

Non-LTE Line Formation: DETAIL and SURFACE

– Oh no not again

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1 Introduction

A few years ago, Jack Giddings and I provided a description of DETAIL and SURFACE (Butler and Giddings, 1985) in which the input was described in great detail (no pun intended, well o.k. it was) but which neglected to inform the reader how to compile the programs. Nor was there any description of the output. For completeness, these descriptions are included here and the formulae now available are to be found in the first appendix. The description of the GRIEM program has been omitted as it has outlived its usefulness. Thomas Schöning has made VCS tables available for almost all conceivable eventualities. Obtain them via my good self or the auspices of the CCP7 library.

Many of you will have noticed that the old description was almost but not completely accurate. Hopefully, there are less errors this time round but this is an uncertain world.

The programs have not evolved much in the intervening period. This will change shortly. However, since the changes are upwardly compatible it will simply be a good opportunity to present them in a later paper. To whet your appetites the new versions will include a velocity field, ALI operators, some parallelisation for the Cray, be much faster (at the cost of a greater core requirement) and, in the case of SURFACE, provide a much more efficient rotational broadening option (the current one is such a hack I am almost embarrassed).

2 Compilation

Well, you've obtained the sources from the CCP7 library (or even, Lord forbid, from me) and you want to know what to do now. You should have three program files, BSFSTR.F, SURFACE.PRE and DETAIL.PRE. I've written .PRE to indicate that these are NOT FORTRAN programs, they must be preprocessed first. To do this compile BSFSTR.F (the only problem will be if your compiler objects to a CDC PROGRAM statement), the string processor. The program requires a data file containing the dimensions for the problem at hand. An example would look like this

```
DETA CRAY
7000 2000 10 200 100 200 2500 600 12 13510000 90 5000 90 2300 8000
8000
FREQS FREQ LATOMS LLEV SXLEV SLEV SINDCS INDRS INDFS INDLSDATA SACTIVCROSFDEPTHCROSLXSECS
MAXGRMXTRBMXALB
```

(BSFSTR does have defaults for all input values but these are totally useless. We deal with so many different models, I couldn't decide what a sensible default might be). The first three lines are the actual input, the last two are the strings they replace in the *.PRE sources. These are a bit more descriptive than they used to be and have the following meanings

FREQS	Total number of frequencies
FREQL	Number of linearized frequencies
ATOMS	Total number of atoms
LLEVS	Total number of L levels
XLEVS	Total number of X levels
SLEVS	Total number of S levels
INDCS	Number of collisions
INDRS	Number of radiative transitions (BF, BX and BB)
INDFS	Total number of free-free transitions
INDLS	Total number of linearized transitions
DATAS	Total number of data entries in data stack
ACTIV	Number of active L Levels
CROSF	Total number of cross section data
DEPTH	Obvious innit?
CROSL	Number of linearized cross sections (lines only)
XSECS	Number of bound free cross sections blank for historical reasons
MAXGR	Number of groups
MXTRB	Size of the microturbulence table
MXALB	Number of albedos

The PRE file must be attached to FORTRAN unit 12, while the actual FORTRAN source will be written to unit 13, the latter may then be compiled and run with an appropriate data set (many are available from the CCP7 library).

If you are building your own model it's always a good idea to use the verify option (see sect. 3) as the last line of input will then be repeated giving an indication of how far the program has got. Dimension problems are amongst the easiest to find as the program states that a dimension has been exceeded and repeats the current value of that dimension. Change the dimension data set and repeat until all dimensions are large enough.

The actual dimensions used are given in the output following the words 'PHYSICAL SETUP' (see appendix D). The output is repeated here together with the corresponding strings from the string preprocessor input. This is particularly useful for the 'CROSS DATA' which are printed BEFORE they are checked.

PHYSICAL SETUP

RUN STATISTICS FULL PART						
ATOMS	2	2		ATOMS	ATOMS	
LEVELS	53	53		LLEVS	LLEVS	
LTE LEVELS	8			XLEVS		
Q.D. SERIES	3			SLEVS		
COLLISIONS	451			INDCS		
FREQUENCIES	2947	1134		FREQS	FREQL	
OPACITIES	325			INDRS		
RATES	325	98		INDRS	INDLS	
FREE FREE	6			INDFS		
CROSS DATA	1522	1304	218	CROSF	CROSL	XSECS
INPUT DATA	1300			DATAS		
DEPTHS	90			DEPTH		

In fact, BSFSTR supports keyword driven input of the dimensions (thanks to Dirk Husfeld) but I haven't used this myself and it has not been maintained so it may not work properly. Anyone interested?

The main problem with preprocessing at present is that some loaders complain (as they should) when they encounter common blocks of differing lengths. The blocks are buffered in DETAIL/SURFACE to be of the same length. Unfortunately, in the current versions this is done using the preprocessor which can cause problems for large cases since the amount of buffering needed can exceed 999999, the largest string provided for. The new versions use PARAMETER statements and so this will soon disappear. The only solution at the moment is to increase the dimensions of the variables in the buffered common blocks to reduce the size of the dummy arrays, certainly not a rewarding enterprise.

The keywords on the first input line give the target program and machine. If you are not lucky enough to have a CRAY, VAX or HP or a machine compatible with one of these, don't despair it is straightforward to add another option. First find out what functions on your machine provide the DATE, TIME and elapsed SECONDS. Then change the routines XDATE, XTIME and CPTIME to reflect these. You also need to know if your machine has single or double precision. If double then search the PRE files for the CDC keywords and duplicate the lines you find (unless your compiler has something against PROGRAM statements), if single then do the same, looking for and duplicating VAX keywords. That's it for the sources. The CRAY option shows places where library matrix inversion routines may be inserted if this is at all relevant. Finally, a suitable machine keyword must be put into BSFSTR to allow the preprocessing to take place.

3 Input

Both SURFACE and DETAIL have the same overall block structure. The overlay and archive files have been removed from the present versions. Communication is now (mostly) via common blocks. In the very latest versions most of this has been shifted to the subroutine calls in the solution code enabling parallelisation to be performed more easily.

The blocks are as follows:-

READ — in which the data are read in and checked. There are various levels of print-out available as an aid to the second of these. All data are read in free-field format so that zeroes must be included explicitly. If all the data requirements are met the next block is executed.

SETUP — from the data given in the previous step, all necessary atomic physics parameters are calculated. At this stage there is a division between background rates that are held fixed during the linearization process and those that are not. The last comment does not apply to SURFACE of course. Again, it is possible to obtain a great deal of information about the atomic data via the print options. If no problems arise then SURFACE will proceed directly to the calculation of the radiation field as the third step. Because of the larger number of options in DETAIL the third step is controlled by

CODE — after an initial compulsory Λ -iteration which must be specified (an estimate of the rates is needed for the linearization), linearizations and Λ -iterations may be freely mixed. This and other options are determined by keywords that are read by CODE.

All the options are now described in terms of the input to DETAIL. The input for SURFACE may be identical but more probably will have Voigt profiles and many more line frequency points in order that they may be delineated accurately.

An important point to note at the outset is that the input is restricted to columns 1 to 80 but the programs see the input as a single stream (You can change this by redimensioning ICARD in COMMON block FRE and changing the call to ENTER in the main program). This can lead to problems for the unwary since a character in column 80 is followed directly by the character in column 1 on the next line. Always set 'V2' for the verify option (see below) when working on a new data set.

A number of more or less mystifying error messages can appear in your output. These are as follows with a few hints as to what to look for, but don't forget the verify option, it's a help!

DUPLICATE The same label has appeared elsewhere

LIMIT EXCEEDED Speaks for itself as does

GARBAGE e.g. A negative atomic weight doesn't make much sense

NOT POSSIBLE Perhaps you want to give a level a parent from the same ion?

MISSING One of our major keywords is missing. FREQ or ATOM for example.

UNKNOWN This keyword hasn't been seen before. Usually when giving the transition list and down to a typo.

MISPLACED A frequency in the wrong order in the **FREQ** list for example.

Data are introduced into the program by the use of keywords. The order of appearance of some keywords (and their associated data) is mandatory and these are indicated by (**) in the following. Other data need not appear but, if they do, they must be positioned appropriately. They are marked with a single asterisk. Still other data may occur anywhere within a given section of the input. These are described at the end of the section in question. Two methods control the amount of data read by a keyword. Either the number of expected quantities is given or a list of input values is terminated by a 0. This will become clearer later but note that a 0 (alone) is therefore not a valid label and that care must be taken to give the correct number of values. To aid in this, the program has three verification levels which may be changed at any time. The control character ':' in the first column interrupts the flow of data to pass instructions to the reading routines. Thus the level of verification is set by

:V_n

where n is 0, 1 or 2. The printout obtained, increases from none for n=0 to all input quantities together with some internal data for n=2. Comments may also be interspersed throughout the data by the use of

:T 'This is a comment'.

The first section gives a set of continuum frequency points in descending frequency order. Thus the first keyword must be

FREQ**

```
labf1  ν1
labf2  ν2
  ⋮      ⋮
labfn  νn
0
```

All labels, both here and throughout the code, consist of one to six characters and the frequencies are in Hz. Frequencies less than 10⁶ are assumed to be wavelengths (they must still appear in the correct order) and are converted to frequencies. The current version of the program uses trapezoidal quadrature for the frequency mesh so that no particular choice is necessary, save for numerical considerations. It is also advantageous to include frequencies at either side of ionization edges of interest.

The levels and transitions of the ions under consideration are read in next. Ions described in this way may be calculated explicitly or may appear only as contributions to the opacity. For the ions that are included in the statistical equilibrium equations, each level must have at least one transition that connects it to another level. If this is not the case, the rates matrix **A** becomes singular. The program has no checks for this so the user should take care that all levels are connected.

Each element is introduced by the keyword

ATOM** Labat Z At. Wt. Abund

and is followed by a label for the atom, the charge, Z, of the lowest ion considered, the atomic weight and the abundance by number density relative to the total number density. A negative value for the abundance implies that the number read is the logarithm (to base 10) of the actual abundance.

The levels of the ions of this element are read in next and may take three forms

```
L**      Labl1      g1      ν1      Parent
X*      Labx      g      ν      Parent
S*      Labs      g0      g1      Ryd      μℓ      n0      n1      Parent
```

After each of **L**, **X** and **S**, there appears a list of the different levels of the ion, each list being terminated by '0'. **L** and **X** differ only in that **X** level populations are held fixed in LTE relative to the parent level

while **L** levels appear in the rate equations explicitly. The data for these are consequently similar. Each **L** and **X** level has a label, a statistical weight g , a frequency and a label detailing the parent level. The frequency is the ionization potential of the level in Hz and the parent label for **L** and **X** levels should be that of the ground state of the next ion so that the transition frequencies are calculated correctly. At each call to **L**, the ionic charge Z is increased by one and it is assumed that the following levels belong to the next ion. Hence, the **X** and **S** levels following a given **L** belong to the same ion.

The **S** level descriptors differ from the other two because they represent upper state sums that appear only in the number conservation equations. The data are statistical weight factors g_0, g_1 such that the weight of a level with principal quantum number n is $g_1 n^2 + g_0$. The g_1 term allows for sums over the angular momentum quantum number ℓ and spin s ; a constant (Ryd) and quantum defect μ_ℓ so that the energy of the levels, relative to their parent is

$$-\text{Ryd}/(n - \mu_\ell)^2$$

(N.B. Ryd is Z^2 times the Rydberg constant for the atom). The sum extends from $n=n_0$ to $n=n_1$ and the series converge to the ‘parent’ level of the ion. The Rydberg constant (in Hz) for an atom of atomic weight AW is given by

$$\text{Ryd} = \frac{109737.312 \times c}{1 + 1./(1836. \times AW)}.$$

The input of levels is terminated by a **K** level which should be the ground state of the most highly charged ion in the model. It has no associated **X** or **S** levels but the same data as for an **L** level is required. Only the statistical weight and label are used however, since no ion lies above it in the model.

The program checks that all ‘parents’ appear in the next ion levels as they ought and that labels are not repeated within an atom. If they are correct it then proceeds to read the data that define the transitions. Each transition is of a given type **TY** which has three attributes. The first is the type of transition, of which there are eight; collisional ionization between two **L** levels, CBF; collisional excitation between two **L** levels, CBB, between an **L** level and an **X** level, CBX, and between an **L** level and a series of **S** levels, CBS. Similarly, there are radiative transitions RBF, RBB, RBX and RFF. The last of these refers to free-free transitions. These types are followed by two integers. The first defines the formula to be used to calculate the cross section while the second specifies the number of data entries that the program is to expect. A transition type is therefore given by

TY** type nformula ndata

and this is followed by further data that depend on the type and formula. The program has some of the more standard formulae built into it and they are described in appendix A. If the formula number does not match any of the built-in functions, it is assumed to be user defined and the program calls a user subroutine of the correct type. They are UBOUND and UTABLE for radiative bound-bound transitions, UPHOTO for radiative bound-free transitions and UFREE for free-free transitions. There are also UCOLBB and UCOLBF for bound-bound and bound-free collisional transitions. Although the user may define these as he wishes, the rates and profiles used in this work are described in the following sections, and are available for general use. The program is unable to check that the formula numbers are permitted, so that they should be inserted carefully.

The first examples of the various types is that of **RBB** which has the following form

RBB** lab_l lab_u f_{lu}

(Note that the type must be repeated once. Thereafter any number of bound bound transitions of this type may follow. See the sample input for examples). The two labels must belong to levels of the same ion and the first value is assumed to be the oscillator strength of the transition. Other data may also be included if necessary, for a Voigt profile, say. The frequency mesh for the line is determined at this point. It may be defined either in terms of a nominal Doppler width or explicitly in Angstrom units. These are set by

DL n $\delta\lambda_1$ $\delta\lambda_2$ \dots $\delta\lambda_n$ for lambda

DB n $\delta\lambda_1$ $\delta\lambda_2$... $\delta\lambda_n$ for Doppler

where there are n frequency points at wavelength $\delta\lambda$ relative to the centre of the line. For the Doppler case a line temperature may be given and is the temperature assumed when depth independent Doppler profiles are adopted. It is used solely in the definition of the frequency mesh and is introduced by the keyword

TL temperature.

The current mesh, as given by the last call to **DL** or **DB**, is used for all transitions thereafter until the mesh is redefined. The frequency at line centre is usually obtained from the difference between the frequencies of the levels given under the **L** and **X** keywords but the observed wavelength may be specified by the use of

CL TY RBB nformula ndata.

If **CL** is quoted, the line wavelength (in Å) should appear immediately after the label of the upper level.

The **CBB** transitions also have a lower level and an upper level which are followed by ndata data values. As with all entries, a type **TY** is terminated by a 0. **RBX** and **CBX** transitions are defined in the same way as for the **RBB** and **CBB** transitions respectively. However, there are now three labels, in that the lower and upper level labels are preceded by the label of a parent. This parent is not necessarily the same as that given in the **X** data. It is used to specify the level to which the rate is added in the rate equation. The form is therefore

CBX* parent₁ lab_l lab_u data
lab_l lab_u data etc.
0
CBX* parent₂ lab_l lab_u data

Note that the same parent applies to all transitions until the **CBX** is terminated by a 0 at which point the parent can be altered or a new **TY** may appear.

A **CBS** transition has the same form as the **CBX** and **RBX** transitions except that the first datum must be a power, **IP**, that is used to scale the collisional cross section of a level of principal quantum number n_0 by a factor of

$$(n/n_0)^{IP}$$

where n_0 is defined by the **S** level. The cross section should be that of the n_0 level and a sum is taken from n_0 to n_1 . There is no upper level for this case and the parent should agree with the one given in the **S** data. Hence,

CBS* parent lab_l IP data.

The **CBF** and **RBF** transitions also use the parent form and again, it is not necessary for the parent to agree with the one given by the **L** data (to allow for inner shell processes). Thus **CBF** transitions are defined

CBF* parent lab_l data.

However, the radiative rates need a frequency mesh for the calculation of the integrals over the radiation field. This is done in terms of the mesh given under **FREQ**

RBF* parent lab_l lab_{f_i} lab_{f_j} data.

The frequency labels must be in descending frequency order and if the transition is to be included in the rate matrices, then the second label should correspond to a frequency just greater than the ionization potential, so that the integral is performed accurately.

The final type, **RFF** has only the parent level specified as it is calculated over the entire frequency mesh

RFF* parent data.

At this point, further atoms may be defined in the same way, beginning with the keyword **ATOM**. If the atomic data have been completed, however, the next word must be

MULTI** n

and the first n atoms are included in the statistical equilibrium calculations. Next comes

LINEAR** n₁ n₂ ... 0.

LINEAR is an instruction to include the radiative rates n₁, n₂, *etc.* as linearized transitions. The numbers n_i are given by the program when the verify option is used. Thus it is necessary to verify the data initially, not only to provide a check but also to obtain the numbers assigned to the radiative transitions.

The temperature-density structure must be input next. It is introduced by the keyword

MODEL**

and this section must contain a

STRUCTURE** ND.

ND is the number of depth points. There is then a title of up to 40 characters

TITLE** This is a title.

and ND values of:

an integer giving the current depth point;

the integrated mass to the current depth;

the temperature;

the total number density;

the electron density;

and two further numbers, which are not used and so are arbitrary (originally Auer/Mihalas atmospheres were used in which b factors were output in these columns)

In addition, a 40 character title for the current calculation may be set by

TITLE This is another title.

TEFF T_{eff} is obvious.

GRAVITY log g is the surface gravity.

If log g is greater than ten, the logarithm of the given value is taken.

The hydrogen and helium abundances may be defined by the use of

YHE Y_{He}

and the abundance of any elements by

ABUNDANCE labat₁ abund₁ labat₂ abund₂ ... 0.

As usual, negative values imply that the logarithm of the abundance has been given. Y_{He} is the helium abundance. The hydrogen abundance is calculated from this value as

$$1 - Y_{He}.$$

Abundances for any given element may be read in more than once and the last one in wins. This means that to set a new abundance while using populations from a previous run as starting values the command must appear *after* the populations have been read. This also applies to things such as microturbulence and albedos which appear in the populations file.

A microturbulent velocity in kms^{-1} may be defined by

TURBULENCE v_T

or as a table

VARTUR ntr logmtr vtr

where a table of microturbulences is read in as a function of the logarithm of the mass column density. v_T is obtained by linear interpolation.

In the same way a table of albedos as a function of frequency may be introduced via

ALBEDO nalb fqalb alb

For SURFACE only!!! A table of Rosseland means will be tabulated if the keyword **ROSS** appears while **LIMB** enables the output of angle-dependent intensities and

ROTATE nrot vrot₁ ... vrot_{nrot}

gives correctly rotationally broadened profiles a la Mihalas and Lockwood (sorry I don't have the reference to hand, it disappeared with our computer manager). The number of angle points can be varied using either

ANGLES nmu

or

GAUSS nmu.

ANGLES distributes the nmu angle points evenly between 0. and 1. (0. is omitted of course). These only apply to the rotation routines, all other calculations are done using the standard Feautrier algorithm.

We have found it useful to introduce a history containing information as to what occurred in any given run. This is a string of text introduced by the **HISTORY** keyword and appearing on a single line. It differs from the :T mechanism in that this text is passed on to the output files. The **DRIVER** and **RYBIKI** routines generate **HISTORY** output as well.

Finally for this section, the populations of some, or all, of the levels may be read in. This provides a restart facility or allows the use of populations from other calculations. The keyword is

POPULATIONS ND₀

where ND₀ is the number of depth points for which populations are available. ND₀ must equal ND. Next comes another title

TITLE Yet another title.

and then an **ATOM** card

ATOM labat Z At. Wt. Abund

(see the earlier discussion). An **L** card gives the level for which the next ND₀ numbers are populations

lab_l g ν parent
pop₁ pop₂ ... pop_{ND₀}

lab_l g ν parent
etc.
0

A new atom may follow. If a level or an atom appears that is not included in the current calculation, the data for that level (atom) are read but ignored. The

GROUP labat oldlab newlab

keyword can be used to assign level populations to L levels with differing labels in the current model atom and to split up or to join pseudolevels together. The labels appear in pairs and are terminated by a 0, at which point the program expects another ATOM label. A further 0 quits the GROUP option. This keyword must appear directly after POPULATION and oldlab refers to the level name as it appears in the populations file, newlab as in the current model atom. The contribution is weighted according to the statistical weights of the two levels thus allowing fine structure level populations to be determined correctly etc.

The structure may be followed by any of

OPACITY*

TABLE*

PRINT* p₁ p₂ p₃ p₄

FIX* labat lab_l lab_u

GO

There is a facility to input opacities other than by explicitly giving the atomic data. The user may add a subroutine UOPAC that defines the opacity and emissivity on the frequency mesh. The subroutine is called only if **OPACITY** is included (there is a version included in the program which introduces the Kurucz line list data as background). Similarly, the calculation of detailed Stark-broadened line profiles is expensive. Therefore, the subroutine UTABLE is available to allow profiles obtained from accurate line-broadening theories to be stored in tabulated form outside the program. UTABLE would then read in these profiles and interpolate from them onto the current temperature, density and frequency grids. **TABLE** ensures that UTABLE is called.

The print options are such that the populations (p₁), collision rates (p₂), foreground and background photoionization cross sections (p₃) and background opacities (p₄) are printed at the first and every p_ith depth point.

The keyword **FIX** states that all levels of atom labat which lie between the level with label lab_l and that with lab_u have their populations held at their initial values, even if they have been declared in the **MULTI** command. This has the effect of forcing two overlapping lines to be calculated at the same frequency points, even if one of the lines belongs to an atom which is to be held fixed. It also allows only part of an atom to be solved for explicitly.

If the word is **GO** the program calculates all the data – collision rates, opacities, cross sections – which are to be held fixed throughout the statistical equilibrium (SE) calculations. Any other keyword causes the program to terminate with an error message.

SURFACE then proceeds to generate the surface radiation field without more ado. For **DETAIL**, further keywords are read in **CODE** and are as follows.

The print levels throughout the SE calculations may be changed at any time, again by the keyword

PRINT p₁ p₂.

This has the same effect as before for p₂, which refers to the active radiative rates and the populations. The radiation field is printed if p₁ is greater than 0. The amount of information increases with p₁ to a maximum for p₁ = 3.

SCRIBE The populations at any stage of the computation may be output to fortran unit 7.

There are two different SE calculations. The first is a Λ -iteration and begins with the keyword

DRIVE.

At this stage, it is possible to hold the bound-bound transition rates fixed by specifying **NOLINE** for a single iteration. **NOLINE** must be respecified if the line rates are to be fixed for further Λ -iterations.

NOLINE is disregarded by the linearization option. The radiative rates may be damped using the keyword **REDUCE** followed by the damping factor (between 0 and 1). There seems to be a problem with the implementation so its use is not recommended.

The second method is initiated by

RYBIKI n_{it} n_{sor} Ω TOL

where n_{it} is the number of linearizations, n_{sor} is the number of iterations in the approximate solution for the changes in the rates δZ_t , Ω is a parameter that controls the amount of successive over relaxations (sor) — 1.67 is generally found to be suitable — and TOL is a tolerance, which may be fairly coarse. Damping may be introduced in the same way as for the driver, this time using **DAMP** but there seems to be a bug somewhere so don't use it.

DRIVE must, of course, appear first, since the Rybicki linearization needs an estimate of the current values for the radiation field *etc.* However, thereafter, **DRIVE** and **RYBIKI** may appear in any desired order. It should be noted that the two systems are mutually inconsistent, unless all transitions are linearized. Hence, the Rybicki solution should prevail in the latter stages. The program provides plots at each overall iteration, so that the convergence of the solution may be seen clearly.

QUIT This keyword terminates program execution gracefully. Any other input causes a termination with an error message.

4 Output

A sample output is provided in appendix D. It has been shortened somewhat to save space but shows all the essential aspects of a typical **DETAIL** output. On occasion timings of the various routines are given on the far right indicating when a particular section has finished its job. The times are elapsed CPU seconds. These do not appear here as I had to reduce the number of columns to make everything fit.

The first section will be printed if a “:V2” appears at the start of the input data set. This should always be the case when developing a new model atom but can be switched off for production purposes. It is simply a repeat of the input data enabling these to be checked (we all make mistakes). The continuum frequency grid is followed by the model atoms with their L, X and S levels and then the transition information. For the latter, the data are repeated and the wavelength at line centre (BB) or at the ionization edge (BF) is also given. “MULTI” then says how many atoms are to be included in the statistical equilibrium equations. Next each linearized transition is listed coupled with the number of the transition in the input data set. There follow two further lists, the background and then the linearized transitions. The original transition number is given in the background list together with the levels involved and the wavelengths. An initial run with “LINEAR 0” saves the user from having to count the transitions by hand, speeding up the choice of transitions to be linearized. The numbering in the list of linearized transitions is important as later plots and tables in the **RYBIKI** section refer to the transition number in this list and not to the original order in the input data set which is what is needed for the **LINEAR** command. The number of the first and last frequencies for any given transition is also listed here which may help in finding the radiation field should it be needed.

The model atmosphere is printed out next including any populations which may have been read in and any comments added to the model atmosphere file. This is followed by the size of the problem described earlier, the print options are listed together with a brief description of the problem at hand. Of particular interest is the list of “FLOATING LEVELS”. The numbering is that used by **DRIVER** for its plots and tables.

The sections that follow are switched on by the **PRINT** option. The LTE populations and Saha factors appear first for each requested depth. The Saha factors are normalized so that the K level of each atom has a factor of one which can be a help when trying to find information for a particular level. For each depth requested three tables then follow. The first contains the collisional rate coefficients C_{ij} in Mihalas (1978) for all transitions. Next comes information for transitions not included in the statistical equilibrium equations including all free-free transitions. The numbers in the introductory line are the depth index, the number of the transition in the appropriate list, the levels involved including their order in the level list and lastly the indices of the first and last frequencies. The cross sections are printed

in this order which means that the cross section at the edge (smallest frequency) is generally the last number in the list.

These background opacities are summed and printed immediately since the populations are known (either they've been read in or are set to LTE values). For each frequency in the grid, two quantities are printed, call them C and E. C includes the electron scattering contribution and the total opacity and emissivity at this frequency are given by

$$\begin{aligned}\chi &= (C - E)/\rho \\ \eta &= 2h\nu^3/c^2E/\rho\end{aligned}$$

ρ being the density. Cross section information for active transitions then follows and the SETUP section closes with a repeat of the model atmosphere structure.

This output can be voluminous but is extremely useful for debugging new model atoms since obvious errors (negative or very large collision rates, cross sections) can be spotted immediately.

With "PRINT 3 1", the output from the DRIVER and RYBIKI subprograms is a maximum (and once more extremely voluminous). The minimum output is the plot from each iteration. For the DRIVER, the surface flux is printed for all frequencies. Frequency, wavelength, Eddington flux, the mass at which an optical depth of 1 is reached, total optical depth and value of the albedo are tabulated. The mass can be used to find the nearest depth point in the atmosphere from which other information, such as the rates or populations of interesting transitions, may be obtained. This is an aid in determining the dominant rates at the depth of line formation giving an idea of how a transition is formed. The fluxes are followed by a plot of the logarithmic relative changes in the populations as a function of depth. Each level is keyed by its index number in the plot. The changes should become smaller with increasing depth as LTE is then a good approximation. The surface is at the top for the DRIVER plot but at the bottom from the RYBIKI iteration allowing them to be distinguished at a glance.

The plot allows those levels to be picked out with unusually large corrections and the depths at which problems occur. This information, coupled with the optical depth information from the surface flux table can give clues as to the underlying physics of numerical problems. The most obvious is that of an ion being calculated at too low or too high a temperature leading to loss of significant figures in the solution of the equations of statistical equilibrium. Inconsistencies in the current model atom compared with that used in the model atmosphere can also lead to numerical instabilities caused by population inversions in the higher levels and subsequent emission. A good solution here is to start from LTE populations.

For each depth, all radiative rate coefficients and net rates followed by the populations are then tabulated. Mihalas writes the rate coefficients as R_{ij} while the net rates are defined by $R_{ij} - (n_j/n_i)R_{ji}$, thus a negative rate implies a net downward rate.

The surface flux for a RYBIKI iteration includes only the linearized frequencies but otherwise the same information as the DRIVER listing. With print option 3 line profiles are also given, flux versus wavelength. The fluxes are normalised simply to the maximum flux within the line. This maximum flux is printed as HMAX in the line header where the mass at the depth of formation (TAUL), maximum optical depth (TAUC) both at line centre and the frequency indices are given. For broad lines, the continuum can change significantly over the line profile which need not therefore be symmetric.

The rate and net rate coefficients come next. The numbering here corresponds to the order in the plot so that troublesome transitions may be found readily. Directly after the rates come the populations together with the b factors, referred to the *ground state of the next ion*. Other definitions are possible so the user should take care when conducting comparisons. As mentioned earlier, the plot which comes next has the innermost point of the atmosphere at the top where the changes should be small. Plotted are the logarithmic changes in the rates, a negative sign indicating that they have decreased during the iteration cycle. The maximum changes in the net rates rates which are tabulated are rarely useful. The depth index at which the maximum occurs is given together with the change for each linearized transition. I find the plot much more helpful.

The keyword "SCRIBE" if present enables the populations to be written to FORTRAN unit 7 which may be stored for use with SURFACE or as input to further DETAIL runs as necessary. The format is straightforward, the interesting part being the populations which are output for each active level at all depths.

The SURFACE output is a subset of the DETAIL output and will not be described further. However, two files are output as two formal solutions are in fact performed, one with the other without line

opacities. This enables Eddington fluxes to be written to FORTRAN unit 7 as with earlier versions while normalised (continuum=1) fluxes are written to unit 70 (as a sort of mnemonic aid) thereby making the measurement of equivalent widths much easier.

A Formulae available in DETAIL for Atomic Data Specification

The following is a list of the different formulae that are currently available within DETAIL for the specification of atomic data. They are given in terms of the type number referred to in the previous section.

RBF

In these formulae, the variable

$$x = \nu_o/\nu$$

is the ratio of the frequency at the ionization edge, ν_o , to the frequency ν . The α_i are parameters where, in general, α_o is a measure of the threshold cross section ($x=1$).

1.

$$\alpha_o x^3$$

Datum is α_o

2.

$$\alpha_o x^{-p}$$

$$\alpha_o x^{-p} + \alpha_1 x^{-q}$$

Data are α_o, p, α_1, q

4.

$$\alpha_o [\alpha_1 + (1 - \alpha_1) x] x^{\alpha_2}.$$

Data are $\alpha_o, \alpha_1, \alpha_2$

The previous formulae are generalizations of the hydrogenic form given next while type 4 is due to Seaton (1958).

5.

$$2.815 \times 10^{29} (Z^2/n^5)(g_{II}/\nu^3)$$

in which n is the principal quantum number and g_{II} is the bound-free gaunt factor (Mihalas 1978 p 99).

Datum is n

6.

$$\alpha_o e^{(\alpha_1 + \alpha_2 \nu)}$$

7.

$$e^{[\alpha_o + \ln(\nu)(\alpha_1 + \alpha_2 \ln(\nu))]}.$$

These last two allow the cross sections to be fitted by linear least squares fit procedures.

Data in both cases are $\alpha_o, \alpha_1, \alpha_2$

RBB

The first datum is *always* the oscillator strength f_{ij} . This will not be listed in the following.

1.

$$e^{-x^2}/(\sqrt{\pi}\Delta\nu_D)$$

where $\Delta\nu_D$ is the Doppler width in frequency units

$$\Delta\nu_D = \frac{\nu_o}{c} \left[\frac{2kT}{M} + \xi^2 \right]^{\frac{1}{2}}$$

and k is Boltzmann's constant, M is the mass of the particle, ξ is the turbulent velocity. The variable x is the displacement of the frequency ν from the frequency at line centre ν_o in terms of the Doppler width

$$x = (\nu - \nu_o)/\Delta\nu_D.$$

Note that this is depth dependent as the temperature at the current depth, T , is used.

2.

$$H(a, x)/(\sqrt{\pi}\Delta\nu_D)$$

where $H(a, x)$ is the Voigt profile

$$H(a, x) = \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{(v - y)^2 + a^2} dy$$

and a is the damping width which is parameterized as

$$\Delta\nu_D a = \Gamma_1 + N_e(\Gamma_2 T^p + \Gamma_3)$$

and hence can allow for pressure broadening. The usual definition for a differs from this by a factor of 4π . Therefore, all the Γ parameters should be divided by 4π before they are input to the program.

Data are $\Gamma_1, \Gamma_2, p, \Gamma_3$

3. The Stark profiles of Griem (1960) may be fitted numerically to the following form up to some limiting electron density N_e . The Stark width $\Delta\nu_S$ is given by

$$\Delta\nu_S^{-1} = c \times (b^2 - a^2)Z^5/(\Delta\nu_o^2)$$

in frequency units and

$$\Delta = 5.5 \times 10^{-5} a^4 b^4 \times 1.25 \times 10^{-9} N_e^{\frac{2}{3}}.$$

For

$$\Delta\nu_S < 0.194\Delta\nu_D$$

the depth dependent Doppler profile is used. Otherwise, with

$$x = (\nu - \nu_o)/\Delta\nu_S,$$

the profile is

$$TH(x)/\Delta\nu_S$$

and $TH(x)$ is the fitted function.

Data are a, b, N_e

4. The Lorentz width is

$$\Delta\nu_L = \Gamma/4\pi.$$

Hence if

$$x = (\nu - \nu_o)/\Delta\nu_L$$

the profile is

$$\frac{1}{\pi\Delta\nu_L} \frac{1}{1 + x^2}.$$

Datum is $\Gamma/4\pi$

5. The depth independent Doppler profile is of the same form as type 1 above except that the fiducial temperature T_{LINE} , mentioned in sect. 3 is used rather than the 'physical' temperature.

RFF

There are only two built-in functions of this type. Both are based on the hydrogenic form, which is the first type

1.

$$3.69 \times 10^8 N_e T^{-\frac{1}{2}} Z^2 g_{III}(\nu, T, Z) \nu^{-3}$$

and g_{III} is the free-free gaunt factor.

2. The second form accounts for the opacity from an infinite series of LTE levels from a given value of the principal quantum number n , upwards. The frequency of the ionization potential of the n level is therefore,

$$\nu_n = 3.29 \times 10^{15} (Z^2/n^2)$$

(3.29×10^{15} is an approximate Rydberg constant in frequency units) and the smaller of the two frequencies, ν and ν_n , is chosen for the exponential factor, *i. e.* ν_{min} is the cutoff frequency

$$\nu_{min} = \min(\nu, \nu_n).$$

The opacity is then

$$3.69 \times 10^8 Z^2 N_e T^{-\frac{1}{2}} \nu^{-3} (e^{h\nu_{min}/kT} - 1).$$

Datum is n

CBF

1. Seaton (1962) has given a formula for the collisional ionization cross section in terms of the photoionization cross section at threshold, α_o , which yields a rate

$$1.55 \times 10^{13} \alpha_o \bar{g} N_e T^{-\frac{1}{2}} e^{-u_o} / u_o$$

where

$$u_o = h\nu_o/kT.$$

The \bar{g} factor is Z dependent, being 0.1, 0.2 or 0.3 for $Z=1$, $Z=2$ and $Z \geq 3$ respectively.

Data are α_o, \bar{g}

2. This and the next form assume simply that the cross section is inversely proportional to the energy or that it is constant. Upon integration over the Maxwellian distribution the rates are then found to be

$$5.436 \times 10^{-11} N_e T^{\frac{1}{2}} e^{-u_o} \alpha_1$$

for the former case and

Datum is α_1

3.

$$5.436 \times 10^{-11} N_e T^{\frac{1}{2}} e^{-u_o} \alpha_o (1 + u_o)$$

for a constant cross section.

Datum is α_o

CBB

The formulae for this type of transition follow the same pattern as for the CBF type. Van Regemorter (1962) gives a form for the collisional excitation cross section that is similar to the Seaton collisional ionization cross section. It is proportional to the oscillator strength, f_{ij} , since bound-bound transitions are involved. The rate is

1.

$$5.465 \times 10^{-11} N_e T^{\frac{1}{2}} [14.5 f_{ij} (u_H^2 / u_o)] e^{-u_o} \Gamma$$

if u_H is the ionization potential of hydrogen scaled by kT . Γ is the maximum of

$$\Gamma = \max[\bar{g}, 0.276 e^{u_o} E_1(u_o)]$$

and $E_1(x)$ is the first exponential integral

$$E_n(x) = \int_1^\infty \frac{e^{-xt}}{t^n} dx.$$

The number \bar{g} is found to be 0.2 if the principal quantum number changes during the transition and 0.7 if it does not.

Data are f_{ij} , \bar{g}

2. The same two forms are provided here as in the CBF case giving the same rates

$$5.465 \times 10^{-11} \alpha_0 N_e T^{\frac{1}{2}} e^{-u_0}$$

and

$$5.465 \times 10^{-11} \alpha_0 N_e T^{\frac{1}{2}} e^{-u_0} (1 + u_0).$$

Datum is α_0 in both cases

B Utility Routines Optionally Available to DETAIL and SURFACE Users

In the course of our work in Munich, many atomic data have been gathered (have you read the papers?); so that they might be accessed the routines UPHOTO, UCOLBF and UCOLBB were written. This section details the various formulae for ease of reference. It also contains a brief outline of two routines, UBOUND and UTABLE, that allow tabulated Stark profiles for hydrogenic ions for example to be used in an efficient manner. The type numbers of sect. 3 are again referenced.

UPHOTO

11. Butler's (1984) photoionization data may be fitted to the quantum defect formulae reviewed by Seaton (1983). These are rather complicated generally, but at low energies the matrices that appear in the theory have only one element. The formulae become easy to manipulate in this region and are described here. However, it should be noted that a code which uses the full theory is available.

For a frequency ν the ejected electron has energy E ,

$$E = EFE - IP \quad \text{in Ryd}$$

the ionization IP should be in Rydberg units while the transition energy EFE may be calculated from

$$EFE = \nu/c\text{Ryd}.$$

The Rydberg constant for an atom of atomic weight AW is

$$\text{Ryd} = \frac{109737.312}{1 + 1/(1836 \times AW)} \quad \text{cm}^{-1}.$$

The fits have a reference energy E_{ref} so x is defined by

$$x = E - E_{ref}$$

and used to calculate

$$\begin{aligned} R &= \sum_{i=1}^{IPP} a_i x^{i-1} + \sum_{j=1}^{NPOLE} \frac{b_j}{E-E_j} \\ G &= \sum_{i=1}^{IPP} c_i x^{i-1} + \sum_{j=1}^{NPOLE} \frac{d_j}{E-E_j} \end{aligned}$$

with E_j , a_i , b_j , c_i , d_j as parameters. The cross section σ is then

$$\sigma = \frac{0.213985}{Z(2L_0 + 1)} EFE \frac{4G^2}{1 + R^2} \quad \text{Mb}$$

where L_0 is total angular momentum quantum number of the bound state. The fits are valid from the threshold up to a maximum frequency ν_{max} . Beyond ν_{max} other methods and data are needed.

Datum is a label for the cross section. See the N3TWOP data set for details. The data are read from FORTRAN unit 8

12. Because the usual form of the cross section given by Seaton (see RBF 4) is non-linear, complicated least squares fitting procedures are needed to obtain the parameters automatically. A similar linear form has already been given in RBF 5 (above) and was incorporated into a version of the single channel quantum defect theory program of Peach (1967). Several cross sections were calculated in this way and the fits are generalized so that

$$\ln \sigma = \sum_i^{NTERMS} a_i [\ln(\nu_0/\nu)]^{i-1}.$$

Data are $a_1 \dots a_6$

13. Pradhan (1980) recommends that his accurate neon cross sections be linearly interpolated between their values at the various threshold energies. This type deals specifically with that case. The threshold cross sections are held in data statements.

14. An extension to the Seaton formula. It reads

$$\sigma = \sigma_0[\alpha + (\alpha_1 + \alpha_2 x)x]^p$$

where x has its usual meaning and $\alpha_1 = \beta - 2\alpha$, $\alpha_2 = 1 + \alpha - \beta$.

Data are α , β , p

15. These are polynomial fits to the Opacity Project data but use 17 below

16. Calls the Storey and Hummer (1991) PIX11 routine for hydrogenic cross sections.

Data are n, l . If $n \geq l$ a total cross section summed over l is provided.

17. He I fits are generated from a subroutine provided by David Hummer. These are Opacity Project data. *Data are n , $2S+1$, L with $n \leq 10$. L, S are angular momenta*

18. Extension to Seaton formula once more (don't ask me why!). See 14.

19. A polynomial fit from ν_{min} to ν_{max} . With

$$x = [2\nu - (\nu_{min} + \nu_{max})]/(\nu_{max} - \nu_{min})$$

the cross section is

$$\sigma = \sum_{i=1}^n a_i x^{i-1}.$$

Data are ν_{min} , ν_{max} , $a_1 \dots a_n$

UCOLBB

Types 11 and 12 are intended to be used for fits to the Γ factor as defined by Mihalas (1978 p133). The Γ factor is defined so that the upward collision rate is

$$5.465 \times 10^{-11} N_e T^{\frac{1}{2}} \Gamma e^{-\frac{h\nu_0}{kT}}$$

and the fits are respectively

11.

$$\Gamma = C_{-2}T^{-2} + C_{-1}T^{-1} + C_0 + C_1T$$

Data are C_{-2}, C_{-1}, C_0, C_1

and

12.

$$\Gamma = C_{-2}(\log T)^{-2} + C_{-1}\log T^{-1} + C_0 + C_1 \log T.$$

Data are C_{-2}, C_{-1}, C_0, C_1

The following (up to and including type 21) are for use with hydrogen and helium although fits of similar form may be suitable in other cases. They are taken from Mihalas and Stone (1968) and from Mihalas (1972).

The close-coupling calculations of Burke *et. al.* (1967) are scaled for $\Delta n > 1$ (Δn is the change in the principal quantum number) to the Sampson and Golden (1971) results. The upward rate is

13.

$$5.465 \times 10^{-11} N_e T^{\frac{1}{2}} \times [4f_{ij} (u_H/u_0)^2] (E_1(u_0) + 0.148u_0 E_5(u_0))$$

where $u_0 = h\nu_0/kT$ and f_{ij} is the oscillator strength of the corresponding radiative transition. For $\Delta n=1$ this is the final result but for $\Delta n > 1$, it is scaled further by a factor of

$$\beta + 2(\alpha - \beta)/\Delta n$$

in which

$$\alpha = 1.8 - 0.4/n^2$$

$$\beta = 3.0 - 1.2/n$$

and n is the principal quantum number of the lower level.

Datum is f_{ij}

14. For He II, the rate is

$$5.465 \times 10^{-11} N_e T^{\frac{1}{2}} (2.71 f_{ij} (u_H/u_0)^2) u_0 [0.693e^{-u_0} + E_1(u_0)]$$

The results are again scaled for $\Delta n > 1$, this time by a factor of

$$\min(n, 1.1) \times \min[\Delta n, n - (n - 1)/\Delta n].$$

Datum is f_{ij}

For allowed transitions from He I ground state Mihalas and Stone (1968) give

15.

$$5.465 \times 10^{-11} N_e T^{\frac{1}{2}} (4f_{ij} (u_H/u_0)^2) u_0 E_1(u_0)$$

Datum is f_{ij}

while from excited states the rate is

16.

$$5.465 \times 10^{-11} N_e T^{\frac{1}{2}} (4f_{ij} (u_H/u_0)^2) u_0 [E_1(u_0) - e^{-0.2(u_0/u_1)} E_1(u_1)]$$

with $u_1 = u_0 + 0.2$.

Datum is f_{ij}

The formula A16 of Mihalas and Stone (1968) for the forbidden rates from the ground state of He I is given by type 17. The form is not repeated here as it is not of direct interest. Other forbidden transitions of He I are variously of the form

18.

$$\log \Gamma = C_0 + C_1 \log T + C_2 (\log T)^{-2}$$

Data are C_2, C_1, C_0

and rates

19.

$$5.465 \times 10^{-11} N_e T^{\frac{1}{2}} a_3 u_0 [e^{-u_0} - u_0 E_1(u_0)]$$

20.

$$5.465 \times 10^{-11} N_e T^{\frac{1}{2}} (2a_3) u_0^2 \left[\frac{2}{3} (1 + u_0) e^{-u_0} (\pi u_0)^{\frac{1}{2}} (1 - \text{erf}(u_0)) \left(1 + \frac{2}{3} u_0\right) \right]$$

21.

$$5.465 \times 10^{-11} N_e T^{\frac{1}{2}} a_3 u_0^2 [E_2(u_0) - E_3(u_0)]$$

Datum for all three formulae is a_3 with the error function defined by

$$\text{erf}(x) = \int_0^x e^{-t^2} dt.$$

Type 22 is the Van Regemorter formula given previously in CBB (formula 1) while type 23 represents fits to some unpublished distorted wave results by Hummer (private communication) for N^{2+} and N^{3+} .

23. If

$$\gamma = \sum_i^{NTERMS} a_i (T/10^4)^{i-1}$$

the upward rate is

$$\frac{N_e g_i}{T^{\frac{1}{2}} g_j} e^{-u_0} \gamma$$

with the statistical weights of the two levels g_i, g_j . For optically allowed transitions the rate is further scaled by a factor

$$f_{obs}/f_{calc}.$$

The calculated oscillator strength f_{calc} is the one obtained with the wavefunctions used in the distorted wave scattering problem while ' f_{obs} ' is an accurate value, either from an experiment or from a more detailed calculation.

Data are $f_{obs}, f_{calc}, a_1 \dots a_8, g_i, g_j$

Allen (1973) gives a semi-empirical cross section so that

24.

$$\Gamma = \frac{\Omega h \nu_H}{g_i k T}.$$

Datum is Ω

The following are fits to the effective collision strength Υ which is related to the upward collision rate via

$$C_{ij} = \frac{8.631 \times 10^{-6}}{g_i T^{\frac{1}{2}}} N_e e^{-u_0} \Upsilon.$$

25.

$$\Upsilon = \sum_{i=1}^{NFIT} a_i x^{i-1}$$

and x is a scaled temperature

$$x = (T - T1)/\text{scale}.$$

Data are $T1, \text{scale}, NFIT, a_1 \dots a_{NFIT}$

26.

$$\Upsilon = \sum_{i=1}^{NFIT} a_i x^{i-1}$$

where x is now

$$x = \log T - T1.$$

Data are $T1, NFIT, a_1 \dots a_{NFIT}$

Merts *et. al.* (1980) provide fits for many ions. Their rates have the form

27.

$$8.631 \times 10^{-6} \frac{N_e}{g_i T^{\frac{1}{2}}} u_0 \left[a_1 \frac{e^{-u_0}}{u_0} + \left(a_2 + \frac{a_4}{u_0} \right) E_1(u_0) + a_3 E_2(u_0) \right]$$

Data are $a_1 \dots a_4$

and

28.

$$\Gamma = \sum_{n=1}^4 a_n \frac{e^{-(u_0 + na_5)}}{(u_0 + na_5)}$$

with the upward rate

$$C_{ij} = 8.631 \times 10^{-6} N_e T^{-\frac{1}{2}} / g_i \times u_0 (a_0 E_2(u_0) + \Gamma)$$

Data are $a_0 \dots a_5$

Formulae 29–32 were inserted for test purposes, while 33 and 34 are from Cochrane & McWhirter (1983) and read

33. and 34.

$$C_{ij} = 4.1105483 \times 10^{11} / (\nu_0 T^{\frac{1}{2}}) e^{-u_0} N_e \bar{g}$$

with

$$fac = 2.0835773 \times 10^{10} (T / \nu_0)$$

and

$$\bar{g} = g_1 + g_2 \ln(fac + g_3)$$

for formula 33 and

$$\bar{g} = g_1 + g_2 \ln \left(\frac{fac + g_3}{fac + g_4} \right)$$

for 34.

Data are $\alpha_0, g_1, g_2, g_3, (g_4 \text{ for } 34)$

35. Calls HECOL from David Hummer. The subroutine is fully commented. The He I levels are indexed. These are the only data required.

Data are n_l, n_u , the indices of the lower and upper levels

36. A formula for constant Ω .

$$C_{ij} = 8.631 \times 10^{-6} / (T^{\frac{1}{2}} g_i) N_e e^{-u_0} \Omega$$

Datum is Ω

37. Van Regemorter (1962) formula for neutrals as implemented by D.G. Hummer.

Datum is f_{ij}

38. Calls David Hummer's HCOL routine but *should not be used* – the fits are in error.

39. Calls David's COLL21 routine. This is an updated version of HECOL and requires the same input (see 35).

40. Calculates classical impact cross sections from a routine written by David Hummer.

Datum is n , principal quantum number of the upper level

UCOLBF

Again, general fits in powers of T and log T have been included.

11.

$$\Gamma = C_{-2} T^{-2} + C_{-1} T^{-1} + C_0 + C_1 T + C_2 T^2$$

Data are $C_{-2}, C_{-1}, C_0, C_1, C_2$

12.

$$\Gamma = C_{-2}(\log T)^{-2} + C_1(\log T)^{-1} + C_0 + C_1 \log T + C_2(\log T)^2$$

Data are C_{-2} , C_{-1} , C_0 , C_1 , C_2
while a hydrogenic scaling is given by

13.

$$\Gamma = (C_0/Z)^4.$$

Data are C_0

Mihalas and Stone (1968) quote results for He I levels such that the rate is

14.

$$5.465 \times 10^{-11} N_e T^{\frac{1}{2}} \sigma_0 [u_0 E_1(u_0) - 0.728(u_0^2/u_1) E_1(u_1) - 0.189(u_0^2/u_2^3) e^{-u_0} (2 + u_2)]$$

and $u_1 = u_0 + 0.27$, $u_2 = u_0 + 1.43$. They also give the relevant values of σ_0 .

Datum is σ_0

The Seaton formula mentioned in the earlier CBF section is repeated as type 15. The Lotz (1968) formula is represented by type 16

16.

$$5.465 \times 10^{-11} N_e T^{-\frac{1}{2}} a_1 (2.5 (u_H/u_0)^2) u_0 [E_1(u_0) - a_2 e^{a_3} (u_0/u_1) E_1(u_1)]$$

with $u_1 = u_0 + a_3$.

Data are a_1 , a_2 , a_3

Moore's (1972) fitted his collisional ionization cross sections for the Boron sequence to a power series in $1/X$ together with a term in $\ln X/X$. Here X is a dimensionless variable

$$X = \nu/\nu_0.$$

The rate is then

17.

$$5.465 \times 10^{-11} N_e T^{\frac{1}{2}} \left[a_0 E_1(u_0) + a_1 e^{-u_0} + u_0 \sum_{i=2}^N a_i E_{i-1}(u_0) \right].$$

Data are N , $a_0 \dots a_N$

The next form in this category are the rates due to Golden and Sampson (1980). These are scaled hydrogenic cross sections that depend on the principal quantum number n , the angular momentum quantum number ℓ , the number of equivalent electrons, $r_{n\ell}$ and a screening factor $\sigma_{n\ell}$ to give an effective charge

$$Z_{eff} = Z - \sigma_{n\ell}.$$

The rate is

18.

$$5.465 \times 10^{-11} N_e T^{-\frac{1}{2}} r_{n\ell} (n^2/Z_{eff})^2 [D'(n, \ell) e^{-u_0} + (A'(n, \ell) + u_0(C'(n, \ell) - 2D'(n, \ell))) E_1(u_0) + u_0(D'(n, \ell) + D''(n, \ell) - C'(n, \ell)) E_2(u_0) - u_0 D''(n, \ell) E_3(u_0)].$$

The parameters A' , D' , C' , D'' have been tabulated by Golden and Sampson and are included in the subroutine as a data statement.

Data are $r_{n\ell}$, n , ℓ , $\sigma_{n\ell}$

19. Was inserted for test purposes.

20. Bell *et al.* (1983) gives fits for the ground states of light ions. Their formula gives

$$5.465 \times 10^{-11} N_e T^{-\frac{1}{2}} (u_H/u_0)^2 [\sigma_0 u_0 E_1(u_0) + \sigma_1 (u_0/u_1)^2 (E_1(u_1) + e^{-u_1})]$$

with $u_1 = u_0 + \Delta u$
 Data are $\sigma_0, \sigma_1, \Delta u$

21. This calls the HECION routine for He I kindly provided by David Hummer. The levels are indexed in energy order.
 Datum is n , the energy level index

UBOUND and UTABLE

These two subroutines are used in conjunction with each other. If type 99 is specified then the keyword **TABLE** should be quoted as indicated in sect. 3. This is discussed further below.

Type 11 utilizes the theory of Barnard *et. al.* (1969) for isolated He I lines and is described further by Auer and Mihalas (1972). The depth independent Doppler profiles are again represented by type 12 and the Griem (1960) theory for Stark broadened hydrogenic lines as implemented by Auer and Mihalas (1972) is given by types 13 and 99. If the type is 99, **UTABLE** is called (providing that **TABLE** has been specified) and the profiles are interpolated from a grid over temperature, density and frequency. If interpolation is not possible, **UBOUND** will calculate the necessary data since the second parameter for type 99 (remembering that the oscillator strength is always the first parameter) is a further type (11 - 14) to be used in this eventuality. The data for the second type should then follow as usual.

The last **UBOUND** type, 14, consists of a Doppler core with power law wings. The width

$$\Delta\nu_S = 8 \times 10^{10} N_e^{\frac{2}{3}} \lambda(\text{\AA})/\nu$$

and

$$x = (\nu - \nu_o)/\Delta\nu_D.$$

For $x < 2$, the profile is

$$e^{-x^2}/(\pi^{\frac{1}{2}} \Delta\nu_D)$$

while for $x \geq 2$ it is the larger of the above or

$$(C_0/y)^{2.5}$$

in which $y = (\nu - \nu_o)/\Delta\nu_S$ and C_0 is a parameter.

C A sample input file

This is a listing of ALIIIAT, available from your local friendly CCP7 data set handler.

```
:V2
:T=====
:T      ALIII DATASET FOR DETAIL
:T      VERSION 1.03
:T      SET UP BY SYLVIA BECKER
:T=====
:V0
:T
:T      EFFECTIVE COLLISION STRENGTHS FOR TRANSITIONS
:T      BETWEEN SOME LEVELS AS IN PAPER BY DUFTON
:T
:T      *****
:T      * OLIVER'S LABELS FOR THE ENERGY-LEVELS *
:T      *****
:T
:T
:T-----
```

:T FREQUENCY MESH

:T-----
FREQ

10	1.E17
20	6.E16
30	5.E16
40	4.E16
50	3.E16
60	2.E16
HHE010	1.3158E16
HHE011	1.3157E16
70	1.E16
80	9.E15
90	8.E15
30101	6.87901E15
30102	6.87871E15
HHE020	5.9487E15
HHE021	5.9486E15
30201	5.26495E15
30202	5.26465E15
100	4.5E15
30301	3.40274E15
30302	3.40244E15
HHE030	3.2929E15
HHE031	3.2928E15
30401	3.09675E15
30402	3.09645E15
30501	2.57142E15
30502	2.57112E15
30601	1.90888E15
30602	1.90858E15
30701	1.85412E15
30702	1.85382E15
30801	1.76346E15
30802	1.74316E15
30901	1.52901E15
30902	1.52871E15
HHE040	1.4632E15
HHE041	1.4631E15
31001	1.21666E15
31002	1.21636E15
31101	1.18669E15
31102	1.18639E15
31201	1.18512E15
31202	1.18482E15
HHE050	1.1528E15
HHE051	1.1527E15
HHE060	9.6034E14
HHE061	9.6033E14
HHE070	8.7612E14
HHE071	8.7611E14
HHE080	8.2238E14
HHE081	8.2237E14
HHE090	8.1472E14
HHE091	8.1471E14
110	6.5E14
HHE100	5.2631E14
HHE101	5.2630E14
HHE110	3.6548E14
HHE111	3.6547E14

HHE120	2.6852E14
HHE121	2.6851E14
HHE130	2.0551E14
HHE131	2.0550E14
HHE140	1.6244E14
HHE141	1.6243E14
HHE150	1.3153E14
HHE151	1.3152E14
120	8.E13
130	5.E13
140	1.E13
150	5.E12
160	1.E12
170	1.E11

0

:V2

:T-----

:T ALUMINIUM ATOM

:T-----

ATOM AL 2.0 27. .273E-4

L

AL32S1	2.	6.87886E15	AL41S1
AL32P1	6.	5.26480E15	AL41S1
AL32D1	10.	3.40259E15	AL41S1
AL32S2	2.	3.09660E15	AL41S1
AL32P2	6.	2.57127E15	AL41S1
AL32D2	10.	1.90873E15	AL41S1
AL32F1	14.	1.85397E15	AL41S1
AL32S3	2.	1.76331E15	AL41S1
AL32P3	6.	1.52886E15	AL41S1
AL32D3	10.	1.21651E15	AL41S1
AL32F2	14.	1.18654E15	AL41S1
AL32G1	18.	1.18497E15	AL41S1

0

S

3NS2S	2.	0.	2.961E16	0.9	6	10	AL41S1
3NP2P	6.	0.	2.961E16	0.6	6	10	AL41S1
3ND2D	10.	0.	2.961E16	0.07	6	10	AL41S1
3NF2F	14.	0.	2.961E16	0.007	6	10	AL41S1
3NG2G	18.	0.	2.961E16	0.0025	6	10	AL41S1
3NH2H	22.	0.	2.961E16	0.0020	6	10	AL41S1
3REST	-72.	2.	2.961E16	0.0	7	10	AL41S1

0

K

AL41S1 1.0 2.90134E16 NONE

:V2

:T-----

:T ALUMINIUM STATISTICS AND OPACITIES

:T-----

TL 30000.

DB 9 -4. -2. -1.33 -.66 0. .66 1.33 2. 4.

TY RBB 1 1 RBB

AL32S1	AL32P1	.854
AL32S1	AL32P2	.0133
AL32S1	AL32P3	.0076
AL32P1	AL32D1	.928
AL32P1	AL32S2	.127
AL32P1	AL32D2	.0039
AL32P1	AL32S3	.0180

AL32P1	AL32D3	.00005
AL32D1	AL32P2	.171
AL32D1	AL32F1	.936
AL32D1	AL32P3	.0097
AL32D1	AL32F2	.166
AL32S2	AL32P2	1.28
AL32S2	AL32P3	.0062
AL32P2	AL32D2	1.28
AL32P2	AL32S3	.229
AL32P2	AL32D3	.0229
AL32D2	AL32P3	.345
AL32D2	AL32F2	.732
AL32F1	AL32D3	.0187
AL32F1	AL32G1	1.339
AL32S3	AL32P3	1.660

0

TY	RBF	12	6							
	RBF	AL41S1	AL32S1	10	30101	-42.363	.1666	-.90357	-.18621	.0 .0
			AL32P1	10	30201	-42.606	3.95E-2	-.84268	-.14762	.0 .0
			AL32D1	10	30301	-40.468	3.0378	-.17911	-.1278	.0 .0
			AL32S2	10	30401	-42.268	.68105	-.44824	-6.37E-2	.0 .0
			AL32P2	10	30501	-42.241	1.3642	.22185	.11694	.0 .0
			AL32D2	10	30601	-39.952	2.8394	2.803E-2	8.471E-2	.0 .0
			AL32S3	10	30801	-42.132	.69576	-.40463	-5.142E-2	.0 .0
			AL32P3	10	30901	-41.690	2.0366	.55522	.13478	.0 .0
			AL32D3	10	31001	-39.560	2.3479	-.20798	-8.091E-3	.0 .0

0

TY	RBF	5	1							
	RBF	AL41S1	AL32F1	10	30701	4				
			AL32F2	10	31101	5				
			AL32G1	10	31201	5				

0

TY	CBB	22	2	CBB						
	AL32S1		AL32P3	.0076	.2					
	AL32P1		AL32D2	.0039	.2					
	AL32P1		AL32S3	.0180	.2					
	AL32P1		AL32D3	.00005	.2					
	AL32D1		AL32F1	.936	.2					
	AL32D1		AL32P3	.0097	.2					
	AL32D1		AL32F2	.166	.2					
	AL32S2		AL32P3	.0062	.2					
	AL32P2		AL32D2	1.28	.7					
	AL32P2		AL32S3	.229	.2					
	AL32P2		AL32D3	.0229	.2					
	AL32D2		AL32P3	.345	.2					
	AL32D2		AL32F2	.732	.2					
	AL32F1		AL32D3	.0187	.2					
	AL32F1		AL32G1	1.339	.2					
	AL32S3		AL32P3	1.660	.7					

0

TY	CBB	24	1	CBB						
	AL32S1	AL32D2	1.0	AL32S1	AL32F1	1.0	AL32S1	AL32S3	1.0	
	AL32S1	AL32D3	1.0	AL32S1	AL32F2	1.0	AL32S1	AL32G1	1.0	
	AL32P1	AL32F1	1.0							
	AL32P1	AL32P3	1.0	AL32P1	AL32F2	1.0				
	AL32P1	AL32G1	1.0	AL32D1	AL32D2	1.0				
	AL32D1	AL32S3	1.0	AL32D1	AL32D3	1.0				
	AL32D1	AL32G1	1.0	AL32S2	AL32D2	1.0				
	AL32S2	AL32F1	1.0	AL32S2	AL32S3	1.0	AL32S2	AL32D3	1.0	
	AL32S2	AL32F2	1.0	AL32S2	AL32G1	1.0	AL32P2	AL32F1	1.0	

AL32P2 AL32P3 1.0 AL32P2 AL32F2 1.0
 AL32P2 AL32G1 1.0 AL32D2 AL32F1 1.0 AL32D2 AL32S3 1.0
 AL32D2 AL32D3 1.0 AL32D2 AL32G1 1.0 AL32F1 AL32S3 1.0
 AL32F1 AL32P3 1.0 AL32F1 AL32D3 1.0 AL32F1 AL32F2 1.0 AL32F1 AL32G1 1.0
 AL32S3 AL32P3 1.0 AL32S3 AL32D3 1.0 AL32S3 AL32F2 1.0 AL32S3 AL32G1 1.0
 AL32P3 AL32D3 1.0 AL32P3 AL32F2 1.0 AL32P3 AL32G1 1.0 AL32D3 AL32F2 1.0
 AL32D3 AL32G1 1.0 AL32F2 AL32G1 1.0

0

TY CBF 15 1
 CBF AL41S1 AL32S1 4.E-19
 AL32P1 3.15E-19
 AL32D1 3.67E-18
 AL32S2 4.35E-19
 AL32P2 4.73E-19
 AL32D2 4.31E-18
 AL32S3 5.E-19
 AL32P3 3.32E-19
 AL32D3 6.54E-18
 AL32F1 3.16E-17
 AL32F2 3.96E-17
 AL32G1 3.96E-17

0

:V2

TY CBB 26 5 CBB
 AL32S1 AL32P1 4.75 3 20.2375 8.5905 4.0476
 AL32S1 AL32D1 4.75 3 3.92094 0.239048 0.244048
 AL32S1 AL32S2 4.75 3 1.09469 -.0209524 0.109127
 AL32S1 AL32P2 4.75 3 0.620625 -.00190476 -.0277777
 AL32P1 AL32D1 4.75 3 45.7625 22.5238 13.4127
 AL32P1 AL32S2 4.75 3 3.27719 1.11429 1.64881
 AL32P1 AL32P2 4.75 3 5.40250 0.490476 0.238095
 AL32D1 AL32S2 4.75 3 10.1181 -3.80667 0.115079
 AL32D1 AL32P2 4.75 3 38.0187 4.63810 -1.78571

0

TY CBB 26 6 CBB
 AL32S2 AL32P2 4.75 4 79.8375 31.7088 21.8254 5.41838

0

:V0

:T -----
 :T HYDROGEN BACKGROUND DETAIL DATASET VERSION 100 RELEASED 13/11/85
 :T -----

ATOM H 0.0 1.008 0.91

L

H11 2. 0.328805282E 16 H21
 H12 8. 0.822013206E 15 H21
 H13 18. 0.365339202E 15 H21
 H14 32. 0.205503301E 15 H21
 H15 50. 0.131522113E 15 H21

0

K

H21 1. 0.0 NONE

:T PHOTOIONIZATIONS FROM H I TO H II

TY RBF 5 1 RBF H21

H11 10 HHE030 1
 H12 10 HHE080 2
 H13 10 HHE110 3
 H14 10 HHE130 4
 H15 10 HHE150 5

0

:T FREE FREE ABOVE H I

```

TY RFF 1 0 RFF H21 0 TY RFF 2 1 RFF H21 (6) 0
:T .....END OF HYDROGEN BACKGROUND DATASET.....
:V0
:T -----
:T HELIUM BACKGROUND DETAIL DATASET VERSION 100 RELEASED 13/11/85
:T VERSION 100 SIMULATES HELIUM LINE BLOCKING 228-261 A.
:T -----
ATOM HE 0.0 4.0026 0.09 L
HE11 1. 5.948620002E15 HE21
HE12S1 1. 9.603359103E14 HE21
HE12P1 3. 8.147174578E14 HE21
HE12S3 3. 1.152845000E15 HE21
HE12P3 9. 8.761150639E14 HE21
HE13 36. 3.65339202E 14 HE21
HE14 64. 2.05503301E 14 HE21
HE15 100. 1.31522113E 14 HE21
0
L
HE21 2. 0.131575659E 17 HE31
HE22 8. 0.328939147E 16 HE31
HE23 18. 0.146195176E 16 HE31
HE24 32. 0.822347868E 15 HE31
HE25 50. 0.526302636E 15 HE31
HE26 72. 0.365487941E 15 HE31
HE27 98. 0.268521753E 15 HE31
HE28 128. 0.205586967E 15 HE31
HE29 162. 0.162439085E 15 HE31
HE210 200. 0.131575659E 15 HE31
0
K
HE31 1. 0.0 NONE
:T PHOTOIONIZATIONS FROM HE I TO HE II
TY RBF 6 3 RBF HE21 HE11 10 HHE020 (7.3E-18 1.373E0 -2.311E-16) 0
TY RBF 2 2 RBF HE21 HE12S1 10 HHE060 (1.079E-17 -1.91) 0
TY RBF 3 4 RBF HE21 HE12P1 10 HHE090 (1.322E-17 -3.5 6.315E-19 -3.3) 0
HE12P3 10 HHE070 (1.726E-17 -2.9 5.627E-19 -3.3) 0
TY RBF 7 3 RBF HE21 HE12S3 10 HHE050 (-2.783E2 1.488E1 -2.311E-1) 0
TY RBF 5 1 RBF HE21 HE13 10 HHE110 3
HE14 10 HHE130 4
HE15 10 HHE150 5
:T FREE FREE ABOVE HE I
TY RFF 1 0 RFF HE21 0 TY RFF 2 1 RFF HE21 (6) 0
:T PHOTOIONIZATIONS FROM HE II TO HE III
TY RBF 5 1 RBF HE31 HE21 10 HHE010 1
HE22 10 HHE030 2
HE23 10 HHE040 3
HE24 10 HHE080 4
HE25 10 HHE100 5
HE26 10 HHE110 6
HE27 10 HHE120 7
HE28 10 HHE130 8
HE29 10 HHE140 9
HE210 10 HHE150 10
0
:T FREE FREE ABOVE HE II
TY RFF 1 0 RFF HE31 0 TY RFF 2 1 RFF HE31 (11) 0
:T .....END OF HELIUM BACKGROUND DATASET.....
MULTI 1
:V2
LINEAR 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26

```

27 28 29 30 31 32 33 34
0

D A sample output file

This is a sample output from our standard Helium dataset. It has been greatly reduced to save space. Also the usual 130 columns have been cut down to 80 for the same reason (and to avoid overfull box messages from T_EX). Dots indicate where some pruning has been done.

CONTINUUM FREQUENCY WINDOW

IJ	LABEL	FRQ(HZ)	WAVE(A)
1	1	1.0000000E+17	29.97925
2	FA	8.0000000E+16	37.47406
3	FB	6.0000000E+16	49.96542
4	2	5.0000000E+16	59.95850
5	01	4.0000000E+16	74.94812

.....
ATOM 1 HE ZEFF 0.00000 WT 4.00260 ABUNDANCE 0.090000

L	LABEL	G	FION	PARENT
1	HE11S1	1.	5.9486200E+15	HE21
2	HE12S1	1.	9.6033591E+14	HE21
3	HE12P1	3.	8.1471746E+14	HE21
4	HE13S1	1.	4.0310167E+14	HE21
5	HE13P1	3.	3.6279150E+14	HE21
6	HE13D1	5.	3.6592734E+14	HE21

.....
S LABEL GS RYD PARENT NS

1	HE19N1	0.00	3.2909000E+15	HE21	9
		1.00			16
2	HE19N3	0.00	3.2902000E+15	HE21	9
		3.00			16

L	LABEL	G	FION	PARENT
28	HE21	2.	1.3157566E+16	HE31
29	HE22	8.	3.2893915E+15	HE31

.....
X LABEL G FION PARENT

1	HE215	450.	5.8478071E+13	HE31
2	HE216	512.	5.1396742E+13	HE31

S	LABEL	GS	RYD	PARENT	NS
3	HE217	0.00	1.3157566E+16	HE31	17
		2.00			32

K	LABEL	G	FION	PARENT
42	HE31	1.	0.0000000E+00	HE31

TL 30000.00

DB 9 -4.8000 -3.2000 -1.6000 -0.8000 0.0000 0.8000 1.6000

* OPTICALLY FORBIDDEN COLLISIONS IN SINGLET HE I

TY	CBB	35	2						
1	CBB	1	HE	1	HE11S1	15	HE12S3	0	TY 35 2
									WAVE 625.1179
								DATA 1.000000	2.000000
2	CBB	1	HE	1	HE11S1	2	HE12S1	0	TY 35 2
									WAVE 600.9932
								DATA 1.000000	3.000000
3	CBB	1	HE	1	HE11S1	16	HE12P3	0	TY 35 2
									WAVE 591.0147
								DATA 1.000000	4.000000

.....
 * COLLISIONAL IONIZATION FROM HE I SINGLET TO HE II

TY	CBF	14	1						
112	CBF	1	HE	1	HE11S1	28	HE21	0	TY 14 1
									WAVE 503.9698
								DATA 1.640000	
113	CBF	1	HE	2	HE12S1	28	HE21	0	TY 14 1
									WAVE 3121.746
								DATA 22.90000	
114	CBF	1	HE	3	HE12P1	28	HE21	0	TY 14 1
									WAVE 3679.711
								DATA 20.40000	
115	CBF	1	HE	4	HE13S1	28	HE21	0	TY 14 1
									WAVE 7437.144

TY	RBB	1	1						
1	RBB	1	HE	1	HE11S1	3	HE12P1	0	TY 1 1
									WAVE 583.9466
								DATA 5.1339025E+15	0.2811000
2	RBB	1	HE	2	HE12S1	3	HE12P1	0	TY 1 1
									WAVE 20587.54
								DATA 1.4561845E+14	0.3621000
3	RBB	1	HE	3	HE12P1	4	HE13S1	0	TY 1 1
									WAVE 7283.309
								DATA 4.1161579E+14	4.6700000E-02

TY	RBF	6	3						
126	RBF	1	HE	1	HE11S1	28	HE21	0	TY 6 3
									WAVE 503.9698
								DATA 7.3000000E-18	1.373000
									-2.3110000E-16
TY	RBF	7	3						
127	RBF	1	HE	15	HE12S3	28	HE21	0	TY 7 3
									WAVE 2600.458
								DATA -278.3000	14.88000
									-0.2311000

TY	RFF	1	0						
1	RFF	1	HE	28	HE18N3	28	HE21	0	TY 1 0
									WAVE 0.0000000E+00
TY	RFF	2	1						
2	RFF	1	HE	28	HE18N3	28	HE21	0	TY 2 1
									WAVE 0.0000000E+00
								DATA 9.000000	

.....
 MULTI 2

* HE11S1-HE12P1 HE12S1-HE12P1 HE12P1-HE13S1 HE12P1-HE13D1 HE11S1-HE13P1

LINEAR	1	RBB	1	HE	1	HE11S1	3	HE12P1
LINEAR	2	RBB	1	HE	2	HE12S1	3	HE12P1
LINEAR	3	RBB	1	HE	3	HE12P1	4	HE13S1
LINEAR	4	RBB	1	HE	3	HE12P1	6	HE13D1
LINEAR	5	RBB	1	HE	1	HE11S1	5	HE13P1

.....
 1BACKGROUND CHANNELS

CHANNEL	ATOM	LOWER	UPPER	VIA	IFL	IFU	WAVELENGTH	
7	RBB	1	HE	4	HE13S1	5	HE13P1	0
					2558	2566	74358.20	74362.61
							74371.44	74373.64
							74384.68	
8	RBB	1	HE	6	HE13D1	5	HE13P1	0
					2907	2915	955851.1	955907.8

956021.3 956049.7
956191.5

127 RBF	1 HE	15 HE12S3	28 HE21	0	1	520	29.97925	2600.431
128 RBF	1 HE	2 HE12S1	28 HE21	0	1	578	29.97925	3121.714
129 RBF	1 HE	16 HE12P3	28 HE21	0	1	626	29.97925	3421.803

1LINEARIZED CHANNELS

CHANNEL	ATOM	LOWER	UPPER	VIA	IFL	IFU	WAVELENGTH	
1 RBB	1 HE	1 HE11S1	3 HE12P1	0	78	86	583.8427	583.8773
							583.9466	583.9639
							584.0506	
2 RBB	1 HE	2 HE12S1	3 HE12P1	0	1931	1939	20583.87	20585.09
							20587.54	20588.15
							20591.20	
3 RBB	1 HE	3 HE12P1	4 HE13S1	0	1134	1142	7282.012	7282.445
							7283.309	7283.525
							7284.606	
36 RBF	1 HE	1 HE11S1	28 HE21	0	1	20	29.97925	503.9644
37 RBF	1 HE	29 HE22	35 HE28	0	256	267	971.9784	972.0361
							972.1226	972.1514
							972.2091	972.2669

MODEL

TITLE HUSFELD/GROTH MODEL ATMOSPHERE PROGRAM
TITLE MODEL STARTED ON1991-09-03 AT 21:04:32
TITLE NLTE-LEVELS IN H/HE1/HE2=5/5/10 , LINE-MODEL
TITLE STATUS:CONV AFTER 14 ITERATIONS
TEFF 42500.0
GRAVITY 3.5500
YHE 0.1401
ABUNDANCE H 0.8598450
ABUNDANCE HE 0.1401550

STRUCTURE 90 TITLE (OUTPUT FROM MOD2AM)

ID	MASS	TEMP	NA	NE
1	3.1325500E-07	36579.3	4.7059700E+07	5.3655300E+07
2	9.9059400E-07	36578.6	1.4881800E+08	1.6967500E+08
3	3.1325000E-06	36576.3	4.7063100E+08	5.3658200E+08
4	3.9435800E-06	36575.5	5.9250300E+08	6.7552800E+08
5	4.9646500E-06	36574.4	7.4593700E+08	8.5045800E+08
6	6.2501000E-06	36573.0	9.3911300E+08	1.0706900E+09

POPULATIONS 90 TITLE NON-LTE H AND HE FROM MODEL

ATOM 2 H ZEFF 0.00000 WT 1.00800 ABUNDANCE 0.859845

L	LABEL	G	FION	PARENT			
1	H11	2.	3.2900000E+15	H21			
1.96426E-05	1.96436E-04	1.96471E-03	3.11407E-03	4.93590E-03	7.82374E-03	1.24015E-02	1.96586
7.83309E-02	1.24204E-01	1.96968E-01	3.12417E-01	4.95655E-01	7.86618E-01	1.24892E+00	1.98402
7.98538E+00	1.27140E+01	2.02403E+01	3.22054E+01	5.12043E+01	8.13304E+01	1.29014E+02	2.04332
5.71337E+02	8.03375E+02	1.12874E+03	1.58471E+03	2.22303E+03	3.11511E+03	4.35903E+03	6.08936

1.63987E+04 2.27082E+04 3.13622E+04 4.31919E+04 5.92945E+04 8.10960E+04 1.10435E+05 1.49662
3.59823E+05 4.75762E+05 6.24434E+05 8.12957E+05 1.17876E+06 1.67376E+06 2.32327E+06 3.14582
6.66000E+06 8.14790E+06 9.78617E+06 1.15923E+07 1.36118E+07 1.59273E+07 1.86622E+07 2.19791
3.75308E+07 4.54565E+07 5.53140E+07 6.75512E+07 8.27029E+07 1.01349E+08 1.24002E+08 1.50943
2.56416E+08 3.00342E+08 3.51655E+08 4.15346E+08 4.99339E+08 6.14933E+08 7.77457E+08 1.00737

.....
POPULATIONS END

TURBULENCE 0.00

PHYSICAL SETUP

RUN STATISTICS FULL PART

ATOMS 2 2
LEVELS 53 53
LTE LEVELS 8
Q.D. SERIES 3
COLLISIONS 451
FREQUENCIES 2947 1134
OPACITIES 325
RATES 325 98
FREE FREE 6
CROSS DATA 1522 1304 218
INPUT DATA 1300
DEPTHS 90

PRINT PARAMETERS

POPULATIONS 90 COLLISIONS 90 CROSS DATA 90 OPACITY 90

ATOMIC DATA TITLE :DETAIL DATASET FOR HE I VERSION 1.02 FROM K.B. MORE LINEAR

MODEL TITLE :HUSFELD/GROTH MODEL ATMOSPHERE PROGRAM
MODEL TITLE :MODEL STARTED ON1991-09-03 AT 21:04:32
MODEL TITLE :NLTE-LEVELS IN H/HE1/HE2=5/5/10 , LINE-MODEL
MODEL TITLE :STATUS:CONV AFTER 14 ITERATIONS

DETAIL PROGRAM VERSION 2.00 ; EXECUTION DATE 08/25/93 TIME 17:40:47

MODEL PARAMETERS :TEFF 42500.
GRAVITY 3.550
NHE/NA 0.1401
TLINE 30000.
ABUNDANCES 1 HE 0.1402
2 H 0.8598
TURBULENCE 1 0.000 0.000
ALBEDO 1 0.000000E+00 0.00000

FLOATING ATOMS :
1 HE T 2 H T

FLOATING LEVELS :
1 HE11S1 T 2 HE12S1 T 3 HE12P1 T
4 HE13S1 T 5 HE13P1 T 6 HE13D1 T
7 HE14S1 T 8 HE14P1 T 9 HE14D1 T

DEPTH 1 SUMUP POPS

7.37694E-11 4.84911E-13 1.45473E-12 1.38480E-13 3.94038E-13

6.59438E-13 1.09044E-13 3.20100E-13 5.34472E-13 7.48068E-13

DEPTH 1 SAHA FACTORS

1.94708E-12 2.79918E-15 6.93710E-15 1.34746E-15 3.83414E-15
6.41657E-15 1.06104E-15 3.11469E-15 5.20061E-15 7.27898E-15

UPWARD COLLISIONS 1

LOWER	UPPER	CU	LOWER	UPPER	CU	LOWER	UPPER	CU	LOWER	UPPER	CU
HE11S1HE12S3	3.150E-04		HE11S1HE12S1	1.563E-04		HE11S1HE12P3	1.197E-04		HE11S1HE12P1	9.316E-	
HE11S1HE13S1	2.145E-05		HE11S1HE13P3	2.249E-05		HE11S1HE13D3	4.804E-06		HE11S1HE13D1	1.109E-	
HE12S3HE12S1	1.241E+00		HE12S3HE12P3	3.289E+01		HE12S3HE12P1	5.645E-01		HE12S3HE13S3	8.526E-	
HE12S3HE13P3	6.077E-01		HE12S3HE13D3	1.250E+00		HE12S3HE13D1	1.015E-01		HE12S3HE13P1	5.267E-	
HE12S1HE12P1	7.780E+01		HE12S1HE13S3	4.597E-01		HE12S1HE13S1	1.052E+00		HE12S1HE13P3	4.785E-	

CROSS SECTIONS 1 2 RFF 28 HE21 28 HE21 1 2947

5.666E-39	1.107E-38	2.623E-38	4.533E-38	8.854E-38	1.426E-37	2.296E-37	3.697E-37	5.954E-37	9
2.486E-36	2.488E-36	2.488E-36	4.004E-36	6.447E-36	1.038E-35	1.672E-35	2.692E-35	2.692E-35	2
2.762E-35	2.762E-35	2.763E-35	2.763E-35	2.763E-35	2.763E-35	2.764E-35	2.764E-35	2.784E-35	2
2.785E-35	2.785E-35	2.786E-35	2.786E-35	2.787E-35	2.818E-35	2.819E-35	2.819E-35	2.820E-35	2
2.821E-35	2.821E-35	2.877E-35	2.878E-35	2.878E-35	2.878E-35	2.879E-35	2.879E-35	2.879E-35	2

FIXED OPACITY 1

1	3.5689E-17	1	8.0489E-87	2	3.5689E-17	2	3.9148E-75	3	3.5689E-17	3	2.3112E-63
5	3.5689E-17	5	1.9437E-51	6	3.5689E-17	6	6.9607E-48	7	3.5689E-17	7	8.0395E-45
9	3.5689E-17	9	6.8264E-40	10	3.5689E-17	10	6.5265E-38	11	3.5689E-17	11	3.4266E-36
13	3.5689E-17	13	1.0793E-34	14	3.5689E-17	14	1.0831E-34	15	3.5689E-17	15	1.0834E-34

CROSS SECTIONS 1 1 RBB 1 HE11S1 3 HE12P1 78 86

1.244E-22 4.509E-18 2.452E-15 1.184E-14 2.001E-14 1.184E-14 2.452E-15 4.509E-18 1.244E-22

CROSS SECTIONS 1 126 RBF 1 HE11S1 28 HE21 1 20

2.649E-27	2.694E-25	2.740E-23	2.763E-22	2.786E-21	1.083E-20	3.447E-20	9.259E-20	2.151E-19	4
1.377E-18	1.377E-18	1.377E-18	2.152E-18	3.149E-18	4.359E-18	5.752E-18	7.287E-18		

1MODEL STRUCTURE

ID	MASS	TEMP	NA	NE	NE SUM
1	3.132550E-07	36579.30	4.705970E+07	5.365530E+07	5.365530E+07
2	9.905940E-07	36578.60	1.488180E+08	1.696750E+08	1.696752E+08
3	3.132500E-06	36576.30	4.706310E+08	5.365820E+08	5.365821E+08
4	3.943580E-06	36575.50	5.925030E+08	6.755280E+08	6.755279E+08

PRINT 3 90

DRIVE

1SURFACE FLUX

IJ	FREQUENCE	WAVELENGTH	HNU	M(TAU=1)	TAUMAX	ALBEDO	
1	1.0000000E+17		29.97925	2.526E-45	6.512E-02	1.861E+02	0.000
2	8.0000000E+16		37.47406	2.839E-45	4.775E-02	2.314E+02	0.000
3	6.0000000E+16		49.96542	5.715E-34	3.077E-02	3.605E+02	0.000
4	5.0000000E+16		59.95850	3.131E-28	2.162E-02	5.218E+02	0.000
5	4.0000000E+16		74.94812	1.328E-22	1.286E-02	8.740E+02	0.000

1LOG CHANGES IN POPULATIONS

RATES

	RU	NET	RU	NET	RU	NET	RU	NE
	1 RBB	1 HE	2 RBB	1 HE	3 RBB	1 HE	4 RBB	1 HE
ID	1 HE11S1	3 HE12P1	2 HE12S1	3 HE12P1	3 HE12P1	4 HE13S1	3 HE12P1	6 HE1
1	1.2943E+07	-5.4726E+05	1.3275E+07	4.6674E+06	2.5073E+06	-2.4046E+06	2.8121E+07	-3.05+05

POPULATIONS

	N	N/N*	N	N/N*	N	N/N*	N	N/
ID	1 HE	1 HE11S1	1 HE	2 HE12S1	1 HE	3 HE12P1	1 HE	4 HE1
1	8.6783E-11	4.2527E-01	4.6823E-13	1.5960E+00	6.3727E-13	8.7651E-01	1.2453E-13	8.81-01

1LOG CHANGES IN RATES

ID	-8	-7	-6	-5	-4	-3	-2	-1	0
90	-89447--95987-73		896849099199311		. -76
89	-35	-876498976594.	66899099931		. -76
88	-35	-87510-746	-8-98979654	-6-73-9316-695		.-76	.	.	.
87	-35	.-87510	--77--98976594	-6-7-932-6-695		.-76	.	.	.
86	-35	.	-876	.3975-9897965462---930--697		.-76	.	.	.
85	-35	.		-875-375-9897654-6---930--6975		. -76	.	.	.
84	-354	.		-8769475-989765-62--9303--695		. -76	.	.	.
83	-35174	.		39.-8756755-98765----9383--697		. -76	.	.	.
82	-35	-17 . 39		47-8763755-98765---9380---695		. -76	.	.	.
81	-3547-20	-17	-39. 5-8767505-98764--93806--695		. -76
80	-35-255	-20	-17 47	-87675--98764---9386---69		. -76	.	.	.
79	-3532-282515	-20	-17473-876757-9875----9386--696.		-76
78	-354-2-32-28-25513-208		-1-8775--9875--73-9386--69.		-76
77	.3531272421-32-2825158840		-94-98793	-73170	-938--69	-76	.	.	.
76	.33	353127242-329-28381-87666479876594.			-939-695	-76	.	.	.
75	.33292623	. 35317242-32-87625164027593639865420--93695			-76
74	.	33292623	35387617-321-6405125750367498643--9396-76		-1
73	.	. 332926	23 353018754074-259753967419864-9389-76		. -1
72	.	.	3329 2623 356875	-3259753467429864-938-76-5		-1	.	.	.
71	.	.	. 33292623.640875	225917545741198549387619-54		-1.	.	.	.
70	.	.	. 339.26264087359	575457475986493986719-5 4		-1	.	.	.
69	.	.	. 332926264879307547431298749328617985		4.-1
68	.	.	. 22.	339 26487357574331986493286713-14		.4-1	.	.	.
67	.	.	. 33292687675743-8985-93985911358.		--1
66	.	.	. -32	. 33292687754829864-938651913 8 41		-14	.	.	.
65	.	.	. 28	. 333916877530984--938651913.8 41		-14.	.	.	.
64	.	.	. 28	82329287554985-7-93865193-8 41		-14	.	.	.
63	.	.	. -2-82	3325968759866--93986-193 841		-14	.	.	.
62	.	.	. -70-829032926879874-7-93876-19 84-2		-14
6182	-572731--687984-7-932876193841-2		-14	.	.	.
60	.	.	. 829-3-789843---938-769384-1-2		-14

RYBIKI LINEARIZATION SOLVED BY BLOCK SOR

1 ITERATIONS 6 SORS OMEGA 1.670000 TOLERANCE 0.100

CORRECTIONS ITERATED 6 TIMES

MAXIMUM CHANGES IN DZ ARE

1 62 -1.3E-01 2 54 -1.7E-01 3 81 1.5E-01 4 88 4.0E+00 5 62 -1.9E-01 6 82 5.8E-01 0

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SCRIBE

References

- Allen, C.W., 1973. *Astrophysical Quantities*, 3rd Edition. London: Athlone Press.
- Auer, L.H., Heasley, J.N. & Milkey, R.W., 1972. Kitt Peak National Observatory No. 555.
- Auer, L.H. & Mihalas, D., 1969. *Astrophys. J.* **158**, 641.
- Auer, L.H. & Mihalas, D., 1972. *Astrophys. J. Supp. Ser.* **24**, 193.
- Barnard, A., Cooper, J. & Shamey, L., 1969. *Astron. Astrophys.* **1**, 28.
- Bell, K.L., Gilbody, H.B., Hughes, J.G., Kingston, A.E. and Smith, F.J., 1983, *J. Phys. Chem. Ref. Data*, **12**, 891.
- Burke, P.G., Ormonde, S. & Whittaker, W., 1967. *PPS* **92**, 319.
- Butler, K., 1984. *Ph.d. Thesis*, University of London.
- Butler, K. and Giddings, J.R., 1985, *CCP7 Newsletter*, **9**, 7.
- Cochrane, D. and McWhirter, P., 1983, *Phys. Scr.*, **28**, 25
- Giddings, J.R., 1981. *Ph.d. Thesis*, University of London.
- Golden, L.B. & Sampson, D.H., 1980. *J. Phys. B: Atom. Molec. Phys.* **13**, 2645.
- Griem, H.R., 1960. *Astrophys. J.* **132**, 883.
- Lotz, W., 1968. *Zeit. für Physik* **216**, 241.
- Merts, A.L., Mann, J.B., Robb, D.W. & Magee, N.H., 1980. Los Alamos Sci. Lab. Rep. LA-8267-MS.
- Mihalas, D., 1972. NCAR Technical Note NCAR - TN/STR 76, Boulder: National Center for Atmospheric Research.
- Mihalas, D., 1978. *Stellar Atmospheres*, Second Edition. W.H. Freeman & Co., San Francisco.
- Mihalas, D. & Stone, M.E., 1968. *Astrophys. J.* **151**, 293.
- Moore, D.L., 1972. *J. Phys. B: Atom. Molec. Phys.* **5**, 286.
- Peach, G., 1967. *Mem. R. astr. Soc.* **7**, 1.
- Pradhan, A.K., 1980. *Mon. Not. R. astr. Soc.* **190**, 5p.
- Sampson, D.H. & Golden, L.B., 1971. *Astrophys. J.* **170**, 169.
- Seaton, M.J., 1958. *Rev. Mod. Phys.* **30**, 979.
- Seaton, M.J., 1962. in "Atomic and Molecular Processes", New York Academic Press.
- Seaton, M.J., 1983. *Rep. Prog. Phys.* **46**, 167.
- Storey, P.J. and Hummer, D.G., 1991, *Comput. Phys. Commun.* **66**, 129
- Van Regemorter, H., 1962. *Astrophys. J.*, **136**, 906.