e}} c} \frac{f_{\mathrm{ij}}}{\Delta \nu_{\mathrm{D}}} e^{-(\Delta\nu/\Delta\nu_{\mathrm{D}})^2}}$$

$$\boldsymbol{\Delta \nu_{\mathrm{D}} = \frac{\nu_0}{c} \sqrt{\frac{2kT}{m_{\mathrm{ATOM}}}}}$$

1 input parameter: f_{ij}

A.3.2 Voigt Profiles, only Radiative Damping

$$\boldsymbol{\sigma_{\mathrm{ij}} = \frac{\sqrt{\pi} e^2}{m_{\mathrm{e}} c} \frac{f_{\mathrm{ij}}}{\Delta \nu_{\mathrm{D}}} H(a, v)}$$

$$\boldsymbol{a = \frac{\Gamma}{4\pi \Delta \nu_{\mathrm{D}}}, \quad v = \frac{\Delta \nu}{\Delta \nu_{\mathrm{D}}}, \quad \Gamma = \Gamma_{\mathrm{low}} + \Gamma_{\mathrm{up}}}$$

2 input parameters: f_{ij}, Γ

A.3.3 Voigt Profiles, Radiative and Collisional Damping (Electrons)

σ_{ij} like in A.3.2, but:

$$\boldsymbol{\Gamma = \Gamma_{\mathrm{rad}} + \Gamma_{\mathrm{St}}}$$

$$\boldsymbol{\Gamma_{\mathrm{St}} = 6.11 \cdot 10^{-5} \frac{n_{\mathrm{e}}}{\sqrt{T}} \left(\frac{n_{\mathrm{eff}}^{\mathrm{up}\,2}}{z} \right)^2}$$

(Cowley 1970, 1971) 3 input parameters: f_{ij}, Γ_{rad}, $\left(\frac{n_{\mathrm{eff}}^{up2}}{z+1}\right)^2$

A.3.4 Voigt Profiles and "Stark Wings" (Linear Stark Effect)

$$\boldsymbol{\sigma_{\mathrm{ij}} = \max \left[\sigma_{\mathrm{ij}}^{Formel\ 3}, \sigma_{\mathrm{ij}}^{St} \right]}$$

$$\boldsymbol{\sigma_{\mathrm{ij}}^{St} = \frac{0.0368 \cdot Z f_{\mathrm{ij}}}{s_{\mathrm{n}} z_{\mathrm{Mikro}}} U \left(\frac{\Delta \nu Z \cdot 1.385}{s_{\mathrm{n}} z_{\mathrm{Mikro}}} \right)}$$

$$\boldsymbol{s_{rmn} = \left\{ n_{\mathrm{up}} \left(n_{\mathrm{up}} - 1 \right) + n_{\mathrm{low}} \left(n_{\mathrm{low}} - 1 \right) \right\}}$$

$$\boldsymbol{z_{\mathrm{Mikro}} = \left[\sum_{\mathrm{i}=1}^{NION} Z_{\mathrm{i}}^{\frac{3}{2}} \cdot n_{\mathrm{i}} \right]^{\frac{2}{3}}}$$

6 input parameters: f_{ij}, Γ_{rad}, $\left(\frac{n_{\mathrm{eff}}^{up2}}{z+1}\right)^2$, Z, n_{low}, n_{up}

A.3.5 Stark Line Broadening following Dimitrijévic

like formula 3

A.4 RBF Transitions

A.4.1 Seaton Formula

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

$$\boldsymbol{\mathrm{hydrogen-like:}\quad \sigma_0 = 2.815 \cdot 10^{29} \frac{z^4 g_{\rm II}\left(\nu_{\rm th}\right)}{n_{\rm eff}^5 {\nu_{\rm th}}^3}}$$

with the effective principal quantum number

$$\boldsymbol{n_{\rm eff} = z\sqrt{\frac{R}{\nu_{\rm th}}}}$$

$\boldsymbol{g_{\rm II}}$ is the bound-free gaunt factor
z core charge of the ion
3 input parameters: σ_0, α, s

A.4.2 Seaton Formula with Gaunt Factor

$$\boldsymbol{\sigma_\nu = \sigma_0 \left(\frac{\nu_{\rm th}}{\nu}\right)^s \left[\alpha + (1-\alpha)\frac{\nu_{\rm th}}{\nu}\right] g_{\rm II}\left(x, y, z\right)}$$

6 input parameters: $\sigma_0, \alpha, s, x, y, z$

A.4.3 Koester Formula for He I

A&A,

$$\boldsymbol{\ln\left(g\sigma_\nu\right) = a_0 + a_1 \ln\lambda + a_2 \ln^2\lambda, \qquad \lambda[\text{Å}]}$$

3 input parameters: a_0, a_1, a_2

A.4.4 Opacity-Project Photoionization Cross-Sections, Seaton tails

See Sect. A.4.10.

A.4.5 Karzas & Latter data with Gaunt Factor

Tables taken from Karzas & Latter (1961) are used to calculate the photoionization cross-sections.
3 input parameters: $z_{\rm eff}$, n (principal quantum number), l (azimuthal quantum number)

A.4.10 Opacity-Project Photoionization Cross-Sections

The Opacity Project data for a level of the ion XXXX are read from the file OP_RBF_XXXX (Sect. 8.1). The programs recognize an A10 label at the begin of the data set which represents the level name in *TMAP* code (Sect. 2.1). For the actual frequency grid *FGRID* (Sect. 3), the cross-sections are interpolated or extrapolated (including possible resonances etc.). Is formula 4 requested and a cross-section of 0.0 inserted, a mean cross-section (at the threshold energy) of the Opacity Project data is calculated and used as threshold cross-section.

no input parameter

A.4.12 DETAIL Fit Formula

$$\ln \sigma_\nu = \sum_{\mathrm{i}=0}^{5} a_\mathrm{i} \cdot \left[\ln\left(\frac{\nu_\mathrm{th}}{\nu}\right)\right]^i$$

6 input parameters: $a_0, \ldots, a_5$

A.5 RFF Transitions

None of the RFF formulae needs an input parameter.

A.5.1 Including Contributions of LTE Levels (Unsöld)

$$\sigma_\mathrm{kk}(\nu, T) = 3.694 \cdot 10^8 e^{h\nu_\mathrm{min}/kT} \frac{Z^2}{\nu^3\sqrt{T}}$$

$$\nu_\mathrm{min} = \min[\nu, \nu_\mathrm{LTE}]$$

ν_LTE is the ionization threshold energy of the lowest LTE level.
(cf. Unsöld 1968)

A.5.2 Including Contributions of LTE Levels with Gaunt Factors

$$\sigma_\mathrm{kk}(\nu, T) = 3.694 \cdot 10^8 \left[g_\mathrm{ff}(\nu, T)(e^{h\nu_\mathrm{min}/kT} - 1)\right] \frac{Z^2}{\nu^3\sqrt{T}}$$

A.5.3 With Gaunt Factors, no LTE Contributions

$$\sigma_\mathrm{kk}(\nu, T) = 3.694 \cdot 10^8 g_\mathrm{ff}(\nu, T) \frac{Z^2}{\nu^3\sqrt{T}}$$

For the free-free Gaunt factors, the default is a calculation following Mihalas (1967, ApJ 149, 169). Since these values are calculated from a fit formula within $100 \leq \lambda \leq 10000$ Å and an extension to longer wavelengths, data (valid from submillimetre to hard X-ray wavelengths and for temperatures from $10 - 10^9$ K) provided by Sutherland (1998) can be chosen by input card (Sect. 5.4).

B Fundamental Constants

In all programs of the Tübingen NLTE Model-Atmosphere Package (*TMAP*) the values of the fundamental constants are the same. They are summarized in Tab. 3.

Table 3: Fundamental constants used in *TMAP*

constant	value		dimension	name
c	2.99792458	$\times 10^{+10}$	cm s^{-1}	velocity of light
e	4.80320425	$\times 10^{-10}$	esu	electron charge
F_o	1.25	$\times 10^{-09}$	esu	Holtsmark normal field strength
h	6.62606957	$\times 10^{-27}$	erg s	Planck constant
k	1.3806488	$\times 10^{-16}$	erg K^{-1}	Boltzmann constant
m_e	9.10938291	$\times 10^{-28}$	g	electron mass
m_p	1.6726217776	$\times 10^{-24}$	g	proton mass
R	109737.31568539		cm^{-1}	Rydberg constant
π	$4 \times \arctan 1$			

C Solar Abundances

Table 4: *TMAP* uses the following values as solar abundances[a] (Asplund et al. 2009; Maiorca et al. 2014; Grevesse et al. 2015; Scott et al. 2015b,a).

Atom (X)	Atomic Number	Atomic Weight	$\log \epsilon_X$	n(X)/n(H) (by number)	n(X)/n(He) (by number)	mass fraction
H	1	1.0079	12.00	$1.000\times10^{+00}$	$1.175\times10^{+01}$	7.375×10^{-01}
He	2	4.0026	10.93	8.511×10^{-02}	$1.000\times10^{+00}$	2.493×10^{-01}
Li	3	6.9410	1.05	1.122×10^{-11}	1.318×10^{-10}	5.698×10^{-11}
Be	4	9.0122	1.38	2.399×10^{-11}	2.818×10^{-10}	1.582×10^{-10}
B	5	10.8110	2.70	5.012×10^{-10}	5.888×10^{-09}	3.964×10^{-09}
C	6	12.0107	8.43	2.692×10^{-04}	3.162×10^{-03}	2.365×10^{-03}
N	7	14.0067	7.83	6.761×10^{-05}	7.943×10^{-04}	6.929×10^{-04}
O	8	15.9994	8.69	4.898×10^{-04}	5.754×10^{-03}	5.733×10^{-03}
F	9	18.9984	4.40	2.512×10^{-08}	2.951×10^{-07}	3.492×10^{-07}
Ne	10	20.1797	7.93	8.511×10^{-05}	1.000×10^{-03}	1.257×10^{-03}
Na	11	22.9898	6.21	1.622×10^{-06}	1.905×10^{-05}	2.728×10^{-05}
Mg	12	24.3050	7.59	3.890×10^{-05}	4.571×10^{-04}	6.918×10^{-04}
Al	13	26.9815	6.43	2.692×10^{-06}	3.162×10^{-05}	5.314×10^{-05}
Si	14	28.0855	7.51	3.236×10^{-05}	3.802×10^{-04}	6.650×10^{-04}
P	15	30.9738	5.41	2.570×10^{-07}	3.020×10^{-06}	5.825×10^{-06}
S	16	32.0650	7.12	1.318×10^{-05}	1.549×10^{-04}	3.093×10^{-04}
Cl	17	35.4530	5.50	3.162×10^{-07}	3.715×10^{-06}	8.203×10^{-06}
Ar	18	39.9480	6.40	2.512×10^{-06}	2.951×10^{-05}	7.342×10^{-05}
K	19	39.0983	5.04	1.096×10^{-07}	1.288×10^{-06}	3.137×10^{-06}
Ca	20	40.0780	6.32	2.089×10^{-06}	2.455×10^{-05}	6.127×10^{-05}
Sc	21	44.9559	3.16	1.445×10^{-09}	1.698×10^{-08}	4.754×10^{-08}
Ti	22	47.8670	4.93	8.511×10^{-08}	1.000×10^{-06}	2.981×10^{-06}
V	23	50.9415	3.89	7.762×10^{-09}	9.120×10^{-08}	2.893×10^{-07}
Cr	24	51.9961	5.62	4.169×10^{-07}	4.898×10^{-06}	1.586×10^{-05}
Mn	25	54.9380	5.42	2.630×10^{-07}	3.090×10^{-06}	1.057×10^{-05}
Fe	26	55.8450	7.47	2.951×10^{-05}	3.467×10^{-04}	1.206×10^{-03}
Co	27	58.9332	4.93	8.511×10^{-08}	1.000×10^{-06}	3.670×10^{-06}
Ni	28	58.6934	6.20	1.585×10^{-06}	1.862×10^{-05}	6.806×10^{-05}
Cu	29	63.5460	4.18	1.514×10^{-08}	1.778×10^{-07}	7.037×10^{-07}
Zn	30	65.4090	4.56	3.631×10^{-08}	4.266×10^{-07}	1.738×10^{-06}
Ga	31	69.7230	3.02	1.047×10^{-09}	1.230×10^{-08}	5.342×10^{-08}
Ge	32	72.6400	3.63	4.266×10^{-09}	5.012×10^{-08}	2.267×10^{-07}
As[a]	33	74.9216	2.30	1.995×10^{-10}	2.344×10^{-09}	1.094×10^{-08}
Se[a]	34	78.9600	3.34	2.188×10^{-09}	2.570×10^{-08}	1.264×10^{-07}
Br[a]	35	79.9040	2.54	3.467×10^{-10}	4.074×10^{-09}	2.027×10^{-08}
Kr	36	83.7960	3.25	1.778×10^{-09}	2.089×10^{-08}	1.090×10^{-07}
Rb	37	85.4678	2.47	2.951×10^{-10}	3.467×10^{-09}	1.846×10^{-08}
Sr	38	87.6200	2.83	6.761×10^{-10}	7.943×10^{-09}	4.334×10^{-08}
Y	39	88.9059	2.21	1.622×10^{-10}	1.905×10^{-09}	1.055×10^{-08}
Zr	40	91.2240	2.59	3.890×10^{-10}	4.571×10^{-09}	2.597×10^{-08}
Nb	41	92.9064	1.47	2.951×10^{-11}	3.467×10^{-10}	2.006×10^{-09}
Mo	42	95.9400	1.88	7.586×10^{-11}	8.913×10^{-10}	5.325×10^{-09}

[a]: from meteorites only

Table 4 continued.

Atom (X)	Atomic Number	Atomic Weight	$\log \epsilon_X$	n(X)/n(H) (by number)	n(X)/n(He) (by number)	mass fraction
Ru	44	101.0700	1.75	5.623×10^{-11}	6.607×10^{-10}	4.159×10^{-09}
Rh	45	102.9055	0.89	7.762×10^{-12}	9.120×10^{-11}	5.845×10^{-10}
Pd	46	106.4200	1.55	3.548×10^{-11}	4.169×10^{-10}	2.763×10^{-09}
Ag	47	107.8682	0.96	9.120×10^{-12}	1.072×10^{-10}	7.198×10^{-10}
Cd[a]	48	112.4110	1.77	5.888×10^{-11}	6.918×10^{-10}	4.843×10^{-09}
In	49	114.8180	0.80	6.310×10^{-12}	7.413×10^{-11}	5.301×10^{-10}
Sn	50	118.7100	2.02	1.047×10^{-10}	1.230×10^{-09}	9.095×10^{-09}
Sb[a]	51	121.7600	1.01	1.023×10^{-11}	1.202×10^{-10}	9.116×10^{-10}
Te[a]	52	127.6000	2.18	1.514×10^{-10}	1.778×10^{-09}	1.413×10^{-08}
I	53	126.9045	1.55	3.548×10^{-11}	4.169×10^{-10}	3.295×10^{-09}
Xe	54	131.2930	2.24	1.738×10^{-10}	2.042×10^{-09}	1.669×10^{-08}
Cs	55	132.9055	1.08	1.202×10^{-11}	1.413×10^{-10}	1.169×10^{-09}
Ba	56	137.3270	2.25	1.778×10^{-10}	2.089×10^{-09}	1.787×10^{-08}
La	57	138.9055	1.11	1.288×10^{-11}	1.514×10^{-10}	1.309×10^{-09}
Ce	58	140.1160	1.58	3.802×10^{-11}	4.467×10^{-10}	3.898×10^{-09}
Pr	59	140.9077	0.72	5.248×10^{-12}	6.166×10^{-11}	5.411×10^{-10}
Nd	60	144.2400	1.42	2.630×10^{-11}	3.090×10^{-10}	2.776×10^{-09}
Sm	62	150.3600	0.95	8.913×10^{-12}	1.047×10^{-10}	9.805×10^{-10}
Eu	63	151.9640	0.52	3.311×10^{-12}	3.890×10^{-11}	3.682×10^{-10}
Gd	64	157.2500	1.08	1.202×10^{-11}	1.413×10^{-10}	1.383×10^{-09}
Tb	65	158.9253	0.31	2.042×10^{-12}	2.399×10^{-11}	2.374×10^{-10}
Dy	66	162.5000	1.10	1.259×10^{-11}	1.479×10^{-10}	1.497×10^{-09}
Ho	67	164.9303	0.48	3.020×10^{-12}	3.548×10^{-11}	3.644×10^{-10}
Er	68	167.2590	0.93	8.511×10^{-12}	1.000×10^{-10}	1.042×10^{-09}
Tm	69	168.9342	0.11	1.288×10^{-12}	1.514×10^{-11}	1.592×10^{-10}
Yb	70	173.0400	0.85	7.079×10^{-12}	8.318×10^{-11}	8.963×10^{-10}
Lu	71	174.9670	0.10	1.259×10^{-12}	1.479×10^{-11}	1.612×10^{-10}
Hf	72	178.4900	0.85	7.079×10^{-12}	8.318×10^{-11}	9.245×10^{-10}
Ta[a]	73	180.9479	−0.12	7.586×10^{-13}	8.913×10^{-12}	1.004×10^{-10}
W	74	183.8400	0.83	6.761×10^{-12}	7.943×10^{-11}	9.094×10^{-10}
Re[a]	75	186.2070	0.26	1.820×10^{-12}	2.138×10^{-11}	2.479×10^{-10}
Os	76	190.2300	1.40	2.512×10^{-11}	2.951×10^{-10}	3.496×10^{-09}
Ir	77	192.2170	1.42	2.630×10^{-11}	3.090×10^{-10}	3.699×10^{-09}
Pt[a]	78	195.0780	1.62	4.169×10^{-11}	4.898×10^{-10}	5.950×10^{-09}
Au	79	196.9666	0.91	8.128×10^{-12}	9.550×10^{-11}	1.171×10^{-09}
Hg[a]	80	200.5900	1.17	1.479×10^{-11}	1.738×10^{-10}	2.171×10^{-09}
Tl	81	204.3833	0.90	7.943×10^{-12}	9.333×10^{-11}	1.188×10^{-09}
Pb	82	207.2000	1.92	8.318×10^{-11}	9.772×10^{-10}	1.261×10^{-08}
Bi[a]	83	208.9804	0.65	4.467×10^{-12}	5.248×10^{-11}	6.830×10^{-10}
Th	90	232.0381	0.03	1.072×10^{-12}	1.259×10^{-11}	1.819×10^{-10}
U[a]	92	238.0298	−0.54	2.884×10^{-13}	3.388×10^{-12}	5.023×10^{-11}

D How to calculate a NLTE model with *TMAP*

A pre-requiste to understand the following scripts is basic knowledge of unix commands. Lists of the most important can be found easily in the WWW.

In addition, knowledge of the emacs text editor is required.

The meaning of the input cards (traditional name adopted from the formerly used FORTRAN punch cards) for *ATOMS2*, *SETF2*, *LTE2*, *PRO2*, *LINE1*, and *LINE1_PROF*, can be found in this User's Guide.

D.1 Basics

First, this is a short explanation of the directory structure:

`${HOME}/adaten` is the directory for the atomic data checked by *ATOMS2*.
`${HOME}/bimod` is the directory for the executable binaries of *LTE2* and *PRO2*.
`${HOME}/fgrids` is the directory for the frequency grids that were produced with *SETF2*.
`${HOME}/jobs` is the directory for all the .job files (*ATOMS2*, *SETF2*, *LTE2*, and *PRO2*).
`${HOME}/models` is the directory for the calculated models from *LTE2* and *PRO2* are.

For our scripts, we use the following definitions / shell variables (typically set in the ∼/.alias file):

```
setenv AA ${HOME}/adaten
setenv BI ${HOME}/bimod
setenv FF ${HOME}/fgrids
setenv JO ${HOME}/jobs
setenv MO ${HOME}/models
```

D.2 Creation of atomic data files with *ATOMS2*

- Change into the directory `/home/${logname}/jobs/atoms2` and copy the template job file to <name>.job. It needs a file <name> with the atomic data in `/home/${logname}/adaten`. The name <name> can be chosen to contain all the elements used in the model (e.g. `H+He`)
- You need to edit both files, test_atmos_lte.job and test_atoms.job (e.g. with emacs). The first one is for *LTE2*, the second one for *PRO2*.
- After editing, execute the job files and create output files for both jobs with

```
<name>_atoms.job     > <name>_atoms.out  and
<name>_atoms_lte.job > <name>_atoms_lte.out .
```

- Check both output files (with emacs) for error messages.
- The jobs create ASCII files, e.g. `/home/${logname}/adaten/<name>.atoms2`.

D.3 Creation of a frequency grid with *SETF2*

- edit both files <name>_lte_setf2 and <name>_setf2 in /home/${logname}/jobs/setf2. Adjust the temperature and make sure that it refers to <name>_lte.atoms2
- run both jobs and create output files with

  `<name>_setf2 > <name>_setf2.out` and
  `<name>_lte_setf2 > <name>_lte_setf2.out` .

- it writes the files <name>_<temperature>_lte.setf2 and <name>_<temperature>.setf2 to `/home/${logname}/fgrids`

D.4 Adaption of the Parameter files

- extract the parameters from the <name>_atoms.out file with `grep para <name>_atoms.out` and from the output file <name>_setf2.out of the frequency grid
- if you want to save the parameters you can write them in a file with `grep para <name>_atoms.out > object.out`
- the parameter files for PRO2 can be found in `/home/${logname}/PARAMETER/pro2`
- copy the existing parameter files to PARA_<name>.INC, PARA1_<name>.INC, PARA3_<name>.INC and adjust them by using the parameters from <name>_atoms.out
  NOTICE: the values in the parameter files should never be 0!
- we have two machines with licenses to compile our codes, *PRO2* has to be compiled on ait320 and *LINE1* on aithp3:

  Examples:
  compile with

  `ssh ait320 load pro2 <name> [x64/p64]`

  (use x64 only to create a unified executable for 64 bit Intel and AMD processors – it takes twice the time compared to p64 that should be used for most of our 64 bit machines. The compiled executable is copied to `/home/${logname}/bimod/pro2_<name>.Linux_[x64]`
  or with

  `ssh aithp3 load line1_prof <name> [x64/p64]`

D.5 Calculation of a start model with *LTE2*

- edit <name>_lte.job with emacs. Adjust the temperature, log g, and the abundances of the elements used (as normalized number fraction) and check if the used files have the right name
- input files: <name>_lte.atoms2, <name>_temperature_lte.setf2
- start the job and write it into an output file with

  `nice +19 <name>_lte.job > <name>_lte.out`
- the lte model is written to `/home/${logname}/model/<name>/lte`. The file is called temperature_logg_numberfraction element a_numberfraction element b, e.g. 0100000_7.00_1.000_0.000

D.6 Calculation of a NLTE model with *PRO2*

- edit the <name>_nlte.job in emacs. Adjust the temperature, log g and the abundances of the used elements and check if the used files have the right name
- input files: <name>.atoms2, <name>_temperature.setf2 and the *LTE2* model as input model
- start the job with

  `nice +19 <name>_nlte.job > <name>_nlte.out`
- the output model is written to `/home/${logname}/model/<name>`

D.7 Strategy to calculate a NLTE model with *PRO2*

To avoid extremely long calculation times, a reasonable way is to calculate first a model using relatively small model atoms and subsequently, after its convergence, perform a so-called line-formation calculation with much more detailed model atmos on a fixed temperature (and density) structure of the model atmosphere. This yields the NLTE occupation numbers of all considered levels. Figure 1 shows the scheme of this startegy.

Some models calculate without any problem using the *LTE2* start model and an atomic data file that contains all lines. This can be tested first. In case that this approach fails, try to follow the steps summarized in Table 5. There is, however, no recipe to guarantee numerical stable models.

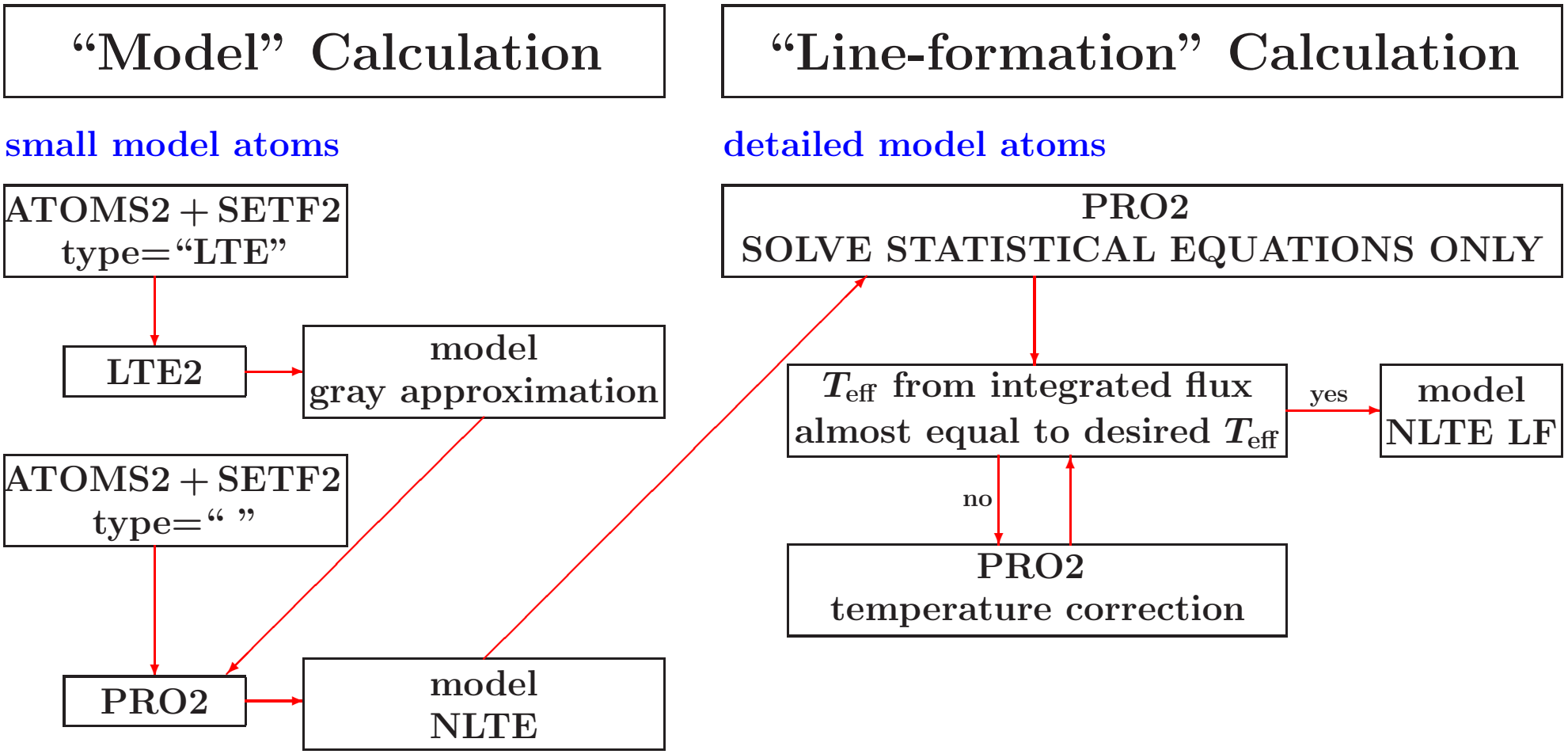

"Model" Calculation
small model atoms
ATOMS2 + SETF2
type="LTE"
LTE2
model
gray approximation
ATOMS2 + SETF2
type=" "
PRO2
model
NLTE
2 atomic-data files
2 frequency files
2 model-atmosphere calculations
"Line-formation" Calculation
detailed model atoms
PRO2
SOLVE STATISTICAL EQUATIONS ONLY
$T_{\rm eff}$ from integrated flux
almost equal to desired $T_{\rm eff}$
yes
model
NLTE LF
no
PRO2
temperature correction
1 atomic-data file
1 frequency file
1 line-formation
and (?) 1 model-atmosphere calculation

Table 5: Steps to calculate a NLTE model with *PRO2*

step	line transitions	temperature correction	ATOMS calculated for	FGRID calculated for	comment
1	no	no	*LTE2*	*LTE2*	very fast due to minimum NF, should work in all cases at least with a `REDUCE LOG CVEC -1` during the very first iterations
2	no	yes	*LTE2*	*LTE2*	very fast
3	no	yes	*LTE2*	*PRO2*	fast, using now the final frequency grid
4	yes	yes	*PRO2*	*PRO2*	initial test with `ITMAX=1` `NEWMAX=0` `LP-PLOT OPTICALLY THICK/THIN,ITERATION:LAST,FILE ONLY` whether the atmosphere is optically thin at the outer boundary (at least two depth points) and optically thick at the inner boundary (at least two depth points) - if this is not fulfilled, recalculate the *LTE2* models with slightly extended τ_{min} and/or τ_{max} (be aware that the following *PRO2* calculation will change the atmospheric structure and the occupation numbers of the atomic levels and, thus, all line strengths - check this $\tau = 1$ limit in the atmosphere by default after all *PRO2* jobs (together with temperature structure and spectral energy distribution)
5	yes	yes	*PRO2*	*PRO2*	test whether all lines can be considered in the temperature correction directly from the outset a) if numerical instabilities are encountered, try first `REDUCE LOG CVEC -1` or `REDUCE LOG CVEC -2` b) if step a is not successful, use the `STEP UP F-VALUES` method, start with unproblematic ions like H I and He II, followed by those that have low ionization fractions, and finally those that are dominating in the line-forming region
6	yes	yes	*PRO2*	*PRO2*	in the final model, neither a `REDUCE LOG CVEC` nor a `UNSOELD-LUCY TEMPERATURE CORRECTION`[a] is allowed

[a] The UNSOELD-LUCY TEMPERATURE CORRECTION may be used in interplay with the standard *PRO2* temperature correction because it yields the temperature of the inner atmosphere quickly and thus stabilizes the numerics. In the outer atmosphere, starting from the line-forming region, the UNSOELD-LUCY TEMPERATURE CORRECTION is not giving a reliable temperature stratification.

D.8 An Example: A model with hydrogen and helium

In the following example, we will use $T_{eff} = 100000\,\mathrm{K}$, $\log g = 7$ and number fractions H=0.9 and He=0.1. The respective parts that have to be changed by a user in the following scripts are marked in red color. Necessary differences in the job files are indicated in blue. Basic H and He model atoms are provided by TMAD (`http://astro.uni-tuebingen.de/~TMAD`). These have to be combined then in one atomic data file in the directory `${AA}/H+He`.

D.8.1 *ATOMS2*

- Copy the job files in `/home/${logname}/jobs/atoms2` to H+He_lte.job and H+He.job. They need a file H+He with the atomic data in `/home/${logname}/adaten`. Edit both files, H+He_lte.job and H+He.job, (with emacs). Make sure you use the atomic data file `H+He`.
- After editing, execute the job file and create an output file for both jobs and check the output files for error messages.

Table 6: Example for *ATOMS2* jobs in the case of LTE (*LTE2*, left) and NLTE (*PRO2*, right) model-atmosphere calculations.

ATOMS2 job for an *LTE2* model

```
#!/bin/sh
set +x;.  ${HOME}/.jobstart
# do not edit the beginning of this file
#########################
## own job following ##
#########################
#
cat > options <<eos
AUTO ION H    I   10  16 -10
AUTO ION HE  II   14  32 -14
CBB-AUTO-FILL
CBF-AUTO-FILL ( NOOP)
CBX-AUTO-FILL
RBB-AUTO-FILL ( NONE)
RBF-AUTO-FILL ( NOOP)
RDI-AUTO-FILL ( NONE)
END OPTIONS
eos
#
cp ${AA}/H+He PROATOM
expand options PROATOM > SOURCE
${BI}/atoms2${sys}
ls -l ATOMS
#
cp ATOMS ${AA}/H+He_lte.atoms2
#
# do not edit the rest of this file
#####################
set +x; ${HOME}/.jobend ${TMPDIR}
```

ATOMS2 job a *PRO2* model job

```
#!/bin/sh
set +x;.  ${HOME}/.jobstart
# do not edit the beginning of this file
#########################
## own job following ##
#########################
#
cat > options <<eos
AUTO ION H    I   10  16 -10
AUTO ION HE  II   14  32 -14
CBB-AUTO-FILL
CBF-AUTO-FILL
CBX-AUTO-FILL
.RBB-AUTO-FILL ( NONE)
RBF-AUTO-FILL
RDI-AUTO-FILL ( NONE)
END OPTIONS
eos
#
cp ${AA}/H+He PROATOM
expand options PROATOM > SOURCE
${BI}/atoms2${sys}
ls -l ATOMS
#
cp ATOMS ${AA}/H+He.atoms2
#
# do not edit the rest of this file
#####################
set +x; ${HOME}/.jobend ${TMPDIR}
```

- Run both jobs and create output files for them, e.g., enter

  ```
  H+He.job > H+He.out
  ```

  on the unix command prompt. The resulting atomic-data files H+He_lte.atoms2 and H+He_0100000.atoms2 are copied to `/home/${logname}/fgrids`.

D.8.2 *SETF2*

- Edit both files H+He_lte.setf2 and H+He.setf2 in `/home/${logname}/jobs/setf2`. Set the temperature in both files to 100000 K and make sure that the jobs files refer to H+He_lte.atoms2 and H+He.atoms2, respectively. In resulting atomic data file for an *LTE2* calculation is temperature independent because not line transitions are considered. The respective parts that have to be changed by a user in the following scripts are marked in red color.

Table 7: Example for *SETF2* jobs in the case of LTE (*LTE2*, left) and NLTE (*PRO2*, right) model-atmosphere calculations.

SETF2 job for an *LTE2* model

```
#!/bin/sh
set +x;.  ${HOME}/.jobstart
# do not edit the beginning of this file
#########################
## own job following ##
#########################
#
TTM=0100000
#
type='_lte'
#
cp ${AA}/H+He${type}.atoms2 ATOMS
#
${BI}/setf2${sys} << eos
${TTM}
PRINT CHECK
1.30E+16
-1
10 10
eos
#
if test -s FGRID
then
cp FGRID ${FF}/H+He${type}.setf2
else
echo 'no FGRID created'
fi
#
#####################
set +x; ${HOME}/.jobend ${TMPDIR}
```

SETF2 job for a *PRO2* model

```
#!/bin/sh
set +x;.  ${HOME}/.jobstart
# do not edit the beginning of this file
#########################
## own job following ##
#########################
#
TTM=0100000
#
type=' '
#
cp ${AA}/H+He${type}.atoms2 ATOMS
#
${BI}/setf2${sys} << eos
$TTM}
PRINT CHECK
1.30E+16
-1
10 10
eos
#
if test -s FGRID
then
cp FGRID ${FF}/H+He_${TT}${type}.setf2
else
echo 'no FGRID created'
fi
#
#####################
set +x; ${HOME}/.jobend ${TMPDIR}
```

- Run both jobs and create output files for them, e.g., enter

  `H+He.job > H+He.out`

  on the command prompt. The resulting f frequency-grid files H+He_lte.setf2 and H+He_0100000.setf2 are copied to `/home/${logname}/fgrids`.

D.8.3 Parameter files

- Extract the parameters from the *ATOMS2* and *SETF2* output files file with

```
cd /home/${logname}/jobs/atoms2
grep para H+He.out
cd /home/${logname}/jobs/setf2
grep para H+He_0100000.out
```

- the parameter files for PRO2 can be found in `/home/${logname}/PARAMETER/pro2`
- copy the already existing parameter files to PARA_H+He.INC, PARA1_H+He.INC, PARA3_H+He.INC and adjust them by using the parameters extracted from the *ATOMS2* and *SETF2* output files (see above).
  NOTICE: the values in the parameter files should never be equal to 0 and none of the parameters ending with MAD (but NRBBMAD) has to be changed by the user!
- compile with `ssh ait320 load pro2 H+He p64`. The executable `/home/${logname}/bimod/pro2_H+He.Linux_x64` is created.

D.8.4 *LTE2*

- Edit `/home/${logname}/jobs/lte2/H+He.job` with emacs. Set $T_{eff} = 100000\,\mathrm{K}$, $\log g = 7$ and number fractions H=0.9 and He=0.1. The input files are H+He_lte.atoms2 and H+He_lte.setf2.
- Start the job (an example is given below) and write its output into a file.

  `nice +19 H+He_lte.job > H+He_lte.out` The *LTE2* model is written to `/home/${logname}/model/H+He/lte`. The model is named 0100000_7.00_0.900_0.100.

```
#!/bin/sh
set +x; . ${HOME}/.jobstart
# do not edit the beginning of this file
############################
## own job  following ##
############################
#
# ------------
# common paths
# ------------
GRP=/home/rauch/group
# ---------
# user part
# ---------
#
# directories etc.
#
code=lte2
 mod=H+He
type='_lte'
#
jobdir=${JO}/lte
flxdir=${JO}/lte
#
# model parameters
  H=0.900
 HE=0.100
#
GGM=7.00
TTM=0100000
#
name=${TTM}_${GGM}
fn=${mod}
#
aa=${AA}/${fn}${type}.atoms2
ff=${FF}/${fn}_${TTM}${type}.setf2
#
MO=${MO}/${mod}/lte/${name}_${H}_${HE}
#
```

```
if test ! -s ${MO}
then
#
echo '2 1 ${H} ${HE}' > normH
echo '2 2 ${H} ${HE}' > normHE
#
 HN=`/home/rauch/bimod/normalize${sys} < normH  2>/dev/null 1>&1`
HEN=`/home/rauch/bimod/normalize${sys} < normHE 2>/dev/null 1>&1`
#
cat > LDATEN << eos
T EFF ${TIM}
LOG G ${GGM}
DAMP=0.1
ITMAX=100
EPS=1.0E-6
TAU SCALE  86 90 -2
PRINT INTEGRATED EDDINGTON FLUX,ITERATION:LAST
PRINT TEMPERATURE CORRECTIONS,ITERATION:LAST,ALL DEPTHS
PRINT MODEL ATOMS (OVERVIEW)
ABUNDANCE H  ${HN}
ABUNDANCE HE ${HEN}
eos
#
cp ${aa} ATOMS
cp ${ff} FGRID
#
${BI}/${code}${sys} < LDATEN
#
if test -s MODELL
then
  cp MODELL ${MO}
  chmod 600 ${MO}
fi
fi
#
# do not edit the rest of this file
#######################
set +x; ${HOME}/.jobend ${TMPDIR}
```

D.8.5 *PRO2*

- Edit the `/home/${logname}/jobs/pro2/H+He.job` in emacs. Adjust the temperature, $\log g$and the abundances of the used elements as before and check if the used files have the right names. The input files are H+He.atoms2, H+He_0100000.setf2 and the model from *LTE2* is the input model.
- Start the job (an example is given in table below) with

  `nice +19 H+He.job > H+He.out`
- The output model is written to `/home/${logname}/model/H+He/.`

```
#!/bin/sh
set +x;. ${HOME}/.jobstart
# do not edit the beginning of this file
############################
## own job  following ##
############################
#
# ------------
# common paths
# ------------
GRP=/home/rauch/group
# ---------
# user part
# ---------
#
# directories etc.
#
code=pro2
 mod=H+He
#
type=''
#
jobdir=${HOME}/jobs/pro2
flxdir=${HOME}/jobs/pro2
#
IONFRAC=HE
#
#--- model parameters
#
fn=${mod}
#
GGM=7.00
#
TTM=0100000
#
  H=0.900
HE=0.100
#
name=${TTM}_${GGM}
```

```
#
#
aa=${AA}/${fn}${type}.atoms2
ff=${FF}/${fn}_${TTM}${type}.setf2
#
name=${name}_${H}_${HE}
#
MI=${HOME}/models/${mod}/0100000_7.00_0.900_0.100_pro2
MO=${HOME}/models/${mod}/${name}_pro2
#
if test -s ${MI}
then
#
# use already existing PRO2 model if not converged yet
if test -s ${MO}
then
  MI=${MO}
fi
#
cat > DATEN << eos
COMMENT: test 4 TMAP
.
.CHANGE ABUNDANCE H  ${H}     MASS FRACTION
.CHANGE ABUNDANCE HE ${HE}    MASS FRACTION
.
.CHANGE LOGG $GGM
.CHANGE EFFECTIVE TEMPERATURE $TT
.
LAMBDA=4
.
OCCUPATION PROBABILITY FORMALISM FOR H1
OCCUPATION PROBABILITY FORMALISM FOR HE1
OCCUPATION PROBABILITY FORMALISM FOR HE2
.
OPACITY PROJECT RBF DATA: START AT EDGE
OPACITY PROJECT RBF DATA: MISSING HYDROGENIC
.
.STEP UP F-VALUES: MODEL-START: H1   1.0E-03 1.5 1
.STEP UP F-VALUES: MODEL-START: HE1  1.0E-04 1.5 1
.STEP UP F-VALUES: MODEL-START: HE2  1.0E-03 1.5 1
.
ITMAX=20
.ERRSCH=1.0E-4
NEWMAX=4
.ERRNEW=1.E-8
.
RADIATIVE EQUILIBRIUM: DIFFERENTIAL/INTEGRAL FORM
.INNER BOUNDARY: LAMBDA-ITERATION
.LINEARIZE HYDROSTATIC EQUATION
.
NO NEGATIVE POPULATION NUMBERS (LTE)
```

```
.
.SWITCH OFF LINES
.
DEPTH DEPENDENT LINE PROFILES, LINEARIZATION: FIRST
.
KANTOROVICH=2,   SWITCH LIMITS  0-->1, 1-->2, 2-->1 : 0.1  0.01  0.5
.SOLVE STATISTICAL EQUATIONS ONLY   RE-SOLVE PARTICLE CONSERVATION
.
.NO TEMPERATURE CORRECTION
.UNSOELD-LUCY TEMPERATURE CORRECTION DAMP=0.1   0.1   0.1
.UNSOELD-LUCY PARAMETERS PRINT LIMIT 0.1 TAU-WIS 0.1  1.
.
.REDUCE LOG CVEC -1
.
.PRINT OPTIONS
PRINT MODEL ATOMS (OVERVIEW)
PRINT ABUNDANCES
PRINT MAX. REL. CORRECTIONS EVERY 1  ITERATIONS
PRINT INTEGRATED SURFACE FLUX,ITERATION:EACH
PRINT CP-TIME/ITERATION,EACH
PLOT  EMERGENT FLUX,ITERATION:LAST
PRINT OUTPUT MODEL,ITERATION:LAST,DEPTH INCREMENT:1    (STRUCTURE ONLY)
PRINT CORRECTIONS OF LAST LINEARIZATION,ITERATION:LAST,DEPTH INCREMENT
    :1
LP-PLOT OPTICALLY THICK/THIN,ITERATION:LAST,FILE ONLY
PLOT IONIZATION FRACTIONS ${IONFRAC}  -8.5  2.5  -10.0  0.5
.
MACHINE `hostname`
eos
#
ls -l ${MI}
cp ${MI} MODIN; chmod 600 MODIN
ls -l ${aa}
cp ${aa} ATOMS
ls -l ${ff}
cp ${ff} FGRID
/home/rauch/data/get_OP > /dev/null
#
ls -l ${BI}/${code}_${mod}${type}${sys}
${BI}/${code}_${mod}${type}${sys} < DATEN
#
if test -s MODOUT
then
  echo "new NLTE  model ${MO} created"
# save input model before replacement
  cp ${MI} ${MI}_`date +%y-%m-%d_%H:%M:%S`
  cp MODOUT ${MO}
  chmod 600 ${MO
  ls -l ${MO
  if test -s STOP
  then
```

```
    cp STOP ${MO}.converged
  fi
else
  echo "no new model ${MO} created" > ${MO}.failed
  touch ${MO}.failed@$HOSTNAME
  echo "no new model ${MO} created"
  if test -s MODTMP
  then
    echo "model found from iteration before failure"
    cp ${MI} ${MI}_`date +%y-%m-%d_%H:%M:%S`
    cp MODTMP ${MO}_tmp
    ls -l ${MO}_tmp
  fi
fi
#
# save plot data files
if test -s IONPLOT
then
  cp IONPLOT ${jobdir}/${name}.${IONFRAC}_ion
fi
if test -s PLLP
then
  cp PLLP ${jobdir}/${name}.lp
fi
if test -s PLOTCORR
then
  cp PLOTCORR ${jobdir}/${name}.corr
fi
if test -s PRFLUX
then
  cp PRFLUX ${flxdir}/${name}.flux
fi
if test -s STRUCTURE
then
  cp STRUCTURE ${jobdir}/${name}.T-structure
fi
#
fi
#
# do not edit the rest of this file
#######################
set +x; ${HOME}/.jobend ${TMPDIR}
```

D.9 Naming the *TMAP* models

In the framework of the Virtual Observatory, *TMAP* models and SEDs that are calculated from them have to follow a general rule. The models' names have to start with $T_{\rm eff}$ (TTTTTTT) and $\log g$ (G.GG), followed by the element abundances in mass fractions. An example is

```
0100000_7.00_H:__9.0000E-01_HE:_1.0000E-01 .
```

This is suitable for a small number of elements, where the level name stays relatively short. Thus, the general form for a model name is then

```
TTTTTTT_G.GG_ABUND_<nnn> ,
```

where nnn is a three digit integer code. ABUND_nnn corresponds to a file with the same name (located e.g. in the model directory). It has the form

```
H␣␣9.0000E-01␣<source ...>
HE␣3.0000E-05␣<source ...>
C␣␣4.0000E-06␣<source ...>
N␣␣2.0000E-06␣<source ...>
O␣␣1.0000E-05␣<source ...>
NE␣2.0000E-03␣<source ...>
SI␣8.0000E-06␣<source ...>
FE␣1.0000E-03␣<source ...>
NI␣2.0000E-05␣<source ...>
```

Please use one line per element, starting with the *TMAP* element code. The abundances are in mass fraction. The entry for the source of the abundances is optional and format free. Avoid to use any string that will be erroneously identified as an element code by a UNIX *grep* command!

In the *TMAP* jobs, the following has to be inserted to set some shell variables (${moddir} is the model directory, ${abund_old} and ${abund_new} may be used for different abundances).

```
#
abund_old="ABUND_001"
abund_new="ABUND_001"
#
#
# abundances in mass fraction (see files)
#
# old abundances
oldabund=${moddir}/${abund_old}
#
Hold=‘grep "H␣␣" ${oldabund} | awk ’{ print $2 }’‘
HEold=‘grep "HE␣" ${oldabund} | awk ’{ print $2 }’‘
Cold=‘grep "C␣␣" ${oldabund} | awk ’{ print $2 }’‘
Nold=‘grep "N␣␣" ${oldabund} | awk ’{ print $2 }’‘
Oold=‘grep "O␣␣" ${oldabund} | awk ’{ print $2 }’‘
NEold=‘grep "NE␣" ${oldabund} | awk ’{ print $2 }’‘
SIold=‘grep "SI␣" ${oldabund} | awk ’{ print $2 }’‘
FEold=‘grep "FE␣" ${oldabund} | awk ’{ print $2 }’‘
```

```
NIold=‘grep "NI␣" ${oldabund} | awk ’{ print $2 }’‘
#
#
# new abundances
newabund=${moddir}/${abund_new}
#
Hnew=‘grep "H␣␣" ${newabund} | awk ’{ print $2 }’‘
HEnew=‘grep "HE␣" ${newabund} | awk ’{ print $2 }’‘
Cnew=‘grep "C␣␣" ${newabund} | awk ’{ print $2 }’‘
Nnew=‘grep "N␣␣" ${newabund} | awk ’{ print $2 }’‘
Onew=‘grep "O␣␣" ${newabund} | awk ’{ print $2 }’‘
NEnew=‘grep "NE␣" ${newabund} | awk ’{ print $2 }’‘
SInew=‘grep "SI␣" ${newabund} | awk ’{ print $2 }’‘
FEnew=‘grep "FE␣" ${newabund} | awk ’{ print $2 }’‘
NInew=‘grep "NI␣" ${newabund} | awk ’{ print $2 }’‘
#
```

In the input files of e.g. *PRO2* respective cards have to use the XXnew variables (XX is the element):

```
CHANGE␣ABUNDANCE␣H␣␣${Hnew}␣␣MASS FRACTION
CHANGE␣ABUNDANCE␣HE␣${HEnew}␣MASS FRACTION
CHANGE␣ABUNDANCE␣C␣␣${Cnew}␣␣MASS FRACTION
CHANGE␣ABUNDANCE␣N␣␣${Nnew}␣␣MASS FRACTION
CHANGE␣ABUNDANCE␣O␣␣${Onew}␣␣MASS FRACTION
CHANGE␣ABUNDANCE␣NE␣${NEnew}␣MASS FRACTION
CHANGE␣ABUNDANCE␣SI␣${SInew}␣MASS FRACTION
CHANGE␣ABUNDANCE␣FE␣${FEnew}␣MASS FRACTION
CHANGE␣ABUNDANCE␣NI␣${NInew}␣MASS FRACTION
```

E Colors

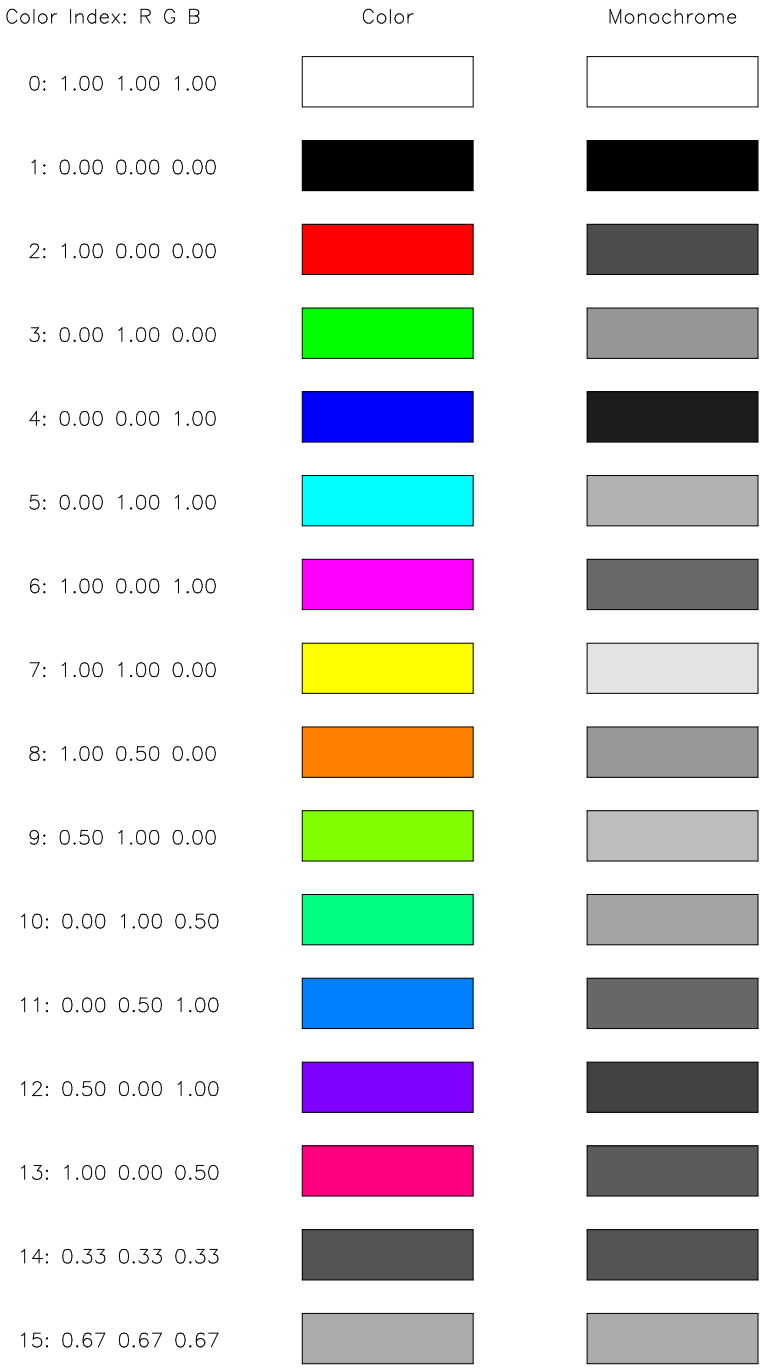


Figure 2: *PLXY* default colors, indices 0-15

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