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About PANDORA

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Pandora ('all gifts'): According to Hesiod, Pandora was the first woman, and was created by Zeus to punish man after Prometheus had created and helped the human race. She came with a box or storage-jar in which all evils and diseases were stored, and when Prometheus's guileless brother Epimetheus married her and opened the box, all these escaped, leaving only Hope at the bottom to be some alleviation of the troubles let loose upon the world. 'Pandora's box' became proverbial . . .

from: "Who's Who in the Ancient World" by Betty Radice (Penguin Books)

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Section 1: Input Language

PANDORA uses free-field self-identified input. The basic input unit is the vector or one-dimensioned array; single variables, on the one hand, and multiply-dimensioned arrays, on the other, are treated as special cases of the vector. A PANDORA input statement specifies the name of the array, and the values to be stored in consecutive locations of it. Several control facilities are provided, to make specifying input statements less tedious.

The general input statement is: **NAME** j(Q).

Each component of that statement (including '(' or ')') is a separate 'field' or a set of fields. PANDORA's input routines use NUDEAL, whose conventions require that every 'field' be preceded by at least one blank, and followed by at least one blank; (i.e. blank is the required 'separator' between fields). In the example above, \mathbf{NAME} is the name of the input quantity (array) whose values follow; j is none or several auxiliary indices; and Q is the sequence of fields and control parameters that specify the values to be stored in memory.

PANDORA's input routines maintain an internal pointer, initially set to 1 and subsequently incremented or set as specified or implied by Q, which identifies that member of the array that will be affected by the next input specification in Q. Therefore, when in the remainder of this section I use phrases like 'the array member currently being read into,' I mean the array member identified by that internal pointer.

The remainder of this section deals with: 1) field format basics; 2) (Q); and 3) examples. The various types of input statements (i.e., combinations of **NAME** and j) are discussed in Section 2; the many **NAME**s recognized by

PANDORA are treated in Section 5.

1. Format Basics

PANDORA reads input file(s) line by line; only the first 80 characters of each line are read. Each line is scanned, character-by-character, from left to right, beginning with the first character, until end-of-line (which normally occurs after the 80. character). Five types of input fields are recognized: 1) null field, 2) excessive field, 3) integer field, 4) floating point field, and 5) alphanumeric field. Only integer, floating point and alphanumeric fields are legal PANDORA input fields, the other two are considered errors.

- 1) Null field: the scan encountered more than 159 successive blanks, without a non-blank character turning up.
- 2) Excessive field: the scan encountered more than 60 successive non-blank characters, without a blank (i.e. break character) turning up.
- 3) Integer field: like an integer constant in FORTRAN, containing up to 9 significant digits. An integer field may contain: digits, and at most a single sign.
- 4) Floating point field: like a real constant in FORTRAN, containing up 16 significant digits, with an exponent value not exceeding 300. A floating point field may contain: digits, at most a single sign for the mantissa, at most a single decimal point for the mantissa, at most a single exponent flag, at most a single sign for the exponent.
- 5) Alphanumeric field: anything that is not one of the field types (1) (4), above.

```
Digits: [ 0 1 2 3 4 5 6 7 8 9 ]
Signs: [ + - ]
Decimal point: [ . ]
Exponent flags: [ E e D d ]
```

Q may contain the following fields: n, M, m, m, l, i, l, r, r, s, s, s and t. Here the **boldface** fields are names (identifiers) of control parameters, and the *italic* fields are numerical values, either of input quantities, or of the control parameters whose names precede them.

n is the quantity (an integer, a floating point number, or an alphanumeric quantity) to be stored in the array member currently being read into; before being stored in memory, the value of n (if an integer or a floating point number) will be multiplied by m.

M or m signal that a value of m will follow.

m is either a floating point number, by which all floating point n's following m will be multiplied before being stored in memory; or is an integer, by which all integer n's will be multiplied before being stored in memory. The modes of m and n must agree (i.e. both integer or both floating point). The default value of m is 1; this value will be used if a different value of m is not specified explicitly in Q. Successive values of m are not multiplied together; it is always the latest value encountered that will be used.

I or **i** signal that a value of i will follow.

i is an integer which explicitly specifies the next array member to be read into (i.e. it is used to reset the internal array pointer). Any n not preceded by an i will be stored in the array member specified by the internal array pointer. If the first n in Q is not preceded by an i, it will be stored as the first array member.

 \mathbf{R} or \mathbf{r} signal that a value of r will follow.

r is an integer specifying the value of the 'repeat' counter. The repeat counter specifies that the next n should be 'used' r times. For example: \mathbf{R} 3 1.7 means that the next array member to be read into, and the two succeeding ones as well, will all be set equal to 1.7; also: \mathbf{I} 7 \mathbf{r} 3 1.0 (which is equivalent to \mathbf{R} 3 \mathbf{i} 7 1.0) means that array members 7 – 9 will all be set equal to 1.0. If the specified value of r implies members beyond the high end of the array, then such 'excess' will be ignored. The default value of r is 1.

S or S signal that the next array member to be read into should be skipped (*i.e.* no value will be specified for it, and its current contents should be left unchanged). The sequence R r S means that the next r array members to be read into should be skipped.

F or **f** signal that the n following **F** should be stored in the current array member to be read into and all succeeding ones as well (*i.e.* the sequence **F** n 'fills' the remainder of the array, or indeed the entire array, with n).

The sequence [A] constitutes a comment or remark. The occurrence of opening square bracket (followed by a blank) signals the beginning of a comment, A, which may comprise any number of fields consisting of any characters, except closing square bracket. The occurrence of closing square bracket (preceded and followed by blank) signals the end of the comment. PANDORA ignores the entire comment (including the delimiting brackets).

The field > ('greater than' sign) indicates end-of-line (*i.e.* the remainder of the input line on which it occurs should be skipped).

Note: only UPPERCASE alphabetic characters were recognized originally; the generalization to mixeD-CAse was implemented later.

3. Examples

Here are some sample lines of input:

```
0001
         N (34)
0002
         KK (13) >
0003
         IOMX (2) > STUFF AFTER 'GREATER THAN' IS IGNORED
0004
         [ THIS IS A REMARK ]
0005
         XK ( I 13 5.5 ) DLU ( 0.1 ) >
0006
         TE (F 10000.)
0007
        NE ( 0. M 1.E1 1. 2. 3. 4. 5.
0008
         R56. F7.)
0009
         [THIS STUFF IS NOT A COMMENT]
0010
         [THIS ALSO IS NOT A R E M A R K]
0011
         A 2 1 ( 1.E8 ) [ ESTIMATE > ]
0012
         CRD 2 1 ( 1.E-5 ) [ ESTIMATE ] >
```

- Lines 1, 4, 6, 7, 8, 9 and 10 are scanned in their entirety (*i.e.*, all 80 characters); the others up to > only.
 - Line 3 shows an alternate form of comment.
- In Line 5, the 13. value of XK is set to 5.5, and DLU is set to 0.1; showing that there may be more than one input statement in a line.
- Lines 7 and 8 show that one input statement may extend over several lines; it is the final ')' that indicates the end of the NE statement. The values in memory of NE will be: 0, 10, 20, 30, 40, 50, 60, 60, 60, 60, 60, 70 ... 70.
- Line 9 would be a valid comment if there were a blank after [, Line 10 likewise if there were a blank before] .
- Line 12 illustrates a pernicious error: it is ignored since it is considered part of the comment begun on Line 11. To get the intended effect, interchange > and] on Line 11.

Note: line numbers are not allowed in PANDORA input.

(Section 1 – last revised: 2003 Aug 01)

Section 2: Input Statements

PANDORA's input routines distinguish among several types of input statements, according to their format.

 ${f 1})$ Input of single quatities:

	NAME (q)
	where q can be a single integer, floating point or alphanumeric variable.
1*\	Input of single quotities with one 7 index.
1)	Input of single quatities with one Z index:
	NAME z $($ q $)$
varia	where z (integer) is a Z index, and q can be a single integer or floating pointable.
2) In	nput of simple arrays:
	$\operatorname{NAME} (q)$
	where q can be an array of integer elements or of floating point elements.
2*)	Input of simple arrays with one Z index:
	NAME Z z (q)

where z (integer) is a Z index, and q can be an array of integer elements or of floating point elements.

3) Input of simple arrays with one level index or one Z index:
NAME k (q)
where k (integer) is either a level index or a Z index, and q can be an array of integer elements or of floating point elements.
3*) Input of simple arrays with one level index and one Z index:
$\operatorname{NAME} k \operatorname{Z} z (q)$
where k (integer) is a level index, z (integer) is a Z index, and q can be an array of integer elements or of floating point elements.
4) Input of single quantities with two level indices:
$\operatorname{NAME} u l (q)$
where u (integer) and l (integer) are two indices specifying a particular transition, $(u > l)$, and q can be a single integer, floating point or alphanumeric variable.

NAME
$$u$$
 l $(q$

where u (integer) and l (integer) are two indices specifying a particular transition, (u > l), and q can be an array of integer elements or of floating point elements.

5*) Input of simple arrays with two level indices and one Z index:

NAME
$$u$$
 l Z z $(q$

where u (integer) and l (integer) are two indices specifying a particular transition, (u > l), z (integer) is a Z index, and q can be an array of integer elements or of floating point elements.

6)	Input	of	WEIGHT:
------------	-------	----	---------

WEIGHT	u	l (m	n	w
--------	---	-----	---	---	---

where u (integer) and l (integer) are two indices specifying a particular transition, (u > l), m (integer) and n (integer) are two indices specifying a particular term, (m > n), and w (floating point) is the weight itself.

7) Input of single quatities with two level indices and one μ index:

NAME
$$u l k (q)$$

where u (integer) and l (integer) are two indices specifying a particular transition, (u > l), k (integer) is an index specifying a particular value of \mathbf{MU} , and q can be a single integer, floating point or alphanumeric variable.

8) Input of simple arrays with two level indices and one μ index:

NAME
$$u l k (q)$$

where u (integer) and l (integer) are two indices specifying a particular transition, (u > l), k (integer) is an index specifying a particular value of \mathbf{MU} , and q can be an array of integer elements or of floating point elements.

NOTE

"NAME," "Z," and "WEIGHT," can be UPPER-, lower-, or MIxed-CasE.

(Section 2 – last revised: 1997 Apr 02)

Section 3: Input Files Set-Up

Years ago I thought it would be ideal if input statements could appear in PANDORA's input files in any order whatever; it seemed to me that this was almost required in the interest of consistency with self-identified free-field input. It became clear, however, that in order to do this I would have to use a two-pass input reading procedure instead of the current single-pass one; since, for programming purposes, certain parameters must already have been specified before others can be accepted. I have not yet been persuaded that the extra complication of a two-pass procedure is worth it. Thus input statements may not appear in whatever order a user might like best, but must conform to the structure described here. (Don't overlook the small number of rather detailed special requirements noted below.)

The set of input statements for a run is divided into nine parts, A - I. Their contents are sketched below. All these nine parts must appear, and in that order. The input statements in parts B, D, F and H may appear in any order (except as noted below). However any of B, D, F and/or H may be empty. Further information about input reading and processing appears in Section 4.

The following subsections describe: 1) overall input file structure; 2) special requirements (concerning maximum array sizes, and specific statement order); and 3) input error handling.

1. Input File Structure

Part A must contain: **HEADING**.

<u>Part B</u> contains mainly table lengths and option settings, as well as other control parameters.

Part C must contain: GO.

<u>Part D</u> contains all the input parameters for the basic calculations, except that populations data appear in part H.

Part E must contain: GO.

<u>Part F</u> contains input parameters for the "spectrum" calculations.

Part G must contain: GO.

Part H contains populations data and related parameters.

Part I must contain: GO.

The **HEADING** is a single comment line, which will be printed on the 'banner' pages at the start of the printed output, and will be inserted at various places in the restart file(s) (see Section 8).

The **GO** lines must appear as shown; they indicate the ends of parts B, D, F and H, respectively. The input statement after **GO** must begin on a new line.

The complete list of all input parameters is given in Section 5. That list specifies which of the parts B, D, F, or H each parameter may appear in. The names of input parameters may be given in UPPER-, lower-, or MixEd-case. The complete set of input statements need not occur in just one file, but may be distributed over several files that are coordinated by **USE** statements (see Section 5, note 44).

2. Special Requirements

In Part B:

- NT must occur before INPAIR;
- **NSL** must be less than 51;
- **NSL** must occur before **MR** and/or **LR**;
- NL must be less than NSL;
- NMT must be less than 51;
- NCL must be less than 100;
- NAB must be less than 100;
- NAB must occur before BANDL, BANDU, or BANDE;
- NVX must be less than 100.

In Part D:

- $\mathbf{LDL}_{i,j}^{u,\ell}$ must not exceed \mathbf{LDLMAX} ; $\mathbf{LDL}_{i,j}^{u,\ell}$ must occur before $\mathbf{DDL}_{i,j}^{u,\ell}$, $\mathbf{CDL}_{i,j}^{u,\ell}$, and the broadening halfwidths for transition (u, ℓ) ;
- $\mathbf{KST}^{u,\ell}$ must not exceed \mathbf{KSTMAX} ;
- $\mathbf{KST}^{u,\ell}$ must occur before $\mathbf{XISYMT}^{u,\ell}$;
- $\mathbf{KBT}^{u,\ell}$ must not exceed \mathbf{KBTMAX} ;
- $\mathbf{KBT}^{u,\ell}$ must occur before $\mathbf{XIBLUT}^{u,\ell}$;
- $\mathbf{KRT}^{u,\ell}$ must not exceed \mathbf{KRTMAX} ;
- $\mathbf{KRT}^{u,\ell}$ must occur before $\mathbf{XIREDT}^{u,\ell}$.

Also:

- the total number of Composite Line Opacity wavelengths, from all bands, must be less than 20001 (see also Section 9);
- MAUX must be less than 51 (see also Section 13).

3. Input Errors

Several types of errors commonly occur: violations of input language syntax; violations of prescribed structure; typos in field names and control character names; logical inconsistencies (*i.e.*, specifying undefined transitions, giving more array members than the stated size); diddly errors related to comments or field separators (too few or too many blanks).

It can be frustratingly time-consuming to correct all errors in a newly-typed input file. Many extensive, detailed error diagnostics have been provided to help with this. Most input error notifications provided by PANDORA display the image of the current input line, and then a single asterisk on the printout line immediately below that input line. This asterisk is positioned beneath the terminating blank (break character) of the input field which triggered the error notification.

When option DELABORT is on, PANDORA attempts to ignore an erroneous input statement (by attempting to find its closing ")") in order to read all the input (perhaps encountering additional errors and attempting to ignore them as well) before stopping. This does not always work well, but when it does work, it saves time.

(Option DELABORT is on by default; turning it off [OMIT (DELABORT)] will affect the reading of the remaining input statements only.)

Note the input parameter **JSTIN** (also, equivalently, available as an option) which stops the run after all input has been read and most of the preprocessing leading up to the first iteration has been done. Such an "input-only" run typically takes little time and provides an efficient means of checking the input for a run starting from scratch.

Since most PANDORA runs are restarts of preceding runs, the input files for a given run are usually obtained through only minor incremental changes to the files of preceding runs. Thus, in practice, only few input errors tend to occur once a new series of runs (restarts) has been launched successfully.

(Section 3 – last revised: 2007 Apr 11)

Section 4: Remarks on the Input Process

PANDORA's input phase must establish all the input data for the subsequent computations. The major activities of the input phase comprise: initialization, setting defaults, reading all input statements, expanding shorthand input notations (e.g. for **KPC** or **TR**), establishing defaults that cannot be pre-set (e.g. for **NP** or **ABD**), extra(inter)polating to **Z** if necessary (see Section 13), and printing out most of the input values.

There are two kinds of defaults: pre-read defaults, which can be set before any input statements are read (e.g. M or TS or TBAR), and post-read defaults, which can only be established by referring to other input, and thus cannot be set until after all the input statements (of a given Part, i.e. B, D, F or H) have been read.

The processing in the input phase proceeds as follows:

- Read, print and write the **HEADING**.
- Set pre-read defaults for Part B, as specified in Section 5 of this writeup.
- Read Part B of the input.
- \bullet Read Part C of the input. After C (= **GO**) has been read, only those of the input parameters in Part B that were explicitly mentioned in input statements will have had new values given them. (These explicit values need not necessarily be different from the defaults.) If any of these parameters were mentioned more than once, they will have the values given them by the respective input state-

ments that were read last.

• Digest the Part B input.

- Set up storage for all the parameters in Parts D and F of the input, and set all this storage to zero (*i.e.* zero is the basic default).
- Set pre-read defaults for Parts D and H, as specified in Section 5. Pre-read defaults for tables are potential defaults only; they will actually be set according to the current values of their respective lengths. (This makes it easy to shorten or lengthen tables *vis-a-vis* their default states. For example, consider the table **MUF** of length **LF**. The pre-read defaults are **LF** = 2 and **MUF** = 1.0, 0.3. If **LF** = 1 resulted from Part B of the input, then the pre-read default is **MUF** = 1.0. If **LF** = 4 resulted from part B of the input, then the pre-read default is **MUF** = 1.0, 0.3, 0.0, 0.0. To replace the two zeroes in this **MUF**-table, a statement in Part F of the form: "**muf** (**I** 3 0.2 0.1)" would be sufficient.
- Read Part D of the input.
- Read Part E of the input. After E = go has been read, only those input parameters of Part D that were explicitly mentioned in input statements will have had new values given them. (These explicit values need not necessarily be different from the defaults.) If any of these input parameters were mentioned more than once, they will have the values given them by the respective input statements that were read last. Provisional input tables of depth-dependent variables will have been inter(extra)polated to \mathbf{Z} (see Section 13); the actual provisional values will have been discarded.
- Digest the Part D input.
- Read Part F of the input.
- Read Part G of the input. After G = go has been read, only those input parameters of Part F that were explicitly mentioned in input statements will have had new values given them. (These explicit values need not necessarily be different from the defaults.) If any of these input parameters were mentioned more than once, they will have the values given them by the respective input statements that were read last. Provisional input tables of depth-dependent variables will have been inter(extra)polated to \mathbf{Z} (see Section 13); the actual provisional values will have been discarded.
- Digest the Part F input.

- Set up storage, in memory and in the random-access scratch file, for the population data of Part H of the input.
- Set pre-read defaults for Part H, as specified in Section 5.
- Read Part H of the input.
- Read Part I of the input. After I (= \mathbf{GO}) has been read, only those input parameters of Part H that were explicitly mentioned in input statements will have had new values given them. (These explicit values need not necessarily be different from the defaults.) If any of these input parameters were mentioned more than once, they will have the values given them by the respective input statements that were read last. Provisional input tables of depth-dependent variables will have been inter(extra)polated to \mathbf{Z} (see Section 13); the actual provisional values, and the auxiliary Z tables as well, will have been discarded.
- Print the input (see Section 11 for more details about this).

Note: default values for unspecified populations and departure coefficients of Part H will be calculated later as part of the various precalculations done before the first iteration. Tables of data for the various population ions are printed, also later, if requested with the corresponding options.

(Section 4 – last revised: 2003 Jul 31)

Section 5: Input Parameters

This section contains the complete list of input parameter specifications, in alphabetical order by name, followed by a set of explanatory notes, and finally by an alphabetized listing of keywords and descriptive phrases for each parameter — this last list should be used when a parameter's significance or function are vaguely known and its name is sought. After the parameter name has been located in the keywords list, the complete specification can then be consulted in the first part of this section.

The list of input parameter specifications has two or more lines of information for each parameter.

Line 1 has the following format: first the parameter **NAME**, in boldface type; then an optional reference, *note, to one of the notes collected at the end of the spefications list; then, if the parameter is a table, the [length] of the table, in square brackets, (if no length is given, then the parameter is a single item; if [@Z] appears, this signifies that the parameter must have as many elements as the associated depth table (**Z** or **ZAUX**) – see Section 13); and then a final group of codes:

- first the letter designating the Part(s) of the input file the parameter may appear in (see Section 3),
- then the number specifying the Statement Form to be used with this parameter (see Section 2), and
- finally the required mode of the parameter.

Line 2 contains a brief description of the function or significance of the input parameter. More information can be found in the *note specified (if any).

Beginning on Line 3 there appears an optional specification of the default

value(s) of the parameter.

If no default(s) are specified, then the default(s) equal(s) zero.

 \mathbf{A} *31, *93 D, 4, floating point Einstein A value *1 ABDD, 1, floating point abundance of the ion of the run **ACE** [NSL] D, 2, floating point

CE (default) addend

ACI [NSL] D, 2, floating point CI (default) addend

ADMAS D, 1, floating point

angular diameter (milliarcseconds) Default: as implied by ADS

ADS D, 1, floating point

star/Sun angular diameter ratio Default: 1.0

ADT[NDT] D, 2, floating point

Type-2 dust opacity function Default: (5.1, 4.7, 4.3, 3.8, 3.4, 3.0, 2.65, 2.4, 2.2, 2.1, 2.1, 2.0, 2.1, 2.3, 2.3, 2.2,

 \mathbf{AEL} [@Z]D, 2*,2, floating point added Helium electrons

 \mathbf{AHM} [MHM]

D, 2, floating point H^- bound-free absorption coefficient

Default: (0.01989, 0.04974, 0.1302, 0.4052, 0.7407, 1.107, 1.485, 1.862, 2.226, 2.571, 2.887, 3.172, 3.419, 3.625, 3.789, 3.906, 3.977, 4.001, 3.977, 3.907, 3.791, 3.632, 3.432, 3.194, 2.923, 2.624, 2.302, 1.965, 1.619, 1.275, 0.9453, 0.7918, 0.6512, 0.5431)

 \mathbf{AL} [NL]D, 2, floating point added recombination fraction

Default: $AL_1 = 1.0$, $AL_i = 0.0,$ $i \le 2 \le NL$

ALBDT [NDT]D, 2, floating point

Type-2 dust albedo Default: 0.9

ALBDUST [LDU] D, 2, floating point

Type-1 dust albedo

ALBK

[NKA]

D, 1, floating point

scattering albedo parameter for Background Line Opacities (see Section 9)

Default: (1.0, 0.0)

ALK

[@Z]

 $H, 2^*, 2$, floating point

singly-ionized Aluminum number density

Default: computed in LTE

ALN

[@Z]

H, 3*,3, floating point

Aluminum-I level populations

Default: ALN_{ij} computed in LTE, for all levels j such that j > NAL

AOWXP

D, 1, floating point

alpha-old weight exponent for Special He-II (Special N-1 calculation, Diffusion)

APARAD

D, 1, floating point

dielectronic recombination parameter

APCDP

D, 1, floating point

dielectronic recombination parameter

APCI

[NAPKNT]

D, 1, floating point

dielectronic recombination parameter

APDDIFC

D, 1, floating point

ambipolar diffusion velocity calculation parameter

Default: 90.7

APDDTFC

D, 1, floating point

ambipolar diffusion velocity calculation parameter

Default: 36.6

APDTEXP

D, 1, floating point

ambipolar diffusion velocity calculation parameter

Default: 1.76

APDXICA

D, 1, floating point

ambipolar diffusion velocity calculation parameter

Default: 1.75

APDXICB

D, 1, floating point

ambipolar diffusion velocity calculation parameter

Default: 4.5

APDXICC

D, 1, floating point

ambipolar diffusion velocity calculation parameter

Default: 0.02

APDXICD

D, 1, floating point

ambipolar diffusion velocity calculation parameter

Default: -3.5×10^5

APEI

[NAPKNT] D, 1, floating point

dielectronic recombination parameter

APETA

D, 1, floating point

dielectronic recombination parameter

APWRA

D, 1, floating point

dielectronic recombination parameter

APWRB

D, 1, floating point

dielectronic recombination parameter

ASMCR *92 D, 1, floating point

sequential smoothing parameter

Default: 0.001

ATOLAB

D, 2, alphanumeric

"name" of ion model data file

Default: "!NONAME!"

AW

[@Z]

D, 5*,5, floating point

integrated diagonal of WN-matrix

BANDE

*77

[NAB]

B, 2, integer

Composite Line Opacities wavelengths bands continuum eclipse calculation switch

BANDL *77 [NAB]

B, 2, floating point

lower limits of Composite Line Opacity wavelengths bands (see Section 9)

BANDU

*77

[NAB]

B, 2, floating point

upper limits of Composite Line Opacity wavelengths bands (see Section 9)

BANDY

[NAB]

D, 2, floating point

method control parameter for Composite Line Opacity (see Section 9) Default: all = -1.0

BD[@Z]D, 3*, 3, floating point departure coefficient of the levels of the ion of the run Default: computed, using input number densities **BDAL** [@Z] $H, 3^*, 3$, floating point departure coefficients of the levels of Aluminum-I Default: computed, using input Aluminum-I level populations BDC[@Z] $H, 3^*, 3$, floating point departure coefficients of the levels of Carbon-I Default: computed, using input Carbon-I level populations **BDCA** H, 3*,3, floating point [@Z]departure coefficients of the levels of Calcium-I Default: computed, using input Calcium-I level populations **BDFE** [@Z]H, 3*,3, floating point departure coefficients of the levels of Iron-I Default: computed, using input Iron-I level populations BDH[@Z]H, 3*,3, floating point departure coefficients of the levels of Hydrogen Default: computed, using input Hydrogen level populations [@Z]H, 3*,3, floating point departure coefficients of the levels of Helium-I Default: computed, using input Helium-I level populations **BDHE2** [@Z]H, 3*,3, floating point departure coefficients of the levels of Helium-II Default: computed, using input Helium-II level populations [@Z]D, 2*,2, floating point departure coefficient of H-minus Default: $BDHM_i = 1.0$, all i [@Z] $H, 3^*, 3$, floating point departure coefficients of the levels of Magnesium-I Default: computed, using input Magnesium-I level populations **BDNA** [@Z]H, 3*,3, floating point departure coefficients of the levels of Sodium-I Default: computed, using input Sodium-I level populations

BDO [@Z] $H, 3^*, 3$, floating point departure coefficients of the levels of Oxygen-I Default: computed, using input Oxygen-I level populations **BDOPT** *43 D, 1, alphanumeric b-ratios selection parameter Default: "BDJ" BDO2 [@Z] $H, 3^*, 3$, floating point departure coefficients of the levels of Oxygen-II Default: computed, using input Oxygen-II level populations BDO3 [@Z]H, 3*,3, floating point departure coefficients of the levels of Oxygen-III Default: computed, using input Oxygen-III level populations BDS[@Z]H, 3*,3 floating point departure coefficients of the levels of Sulphur-I Default: computed, using input Sulphur-I level populations **BDSI** [@Z]H, 3*,3 floating point departure coefficients of the levels of Silicon-I Default: computed, using input Silicon-I level populations **BHORIZ** [@Z]D, 2*,2, floating point magnetic field strength **BLCSW** *14 D, 4, integer broadening components switch (a.k.a. damping components selector) Default: 31 **BLIMG** *34 D, 1, floating point absorption contributors graph axis limit Default: $-1.301 [= \log(0.05)]$ $\mathbf{B}\mathbf{M}\mathbf{W}\mathbf{A}\mathbf{C}$ D, 1, floating point beam width parameter for continuum eclipse calculation

5.7

Default: (0., .03, .06, .1, .15, .22, .3, .4, .6, .9, 1.2, 1.5, 2., 3., 5., 10., 20., 40.,

D, 2, floating point

[KBX]

background lines frequency table (half profile)

70., 110., 200., 500., 1000., 2000., 5000.)

Default: 0.1

*66

BXI

CAK [@Z] H, 2*,2, floating point

singly ionized Calcium number density

Default: computed in LTE

CAN [@Z] H, 3*,3, floating point

Calcium-I level populations

Default: CAN_{ij} computed in LTE, for all levels j such that j > NCA

CCHX *95 D, 1, floating point

upper-level charge-exchange cross-section multiplier

Default: 1.0

CDL *77, *105 [LDL] D, 4, floating point

weights for blended line components

Default: 1.0

CDZ *82 D, 1, floating point

fluid velocity parameter

Default: 100.

CE *25, *93 [NTE] D, 5, floating point

collisional excitation coefficient

Default: computed (see Section 19)

CEDMN D, 1, floating point

impact-parameter CE-value calculation parameter (for integration)

Default: 10^{-6}

CEDMX D, 1, floating point

impact-parameter CE-value calculation parameter (for integration)

Default: 10^3

CEFEQ D, 1, floating point

impact-parameter CE-value calculation parameter (for integration)

Default: 10^{-2}

CEMETHOD *93, *139 D

CE-method selectors

Default: for Hydrogen: (SCHOLZ, GIOVAN, JOHNSON); otherwise: (SEATON, VREGE)

CEQMX D, 1, floating point

H2 number density control parameter

Default: 10^6

CGR

D, 1, floating point

gravity ratio, with respect to Sun

Default: 1.0

CHEFLOW

D, 1, floating point

Helium flow constant for RHEAB calculation

 \mathbf{CHI}

[@Z]

D, 5*,5, floating point

RHO-like line transfer quantity

CHLIM *19

D, 1, floating point

RHOW parameter

Default: 0.5

CHOP *19

D, 1, floating point

a RHO selection parameter

Default: 1.0

 \mathbf{CI}

*93

[NTE]

D, 3, floating point

collisional ionization coefficient

Default: computed (see Section 19)

CIJADD *91

[@Z]

D, 5*,5, floating point

term to be added to CIJ

CIMETHOD *93, *139

9

D

CE-method selectors

Default: for Hydrogen: (SHAH, CLARK); otherwise: (AR, CLARK)

 ${f CK}$

 $H, 2^*, 2$, floating point

singly-ionized Carbon number density

Default: computed in LTE

CKADD

[@Z]

[@Z]

D, 3*, 3, floating point

term to be added to CK

CLEVELS

D, 1, floating point

diffusion calculation parameter

Default: 2.0

 \mathbf{CLM}

D, 1, floating point

scattering albedo parameter for Background Line Opacities (see Section 9)

Default: 1.0

CLOGG

D, 1, floating point

log(surface gravity)

Default: as implied by CGR

CLNH

D, 1, floating point

HSE calculation parameter

Default: 2.0

 \mathbf{CN}

[@Z]

 $H, 3^*, 3$, floating point

Carbon-I level populations

Default: CN_{ij} computed in LTE, for all levels j such that j > NLC

CN1S

D, 1, floating point

rcheck-criterion for Special-N1 (diffusion)

Default: 0.01

COLINES *112

D

CO lines control parameters Default: see Note *112

COMU

D, 1, floating point

mu-value for CO lines opacity calculation

CORMAX *130

D, 1, floating point

limit parameter for ORIGINS and CONTRIBUTORS print outs $% \left(1\right) =\left(1\right) \left(1$

Default: -1.0

CORMIN *130

D, 1, floating point

limit parameter for ORIGINS and CONTRIBUTORS printouts

Default: -1.0

 \mathbf{CP}

*56, *93

[NSL]

D, 2, floating point

photoionization cross-section

Default: computed (see Section 19)

CPRESS

D, 1, floating point

specified constant pressure

 \mathbf{CQA}

*117

[NCQ]

D, 2, floating point

'Line Opacity' scattering albedo parameter

Default: $(10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1.0)$

 \mathbf{CQM}

D, 1, floating point

scattering albedo parameter for Background Line Opacities (see Section 9)

 \mathbf{CQT} *117 [NCQ]D, 2, floating point 'Line Opacity' scattering albedo parameter Default: (4000, 5000, 6000, 7000, 8000) CRD*77, *93,* 105 [LDL] D, 4, floating point radiative broadening halfwidth CRS *93 D, 4, floating point resonance broadening halfwidth CSDWD, 1, floating point number of Doppler widths from line center at which the Hydrogen Stark components strengths are reduced by the factor 1/e Default: 1.0 **CSFCRIT** D, 2, floating point convergence criterion for CSF iteration Default: 10^{-5} CSK*93, *105 D, 4, floating point Stark broadening halfwidth **CSTARK** *107 D, 4, floating point Hydrogen Stark broadening (convolution) switch **CUTFE** D, 1, floating point cut-off criterion for injection function integration (fast electrons) Default: 10^{-8} **CTCO** D, 1, floating point NCO calculation temperature enhancement factor CTMXD, 1, floating point maximum NCO temperature enhancement Default: 0.2 \mathbf{CVSB} *82 D, 1, floating point fluid velocity parameter for VSB

CVW *93, *105 D, 4, floating point

van der Waals broadening halfwidth

CVX *82 [NVX] F, 2, floating point fluid velocity parameters for VX

CVXF *82 F, 1, floating point fluid velocity parameter for flow broadening velocities

 $Default:\ 25.0$

CVXM

F, 1, floating point

fluid velocity parameter for flow broadening velocities

CVXS *82

D, 1, floating point

fluid velocity parameter for VXS

*82

CVZ *82

D, 1, floating point

fluid velocity parameter

Default: smallest Z_i such that $NH_i > 10^{11}$

CWJ *19

D, 1, floating point

a RHOJ calculation parameter

Default: 0.5

CWR *19

D, 1, floating point

a RHO selection parameter

Default: 0.1

DDL *77, *105 [LDL]

D, 4, floating point

displacements from reference wavelength of blended line components, in Angstroms (see also DWN)

DDR *42 [NDR]
DR parameter, PRD transitions

Default: (1.0, 0.9, 0.65, 0.4, 0.1, 0.05, 0.0)

DDT

D, 1, floating point

D, 2, floating point

Type-2 dust opacity calculation convergence criterion

Default: 0.01

DELLIM

D, 1, floating point

DEL-criterion for using DIRECT instead of FULL solution

Default: 10^{-6}

DELTB

D, 1, floating point

departure coefficients editing parameter

Default: 0.01

DELWAVE *76

[NWS]

D, 2, floating point

'subtractional' wavelengths for continuum calculations

DFDUST [LDU] D, 2, floating point

Type-1 dust factor

DGM *138 [@Z] D, 2*,2, floating point

depth-dependent G multiplier (HSE)

Default: all = 1.0

DGMZ *138 [NGM] D, 2, floating point

standard table of DGM (as a function of ZGM) for the quiet sun

Default: (.64, .645, .66, .68, .71, .74, .77, .81, .86, .89, .92, .95, .97, .985, .99,

.995, .995, .995, .99, .98, .97, .965, .96

DLU D, 1, floating point

dilution factor Default: 1.0

DO [variable] B, 2, alphanumeric enable program options (see Section 6 for further details)

DOFDB *80 $[\le 2 \times NT]$ D, 2, integer

alternate form of LSFFDB

DOFLUX *79 $[\le 2 \times NT]$ D, 2, integer alternate form of LFLUX

DOPROF *78 $[\le 2 \times NT]$ D, 2, integer

alternate form of PROF

DOSFPRNT *81 $[\le 2 \times NT]$ D, 2, integer alternate form of LSFPRINT

DPMULT D, 4, floating point

damping multiplier Default: 1.0

DQMAX D, 1, floating point parameter for injection function integration (fast electrons)

Default: 2.0

DQMIN D, 1, floating point

parameter for injection function integration (fast electrons)

Default: 0.01

DRHO D, 4, floating point

RHO editing parameter

Default: 0.05

DRLIM *42

D, 1, floating point

DR parameter, PRD transitions

Default: 0.01

DWAVE *65

[NDV]

D, 2, floating point

Continuum Source Function dump wavelengths table

DWN *77

[LDL]

D, 4, floating point

= DDL, but in wavenumbers

DZMSS

D, 1, floating point

Z-from-Mass calculation parameter

Default: 0.01

ECLI *58

D, 4, integer

Eclipse line profiles computation switch

EIDIF

D, 1, floating point

NE-iterations convergence criterion

Default: 10^{-4}

ELEMENT

D

element data (see Section 10)

ELLED

D, 1, floating point

particle energy dissipation calculation parameter 'L' (fast electrons)

Default: 2.4×10^{-11}

ELSYM *93

D, 1, alphanumeric

chemical symbol of the ion of the run

Default: "ZZ"

EMXED

D, 1, floating point

particle energy dissipation calculation parameter 'EMAX' (fast electrons)

Default: 10^{-6}

EPCBR

D, 1, floating point

branching ratio for supplementary levels in Lyman EPSILON-1

EPDUST

[LDU]

D, 2, floating point

Type-1 dust dilution factor

EP1

[@Z]

D, 2*,2, floating point

Lyman EPSILON-1

 $\mathbf{EP2}$

[@Z]

D, 2*,2, floating point

Lyman EPSILON-2

ESCTAU *48

D, 1, floating point

TAU criterion for automatic use of escape probability solution

Default: 5.0

EXLYM *67 D, 1, floating point

Lyman change-over TAU parameter

Default: 10.

FABD

D, 1, floating point

multiplier for element abundances

Default: 1.0

FBVMX

F, 1, floating point

maximum velocity value for flow broadening

Default: 100.

FCE

[@Z]

D, 5*,5, floating point

CE-enhancement factors

FEK

[@Z]

 $H, 2^*, 2$, floating point

singly-ionized Iron number density

Default: computed in LTE

FEN

[@Z]

 $H, 3^*, 3$, floating point

Iron-I level populations

Default: FEN_{ij} computed in LTE, for all levels j such that j > NFE

FILE

*44

B,D,F,H alphanumeric

input file designation

FINK

[INK]

D, 2, floating point

incident radiation input values

Default: $(0., 3.0 \times 10^{-12}, 3.0 \times 10^{-12}, 1.5 \times 10^{-12}, 1.5 \times 10^{-12}, 0.)$

FKUR

[KURNWV] D, 2, floating point

multiplier for Statistical Line Opacity (see Section 9)

Default: all = 1.0 (KURNWV = 53, built in)

FMCDL

D, 1, floating point

Hydrogen Stark splitting components elimination criterion

Default: 0.1

FMVLIM *82

D, 1, floating point

fluid velocity multiplier limit

Default: 10^{-4}

FNH

[NFH]

F, 2, floating point

standard tabel of flow velocity for flow broadening

Default: (10., 9., 7., 5., 3., 2., 1., 0.)

FNRMLA

65

D, 2, floating point

normalizing factor for simulated background H Ly α profile

Default: all = 1.0

FNRMLB

65

D, 2, floating point

normalizing factor for simulated background H Ly β profile

Default: all = 1.0

FRCDL

D, 1, floating point

Hydrogen Stark splitting components elimination criterion

Default: 0.01

FROSCE *93

D, 1, floating point

 $fraction-of-classical-oscillator-strength\ used\ in\ the\ calculation\ of\ collision\ rates$

for forbidden transitions

Default: 0.01

 \mathbf{FRR}

[MRR]

D, 2, floating point

radius fraction

Default: (0.0, 0.5, 0.8, 0.9, 0.95, 1.0)

FSTKM

D, 1, floating point

Hydrogen Stark splitting reduction factor

Default: 1.0

FZION

D, 1, floating point

ZION-multiplier for diffusion calculation

Default: 1.0

FZLIM

D, 1, floating point

Z-from-Mass calculation parameter

Default: 1.5

 $\mathbf{G}\mathbf{K}$

*123

D, 2, floating point

Gaunt factors for Level-KOLEV-to-Continuum calculation

[KK]

Default: RRCP(KOLEV)

GMMA *42

D, 4, floating point

gamma-parameter, PRD transitions

Default: -1.0

HEABL

D, 1, floating point

Helium abundance limit factor for RHEAB calculation

Default: 3.0

HEK

[@Z]

 $H, 2^*, 2$, floating point

singly-ionized Helium number density

Default: computed in LTE

HEL

D, 1, floating point

weight for HSE calculation

Default: 1.0

HEN

[@Z]

H, 3*,3, floating point

Helium-I level populations

Default: HEN_{ij} computed in LTE, for all levels j such that j > NLZ

HE2K

[@Z]

 $H, 2^*, 2$, floating point

doubly-ionized Helium number density

Default: computed in LTE

HE2N

[@Z]

H, 3*,3, floating point

Helium-II level populations

Default: HE2N_{ij} computed in LTE, for all levels j such that j > NZ2

HE304

[@Z]

 $D, 2^*, 2,$ floating point

He-II $\lambda 304$ line mean intensity

HN

[@Z]

H, 3*,3, floating point

Hydrogen level populations

Default: HN_{ij} computed in LTE, for all levels j such that j > NLH

HNAJL

D, 1, floating point

limit for NH-adjustment factor in HSE calculation

Default: 10^{20}

HNDF

[NFH]

F, 2, floating point

Hydrogen density table for FNH

Default: $(1.0\times10^{11},\ 3.0\times10^{11},\ 1.0\times10^{12},\ 3.0\times10^{12},\ 1.0\times10^{13},\ 3.0\times10^{13},\ 1.0\times10^{14},\ 3.0\times10^{14})$

HNDV *90 [NVH] D, 2, floating point

Hydrogen density table for VNH

 $\begin{array}{l} \textit{Default:} \ (1.0\times10^9,\, 2.0\times10^9,\, 5.0\times10^9,\, 1.0\times10^{10},\, 2.0\times10^{10},\, 5.0\times10^{10},\, 8.38\times10^{10},\\ 1.07\times10^{11},\, 1.61\times10^{11},\, 3.17\times10^{11},\, 7.73\times10^{11},\, 2.71\times10^{12},\, 9.32\times10^{12},\, 2.04\times10^{13},\\ 6.69\times10^{13},\, 9.82\times10^{13},\, 2.25\times10^{14},\, 3.55\times10^{14},\, 6.01\times10^{14},\, 9.87\times10^{14},\, 1.64\times10^{15},\\ 2.09\times10^{15},\, 3.37\times10^{15},\, 4.22\times10^{15},\, 6.58\times10^{15},\, 1.02\times10^{16},\, 2.33\times10^{16},\, 4.24\times10^{16},\\ 6.05\times10^{16},\, 8.33\times10^{16},\, 1.03\times10^{17},\, 1.15\times10^{17},\, 1.22\times10^{17},\, 1.27\times10^{17},\, 1.30\times10^{17},\\ 1.32\times10^{17},\, 1.34\times10^{17},\, 1.35\times10^{17}) \end{array}$

HSBDMN

D, 1, floating point

Hydrogen Stark broadening parameter, for convolution calculation $Default: 10^{-5}$

HSBDMX

D, 1, floating point

Hydrogen Stark broadening parameter, for convolution calculation $Default: 10^3$

HSBFEQ

D, 1, floating point

Hydrogen Stark broadening parameter, for convolution calculation Default: 0.1

HSBM

D, 1, floating point

Hydrogen Stark broadening parameter, for convolution calculation

Default: 20.0

HSEC *15

D, 1, floating point

weight for HSE calculation

Default: 1.0

HSLITER

D, 1, floating point

number of HSL iterations

Default: 1

HTAU

D, 1, floating point

HSE calculation parameter

Default: 1.0

IBETSW *126

D, 1, integer

beta-equation selection switch, diffusion

IBNVIEW

D, 1, integer

depth index for illustration of BD- and ND-calculations trace Default: (JEDIT+1)

IBRDP D, 1, integer

diffusion d-coefficients debug dump switch

ICDIT *101 D, 1, integer

 $\mathrm{d} I/\mathrm{d} h$ continuum wavelengths selector

Default: 1

ICHDP D, 1, integer

hydrogen collision rates calculation dump depth index

ICHSW *136 D, 1, integer

collision-with-Hydrogen switch

ICR [NCR] D, 2, floating point

values of incident coronal radiation

ICXDP *95 D, 1, integer

upper-level charge-exchange dump depth index $\,$

IDEDP D, 1, integer

ion broadening (Hydrogen) dump switch

IDEX D, 1, integer

extra information switch for standard-output (or log file)

Default: 10

IDFDI *89 D, 1, integer

d-coefficients dump index

Default: N/4

IDFDM *89 D, 1, integer

d-coefficients method selection switch

Default: 1

IDFDS D, 1, integer

d-coefficients smoothing

Default: 1

IDFSW D, 1, integer

dI/dh details print switch

IDNRT D, 1, integer

switch for calculation of DNRT, DNRTC in Lyman

Default: 1

IDRCD

D, 1, integer

index of disk ray for CSF debug printout

Default: 1

IDRDP

D, 1, integer

depth index for option DRDMP

Default: N/2

IDWIN

D, 1, integer

DW-dump index increment

*42

IFXDS *70

D, 1, integer

continuum flux detail output control

IGII

D, 1, integer

RII-approximation selector (PRD)

Default: 1

IGMSW *42

D, 1, integer

alternate GMMA for H Lyman alpha and beta (PRD)

IHDMP

D, 1, integer

dump output control switch for Line Flux Distribution calculation

IHEAB

D, 1, integer

reference depth index for RHEAB calculation

IHSDD *106

D, 1, integer

Hydrogen Stark broadening dump switch

IHSDP

*106

D, 1, integer

Hydrogen Stark broadening dump switch

IHSKM

D, 1, integer

Hydrogen Stark broadening calculation table limit

 $Default:\ 100$

IHSSM

D, 1, integer

Hydrogen Stark broadening calculation table limit

Default: 2000

IHSSP

D, 1, integer

Hydrogen Stark splitting control switch

IHSSW

D, 1, integer

Hydrogen Stark broadening (convolution) switch

ILI *19 D, 1, integer

a RHO selection parameter

IMUCD D, 1, integer

index of XMU for Continuum Source Function debug printout

Default: 1

INCEI *93 D, 1, integer

depth index for CI and CE comparison calculations

Default: index of TE-value closest to 8000 K, going in

INCH D, 1, floating point

RHO weight adjustment parameter

Default: 0.1

INDRN D, 1, integer

input number densities renormalization switch

Default: 1

INFSM D, 1, integer

Lyman RK-Kolev smoothing delimiter

 $Default:\ 1$

INK B, 1, integer

length of XINK Default: 6

INLSM D, 1, integer

Lyman RK-Kolev smoothing delimiter

Default: N

INPAIR *2, *77 $[2 \times NT]$ B, 2, integer

list of transition indices

INRHO D, 4, integer

input-RHO use switch

IOMX D, 1, integer

number of overall iterations

Default: 1

IONSTAGE *93 D, 1, integer

stage of ionization of the ion of the run

Default: 1

IORIC

D, 1, integer

line-center depths-of-formation print switch $Default:\ 1$

IPDEE *125

D, 1, integer

d-coefficients printout switch, diffusion calculation

IPDIJ *127

D, 1, integer

DIJ printout switch, diffusion analysis

IPERFA

D, 1, integer

performance data archive record switch

Default: 1

IPEX *113

D, 1, integer

switch for extra debug output

IPIJG

D, 1, integer

fudge GNV in the equation for PIJ $\,$

Default: 1

IPPOD *52

D, 1, integer

'population ion' absorption/emission calculation dump switch

IPR01 *59

D, 1, integer

Line Source Function debug printout limiting index

Default: 1

IPR02 *59

D, 1, integer

Line Source Function debug print out limiting index Default: 5

IPR03 *59

D, 1, integer

Line Source Function debug print out limiting index Default: 10

IPR04

D, 1, integer

Line Source Function debug printout limiting index

Default: 15

IPRDD *30

D, 1, integer

depth interval for PRD printout

*59

Default: 1

IPRDF *30 D, 1, integer

frequency print out for PRD printout

Default: 1

IPZER *71 D, 1, integer

dump printout selector for subroutine DIVIDE

IRATE *100 D, 1, integer

depth index for 'minimal' rates printout

IRFNC *111 D, 1, integer

depth index of reference value of charged particle number density for printed sample values of Hydrogen CE and CI

Default: i such that TE_i "equals" the middle value of TER, where i is the smallest such value

IRKCOMP *45 [NSL] D, 2, integer

 $\ensuremath{\mathrm{RK}}\xspace$ compute switches

Default: all =1

IRLCOMP *45 [NSL] D, 2, integer

RL-components compute switches

Default: all =1

IRLSN *39 D, 1, integer

RL integration methods switch

Default: 1

IRLS1 *39 D, 1, integer

RL integration methods switch

Default: 1

IRPUN *84 D, 1, integer

RABD calculation data output switch

Default: 1

IRTIS *63 D, 1, integer

incident radiation table interpolation selector

Default: 2

IRUNT ***74**, ***84** D, 1, integer

run type switch

ISCOMP D, 1, integer

line source functions comparison printout details switch

ISCRS *20, *84

scratch I/O mode switch

ISRCD D, 1, integer

index of shell ray for Continuum Source Function debug printout Default: 1

B, 1, integer

ISMBD D, 1, integer

intensity integration (SIMBA) dump interval

ISMSW *99 D, 1, integer

iteration summaries format switch

ISMVE D, 1, integer

small-values editing switch

Default: 1

ISNDD *121 D, 1, integer

S(n) calculation dump switch

ISNUD D, 1, integer

PRD SNU-shift debug dump switch

ISOD D, 1, integer

depth index for Sobolev integration dump

ISSV *55 [NVX] F, 2, integer

shock velocity depth indices

ISTARK D, 1, integer

default value of NE-index for Stark splitting of Hydrogen lines

Default: largest index where NE $\approx 10^{12}$

ISUB D, 1, integer

number of sub-iterations (= RHO-iterations)

Default: 1

ITKZA D, 1, integer

Z-augmentation (diffusion) iteration limit

Default: 1

ITN1R D, 1, integer

"Special N1" iterations limit (diffusion calculations)

Default: 10

ITPRD *42 D, 1, integer,

PRD-iterations limit

Default: 4

ITRFI D, 1, integer

TR-iteration debug output control

IVOIT *50 D, 1, integer

Voigt profile methods selector

Default: 1

IWEIT D, 1, integer

weighting details print switch

IWSMD D, 1, integer

WAVELENGTHS summary Part-2 switch

XASM D, 1, integer

smoothing dump (IPEX=25) detail control index

IXNCS *111 D, 1, integer

switch controlling calculation of on-the-fly Hydrogen CE and CI values

IXSTA *84 D, 1, integer

performance statistics printout control

Default: 1

IZOPT *38 D, 1, integer

graph Z-scale (axis) option

Default: 1

I4DEQ *122 D, 1, integer

four-diagonal method ("Special N1"), equation selector

I4DFM *122 D, 1, integer

four-diagonal method ("Special N1"), version selector

Default: 1

I4DIO *122 D, 1, integer

four-diagonal method ("Special N1"), flow direction specifier

Default: 1

JATAW D, 1, integer

write values of WRAT and RRCP as part of atomic data defaults output

JBAR [@Z] D, 5*,5, floating point

mean intensity

JBDNC *84 D, 1, integer

Rho and b-ratio calculation bypass switch

JBFSW D, 1, integer

b calculation method selector for supplementary levels Default: 1

JDMCE *115 D, 1, integer

debug dump switch for default calculation of Hydrogen CE values

JDMCI *115 D, 1, integer

debug dump switch for default calculation of Hydrogen CI values

JEDIT D, 1, integer

depth index for N-editing

Default: N/2

JHBFD D, 1, integer

debug dump switch for H-bf background absorption and emission

JHEAS D, 1, integer

secret HEABD switch

JHLSK *137 D, 1, integer

Stark broadening in H Lyman lines background opacity Default: 1

JH1 *102 D, 1, integer

photoionization rates multiplier index

JH2 *102 D, 1, integer

photoionization rates multiplier index

JM B, 1, integer

lenght of LMM

Default: 1

JNEDP D, 1, integer

N-editing dump switch

JNUNC *46 D, 1, integer

JNU input switch

JSFEX D, 1, integer LSF-solution-explanation print switch Default: 1 \mathbf{JSSV} * 55 D, 1, integer shock temperature depth index *5, *6, *11 **JSTCN** D, 1, integer Continuum-only run type selector *6, *40, *84 **JSTIN** D, 1, integer input-check only switch **JZATMO** *133 D, 1, integer zero-print mode switch for ATMOSPHERE

JZATOM *133 D, 1, integer zero-print mode switch for ATOM

JZOPT *38 D, 1, integer graph Z-scale (axis) option

 \mathbf{K} B, 1, integer = KS

KALHD *73 B, 1, alphanumeric Hi/Bye/Abort-system control parameter Default: "" (i.e., blank)

KALOR *73 B, 1, integer Hi/Bye/Abort-system control parameter Default: 1

KANTNU *129 D, 1, integer TNU-analysis switch

KAPDB D, 1, integer continuum contributors control debug switch

KARB *75 B, 1, integer 'print character' selector for 'banner' page Default: 1

 $\begin{array}{ccc} \mathbf{KB} & \textbf{*66} & \mathbf{B}, \ 1, \ \mathrm{integer} \\ \mathrm{length} \ \mathrm{of} \ \mathrm{XIBLU} \\ \mathit{Default:} \ \mathrm{KS} \end{array}$

KBNDS *122

D, 1, integer

boundary condition switch for diffusion ("Special N1")

Default: 1

KBT *66

D, 4, integer

length of XIBLUT Default: KST

KBTMAX

B, 1, integer

maximum of the various values of KBT occurring in ${f Part}\ {f D}$

KBX *66

B, 1, integer

length of BXI Default: 25

KB1WA *128

D, 1, integer

B1-weights depth index

KB1WB *128

D, 1, integer

B1-weights depth index

KB1WS *128

D, 1, integer

B1-weights type selection switch

Default: 2

KCOAA

D, 1, integer

switch of short form of Composite Line Analysis output

KDAMP *122

D, 1, integer

matrix solution damping switch for "Special N1" (diffusion)

KDIAG *122

D, 1, integer

diagonal method selector for diffusion ("Special N1")

Default: 3

KDIFD1 *119

D, 1, integer

method switch for derivatives in diffusion calculations

Default: -1

KDIFGA *124

D, 1, integer

GNV-fudging depth index

Default: -1

KDIFGB *124 D, 1, integer

GNV-fudging depth index

Default: -1

KDIFGS *124 D, 1, integer

GNV-fudging switch

KDRDP D, 1, integer

frequency index for option DRDMP

Default: K/2

KDUST D, 1, floating point

dust constant

KHFFS *41 D, 1, integer

H free-free contribution to Total Hydrogen cooling

Default: 1

KININT D, 1, integer

plot index selection increment for Line Background opacities (see Section 9)

Default: 5

KINMAX D, 1, integer

plot index for Line Background opacities (see Section 9)

Default: index of depth near the minimum of TE

KK B, 1, integer

length of XK

Default: MR(KOLEV)

KKPR D, 1, integer

frequency index for detailed Lyman printout

Default: KK

KLDIN D, 1, integer

Lyman dump depth interval

KLFIN D, 1, integer

Lyman dump frequency interval

KMMAX *66 D, 1, integer

maximum XIFUL length

KODNT D, 1, integer

Composite Line Opacity raw data dump interval (see Section 9)

KOELS

D, 1, integer

every-line switch for ORIGIN printout

Default: 1

KOLEV

B, 1, integer

level index $(i.e. \mathcal{N})$ for 'Level- \mathcal{N} -to-Continuum' transfer calculation

Default: 1

KONFORM *12

D, 1, integer

detail contributions printout format selector

Default: 2

KOOLSUM *41

D, 1, integer

control for components added into Total Cooling Rate for Hydrogen runs

KPC

*10

[@Z]

D, 5*,5, floating point

continuous opacity

Default: $KPC^{u,\ell} = KPC^{MS,NS} \times KPCR^{u,\ell}$, for $u \neq MS$, $\ell \neq NS$

 \mathbf{KPCR}

D, 4, floating point

ratio of the continuous opacity with respect to that of transition (MS,NS)

 $\mathbf{K}\mathbf{R}$

*66

B, 1, integer

length of XIRED Default: KS

KRATE

*118

D, 4, integer

single-vs.-net rate switch for transition terms

Default: 1

 \mathbf{KRT}

*66

D, 4, integer

length of XIREDT

Default: KST

KRTMAX

B, 1, integer

maximum of the various values of KRT occurring in ${f Part}\ {f D}$

KS

*66

B, 1, integer

length of XISYM $\,$

 $Default:\ 24$

KST

*66

D, 4, integer

length of XISYMT $\,$

Default: KS

KSTMAX

B, 1, integer

maximum of the various values of KST occurring in Part D

KTRANS *33

D, 4, alphanumeric

 $\begin{array}{l} {\it transition \ descriptor} \\ {\it Default: \ "RADIATIVE"} \end{array}$

KUDNT

D, 1, integer

Statistical Line Opacity raw data dump interval (see Section 9)

KURIN

D, 1, integer

step selection index for Statistical Line Opacity data (see Section 9)

KURMA

D, 1, integer

long-wavelength cutoff for Statistical Line Opacity data (see Section 9) Default:~9000.0

KURMI

D, 1, integer

short-wavelength cutoff for Statistical Line Opacity data (see

Section 9)
Default: 1682.0

KXLYM

D, 1, integer

XK-table augmentation switch

 ${f L}$

*24

B, 1, integer

length of MU Default: LF

LCEX

D, 1, integer

charge exchange index

Default: 1

 \mathbf{LCH}

*136

[NSL]

D, 2, integer

collisions-with-Hydrogen codes

LCOA

[NCB]

D, 2, floating point

CO-lines opacity wavelength band lower limit

LCOB

[NCB]

D, 2, floating point

CO-lines opacity wavelength band upper limit

LCOD

D, 1, floating point

CO-lines opacity dump printout wavelength

LCR [LCR] D, 2, floating point wavelengths at which incident coronal radiation is specified LDFD1 D, 1, integer smoothing control switch for computed derivatives LDINT *54 D, 1, integer depth increment for detailed printout of transition terms Default: 5 LDL*77, *105 D, 3, integer length of DDL Default: 1**LDLMAX** B, 1, integer maximum of the various values of LDL occurring in Part D LDT[NDT]D, 2, floating point wavelengths tables for Type-2 dust opacity calculation Default: (910.0, 952.0, 1000.0, 1050.0, 1110.0, 1180.0, 1250.0, 1330.0, 1430.0,1540.0, 1670.0, 1820.0, 2000.0, 2080.0, 2170.0, 2270.0, 2380.0, 2500.0, 3330.0, $5000.0, 1.0 \times 10^4, 3.0 \times 10^4, 1.0 \times 10^5, 3.0 \times 10^5, 1.0 \times 10^6, 3.0 \times 10^6, 1.0 \times 10^7,$ 3.0×10^7 , 1.0×10^8) LDTYP *54 D, 1, integer type control for detailed printout of transition terms Default: 1 LDUB, 1, integer length of LMDUST

Default: 1

LEEDS

He-I background lines opacity calculation debug switch

LEVDES *53 [NSL] D

level designation (term designation)

 \mathbf{LF} *17, *24 B, 1, integer length of MUF

Default: 2

LFLUX *72

D, 1, integer

LG

B, 1, integer

length of XMU Default: 8

LHEDS

D, 1, integer

He-II background lines opacity calculation debug switch

LHHSF

D, 1, integer

reference depth index for H and M in HSE

LHM

[MHM]

D, 2, floating point

wavelengths for H-minus continuum calculations

 $Default: (16300.0, 16200.0, 16000.0, 15500.0, 15000.0, 14500.0, 14000.0, \\ 13500.0, 13000.0, 12500.0, 12000.0, 11500.0, 11000.0, 10500.0, 10000.0, 9500.0, \\ 9000.0, 8500.0, 8000.0, 7500.0, 7000.0, 6500.0, 6000.0, 5500.0, 5000.0, 4500.0, \\ 4000.0, 3500.0, 3000.0, 2500.0, 2000.0, 1750.0, 1500.0, 1250.0)$

LLY

B, 1, integer

length of LMXX

LMA *104

D, 1, floating point

Lyman EP-1 edit parameter

Default: 0.3

LMB *104

D, 1, floating point

Lyman EP-1 edit parameter

Default: 10^4

LMCR *137

D, 1, floating point

Hydrogen Lyman lines background opacity parameter

Default:~85.0

LMDL2 *137

D, 1, floating point

DR parameter, Hydrogen Lyman lines background opacity Default: 0.01

LMDL3 *137

D, 1, floating point

DR parameter, Hydrogen Lyman lines background opacity

Default: 0.01

LMDR *137

[LLY]

D, 2, floating point

DR parameter, Hydrogen Lyman lines background opacity

LMDUST [LDU] D, 2, floating point

wavelengths table for Type-1 dust opacity data

Default: 5000.0

LME *104 D, 1, floating point

Lyman EP-1 edit parameter

Default: 10^{-4}

LMF *104 D, 1, floating point

Lyman EP-1 edit parameter

Default: 10^{-5}

LMH *137 D, 1, floating point

wavelength cutoff for highest H Lyman lines background opacity *Default:* 950.

LMM [JM] D, 2, floating point

wavelengths table for opacity multiplier

 $Default:\ 1682.0$

LMR *104 D, 1, floating point

Lyman EP-1 edit parameter

Default: 10^4

LMT *104 D, 1, floating point

Lyman EP-1 edit parameter

Default: 0.3

LMXC *137 D, 1, floating point

DR parameter, Hydrogen Lyman lines background opacity Default: 2.0

LMXP *137

D, 1, floating point

DR parameter, Hydrogen Lyman lines background opacity Default: 3.0

LMXX *137 [LLY] D, 2, floating point DR parameter, Hydrogen Lyman lines background opacity

LMZ D, 1, floating point

Lyman alpha wing background opacity cut-off wavelength $Default:\ 2500.0$

LN *67 D, 1, integer

depth index limit for saturation approximation in "Lyman" calculation Default: 8

LODCG *88 D, 1, integer

depth index for diffusion calculation graphs Default: -1

LOGAS *114 D, 1, integer

location analysis graph switch

LOXDS D, 1, integer

O-I background lines opacity calculation debug switch

LPMLR F, 1, integer

mass-loss-rates print switch (used with LPVEL) $\,$

Default: 1

LPVEL F, 1, integer

profile-velocities print switch

Default: 1

LR *77 [NL] B, 2, integer

number of RKC values (one LR for each level)

LSFBOC *16 D, 4, integer

Line Source Function background opacity control

LSFFDB *36 D, 4, integer

Line Source Function background type selector

LSFGC *68 D, 1, integer

Line Source Function graph control code

Default: 1

LSFPRINT *81 D, 4, integer

Line Source Function printout switch

LSTMP D, 1. integer

STIM-for-GTN details print switch

LSFTYP *48 D, 4, integer

Line Source Function solution method selector

LWNT

D, 1, integer

'Line Opacity' printout wavelengths interval (see Section 9) Default: 1

LX2DS

D, 1, integer

O-II background lines opacity calculation debug switch

LX3DS

D, 1, integer

O-III background lines opacity calculation debug switch

LYMITER

D, 1, integer

number of Lyman iterations

Default: 1

LYODS

D, 1, integer

H Lyman background lines opacity calculation debug switch

LZA

B, 1*, integer

length of ZAUX

 ${\bf M}$

B, 1, integer

length of TS Default: 33

MAMAS

D, 1, integer

matrix elements magnitude scan switch

Default: 1

MASS

D, 1, floating point

atomic mass

MATRIX *140

 \mathbf{D}

matrix manipulation control data

MAUX

D,F,H, 1, integer

index specifying a ZAUX table

MCE

[NSL]

D, 2, floating point

CE (default) multiplier

Default: 1.0

MCI

[NSL]

D, 2, floating point

CI (default) multiplier

Default: 1.0

MCOA

D, 1, floating point

mulitplier of van der Waals damping for CO-lines profiles Default: all = 1.0

MCON

D, 1, integer

CO number density output switch

MDFG

D, 1, integer

diffusion terms (GVL) output switch

 $Default:\ 1$

MDFV

D, 1, integer

diffusion velocities output switch

Default: 1

MDTR1

D, 1, integer

Type-2 dust opacity calculation iteration limit

Default: 10

MDTR2

D, 1, integer

Type-2 dust opacity calculation iteration limit

Default: 20

METEP *21

D, 1, integer

Lyman EP-1 and EP-2 calculation methods selector

Default: 3

METSE

D, 4, integer

Statistical Equilibrium equations calculation methods selector

Default: METSEDG or METSEDW

METSEDG *35

D, 1, integer

general default value of METSE

*35

Default: 1

METSEDW *35

D, 1, integer

default value of METSE for transitions down to Level 1

Default: 3

MFONT

D, 1, integer

Fontenla atmosphere data output switch

Default: 1

MGK [@Z]

 $H, 2^*, 2$, floating point

singly-ionized Magnesium number density

Default: computed in LTE

MGN

[@Z]

H, 3*,3, floating point

Magnesium-I level populations

Default: MGN_{ij} computed in LTE, for all levels j such that j > NMG

 $\mathbf{M}\mathbf{H}\mathbf{M}$

B, 1, integer

length of LHM Default: 34

MH2N

D, 1, integer

H2 number density output switch

MKURU

D, 1, integer

Kurucz spectrum data output switch

Default: 1

MLC

[JM]

D, 2, floating point

opacity multiplier Default: 1.0

MN1

D, 1, integer

depth limit for N1 recalculation in the ambipolar diffusion calculation

Default: N

MNG1

D, 1, integer

depth limit for GNV-1 replacement in the ambipolar diffusion calculation

Default: -MN1

MODLAB *37

D, 1, alphanumeric

name of atmospheric model Default: "!NONAME!"

MOPRNT

D, 1, integer

switch to print built-in population-ion models

Default: 1

MQT

B, 1, integer

length of QTAIL

Default: 3

MR

*29, *77

[NSL]

B, 2, integer

number of WRAT values (one MR for each level)

 $\mathbf{M}\mathbf{R}\mathbf{R}$

B, 1, integer

length of FRR Default: 6

MS

*2, *59

D, 1, integer

index of upper level of 'reference transition'

Default: from INPAIR; see Note *2

MSKIP *62

D, 1, integer

ray selection parameter for computing weight matrices in spherical coordinates

MSSPR

D, 1, integer

print switch for matrix of simultaneous "Special N1" solution (diffusion)

Default: 1

MTHEI *83

D, 1, integer

exponential integral method selector

Default: 1

MTREF

D, 1, integer

TR-effective output switch

MU

*24

[L]

F, 2, floating point

cosine-of-lookangle values for emergent intensity calculation

Default: MUF

MUF *24

[LF]

F, 2, floating point

cosine-of-lookangle values for emergent flux calculation

Default: (1.0, 0.3)

MXPPI

D, 1, integer

limit for individual KZAUG values (Z-augmentation, diffusion)

Default: 5

MXTAP

D, 1, integer

limit for sum of KZAUG values (Z-augmentation, diffusion)

Default: 100

M304

D, 1, integer

index of reference value of He-II $\lambda 304$ line mean intensity

Default: 10

 \mathbf{N}

B, 1, integer

length of Z

NAB *77 B, 1, integer

length of BANDL (see Section 9)

NABS *7 [37] D, 2, integer

absorber/emitter switches $Default: NABS_i = on, for all i$

 \mathbf{NAK} [@Z] H, 2*,2, floating point

singly-ionized Sodium number density

Default: computed in LTE

NAL B, 1, integer

number of levels for which Aluminum populations are specified

 $\mathbf{NAME} \qquad \qquad \mathbf{*3} \qquad \qquad \mathrm{D, 1, alphanumeric}$

name of ion of run

NAN [@Z] H, 3*,3, floating point

Sodium-I level populations

Default: NAN_{ij} computed in LTE, for all levels j such that j > NNA

NANAL1 D, 1, integer

profile ANALYSIS depth selection parameter

Default: 1

NANAL2 D, 1, integer

profile ANALYSIS depth selection parameter

Default: 5

 $\mathbf{NAPKNT} \hspace{1.5cm} \mathrm{D}, \ 1, \ \mathrm{integer}$

recombination parameter

NAPWRA D, 1, integer

recombination parameter

Default: 1

NAPWRB D, 1, integer

recombination parameter

Default: 2

NARB ***75** B, 1, integer

number of 'banner' pages

NBS D, 1, integer

b-smoothing control (level) index

Default: 2

 \mathbf{NC} [@Z] H, 2^* ,2, floating point

charged particle number density

NCA B, 1, integer

number of levels for which Calcium populations are specified

NCB B, 1, integer

length of LCOA, LCOB

NCL *29, *109 B, 1, integer

length of XCOL

Default: 5

NCOI [@Z] D, 2^* , 2^* , floating point

CO number density, input (to replace computed values)

NCOPT D, 1, integer

CO-lines opacity calculations statistics-keeping switch

NCOSW D, 1, integer

Carbon Monoxide abundance correction computation method selector

Default: 1

NCQ B, 1, integer

length of CQT Default: 5

NCR B, 1, integer

length of LCR

ND *32 [@Z] D, 3*,3, floating point

number densities of the levels of the ion of the run

Default: computed in LTE

NDR B, 1, integer

length of XDR Default: 7

NDSN1 D, 1, integer

skip Special N-1 recalculation in first overall calculation

NDT B, 1, integer

length of LDT Default: 29

NDV

B, 1, integer

length of DWAVE

NDW

D, 1, integer

depth index for reference value of DW (Doppler width)

Default: either index of Z-value closest to ZNDW, or N/2

NDWM

D, 1, integer

depth index for reference value of DW (Doppler width), for atmospheric model

Default: NDW

NE

[@Z]

D, 2*,2, floating point

electron number density

NECLIP

D, 1, integer

continuum eclipse printout quantity selector

 \mathbf{NED}

D, 4, integer

RHO editing index

Default: N

NEFDF *125

D, 4, integer

switch for NE for d-coefficients in diffusion calculation

Default: 1

NERM *85

D, 1, integer

limit for some error messages from EDITH

Default: 10

NEWELE

D

element data (see Section 10)

 \mathbf{NFB}

B, 1, integer

number of isotropic flow broadening velocities

Default: 6

NFE

B, 1, integer

number of levels for which Iron populations are specified

 $\mathbf{1FH}$

B, 1, integer

length of HNDF Default: 8

 \mathbf{NGM} *138 B, 1, integer length of DGMZ

Default: 23

NGNV *116 D, 1, integer

GNVL-suppression level limit

NGRL *38 D, 1, integer graphs Z-scale (axis) limit

NGRR *38 D, 1, integer

graphs Z-scale (axis) limit

NH [@Z] D, 2*,2, floating point

total Hydrogen number density

NHN

= "HN 1 "

NHTSW *64 D, 1, integer

H2 abundance correction method selector

Default: 2

NIASM D, 1, integer

sequential smoothing parameter $\,$

Default: 20

NIL *19 D, 1, integer

a RHO selection parameter

Default: 2

NK [@Z] D, 3*,3, floating point

ionized number density of the ion of the run

Default: computed in LTE

NKA B, 1, integer

length of ZALBK (see Section 9)

Default: 2

NL *29, *77 B, 1, integer

number of levels of the ion of the run

Default: 2

NLC B, 1, integer

number of levels for which Carbon populations are specified

NLH B, 1, integer number of levels for which Hydrogen populations are specified NLO B, 1, integer number of levels for which Oxygen populations are specified \mathbf{NLPAIR} *94, *95 $[2\times NL]$ B, 2, integer list of quantum numbers NLS B, 1, integer number of levels for which Silicon populations are specified NLUB, 1, integer number of levels for which Sulphur populations are specified NLY D, 1, integer H Ly lines background opacity limit Default: 15 B, 1, integer number of levels for which Helium populations are specified

NLZ

B, 1, integer

number of levels for which Magnesium populations are specified

NMLR D, 1, integer mass-loss-rate index

Default: NDW

 \mathbf{NMT} *16, *77 B, 1, integer number of rows in the table ELE (see Section 10) Default: 38

NNAB, 1, integer number of levels for which Sodium populations are specified

NNDFE D, 1, integer dump control for injection function FJIN (fast electrons) Default: -1

NODCG *88 D, 1, integer depth index for diffusion calculation graphs Default: -1

NOION *11, *84 B, 1, integer 'no ion' switch

NO2

number of levels for which Oxygen-II populations are specified

B, 1, integer

NO3 B, 1, integer

number of levels for which Oxygen-III populations are specified

 \mathbf{NP} [@Z] H, 2^* ,2, floating point

proton number density

Default: computed in LTE

NQLYM *137 D, 1, integer

weight limit for highest H Lyman lines background opacity

NS *2, *59 D, 1, integer

index of lower level of 'reference transition'

Default: from INPAIR; see Note *2

NSL *29, *77 B, 1, integer

total number of levels of the ion of the run (including supplementary levels) Default: NL

NSPED D, 1, integer

particle energy dissipation calculation parameter "NS" (fast electrons)

Default: 1

NSPRD D, 1, integer

secret PRD switch

NSW *134 B, 1, integer

length of SCOW

NT *29, *77 B, 1, integer

number of transitions specified in INPAIR

NTAN *62 B, 1, integer

ray selection parameter for computing weight matrices in spherical coordinates Default: 4

NTE B, 1, integer

length of TER Default: 1

NU *93 [NSL] D, 2, floating point

frequency intervals between levels of the ion of the run, in frequency units (see also WNU)

NUC *93 [NSL] D, 2, floating point

auxiliary continuum frequency intervals of the ion of the run, in frequency units (see also WNUC)

Default: NUK

NUK *93 D, 1, floating point

continuum frequency interval of the ion of the run, in frequency units (see also WNUK)

NVDFE D, 1, integer

dump control for injection function FINJ (fast electrons)

Default: -1

NVF B, 1, integer

number of velocity values (fast electrons)

Default: 30

NVH *90 B, 1, integer

length of HNDV

Default: 38

NVOIT *50, *84 D, 1, integer

Voigt profiles subroutine execution statistics printout switch

Default: 1

NVX *29, *82, *108 B, 1, integer

number of VX tables

NWS B, 1, integer

length of DELWAVE

NWV B, 1, integer

length of WAVES

NXF B, 1, integer

maximum number of integrand values for injection functions (fast electrons)

Default: 1000

NZDFE D, 1, integer

dump control (fast electrons)

Default: -1

NZE B, 1, integer

length of ZECL

NZ2

B, 1, integer

number of levels for which Helium-II populations are specified

N₁MET

D, 1, integer

"Special N1" (diffusion calculation), method selector

Default: 2

N₁NUP

D, 1, integer

populations-of-the-run update switch, "Special N1" calculation

Default: 1

 \mathbf{OK}

[@Z]

 $H, 2^*, 2$, floating point

singly-ionized Oxygen number density

Default: computed in LTE *18

 \mathbf{OLL}

D, 4, floating point

line opacity multiplier

Default: 1.0

OMIT

[variable]

B, 2, alphanumeric

disable program options (see Section 6 for further details)

 \mathbf{OML} *16 D, 4, floating point

line-background opacity multiplier

Default: 1.0

on

[@Z]

H, 3*,3, floating point

Oxygen-I level populations

Default: ON_{ij} computed in LTE, for all levels j such that j > NLO

OPF

D, 1, floating point

incident radiation extinction factor

Default: 1.0

OUTPUT *23

B, 1, alphanumeric

'general printout' file scope switch

Default: "MERGE"

O2K

[@Z]

 $H, 2^*, 2$, floating point

doubly-ionized Oxygen number density

Default: computed in LTE

O2N[@Z]H, 3*,3, floating point Oxygen-II level populations Default: O2N_{ij} computed in LTE, for all levels j such that j > NO2O3K[@Z] $H, 2^*, 2$, floating point triply-ionized Oxygen number density Default: computed in LTE O3N[@Z]H, 3*,3, floating point Oxygen-I level populations Default: O3N_{ij} computed in LTE, for all levels j such that j > NO3 \mathbf{P} *93 [NSL] D, 2, floating point statistical weight **PALBET** [@Z]D, 2*,2, floating point Helium diffusion parameter **PART** *61 D, 1, floating point partition function for the ion of the run **PARTLIM** D, 1, floating point partition functions component limit (for ions in table ELE) Default: 3.0**PBETAL** D, 2*,2, floating point [@Z]Helium diffusion parameter D, 2*,2, floating point **PBETGM** [@Z]Helium diffusion parameter PCE D, 5, floating point FCE adjustment factors **PGMBET** [@Z]D, 2*,2, floating point Helium diffusion parameter **PMSK** D, 1, floating point multiplier of default Stark half-width

scattering albedo parameter for Background Line Opacities (see Section 9)

POPION *28
'population update' ion data

Default: 1.0

PNH

Η

D, 1, floating point

POPRCP *28

Η

'population update' ion data

POPUP *8

D, 1, alphanumeric

populations data update switch

POPXLM *28

Η

'population update' ion data

PRDCV *42

D, 1, floating point

PRD-iterations convergence criterion

Default: 0.1

PROF *1

D, 4, integer

emergent line profiles calculations switch

PROGLI *98

D, 4, floating point

profile graphs control parameter

 \mathbf{PW}

D, 1, floating point

exponent for Stark broadening term

Default: 1.0

PZERO *103

D, 1, floating point

Z-from-TAUKIN recalculation parameter

QIN

[@Z]

D, 2*,2, floating point

K-shell ionization calculation data

 \mathbf{QNL}

[NSL]

D, 2, integer

number of " $n\ell$ " electrons

Default: all = 1

QTAIL

[MQT]

D, 2, floating point

Lyman EP-1 Q-smoothing tail

Default: (0.5, 0.1, 0.01)

RABD

*120

[@Z]

 $D, 2^*, 2,$ floating point

depth variation of abundance ratio

Default: antilog(RABDL_i), or RABD_i = 1.0, for all i

[@Z]

RABDL

*120

D, 2*,2, floating point

depth variation of log of abundance ratio

RCCFE

D, 1, floating point

accuracy criterion for injection function integrations (fast electrons) Default: 0.1

RCHX *95, *97

D, 4, floating point

upper-level charge-exchange parameter

RCOMIN

D, 1, floating point

CO abundance lower limit

Default: 10^{-10}

REFLM *103

D, 1, floating point

wavelength to which TAUKIN values correspond

Default: 911.1236

RFAC

D, 1, floating point

reduction factor for all collision rates

Default: 1.0

RFHEAB

D, 1, floating point

Helium abundance coefficient reduction factor for RHEAB calculation

Default: 1.0

RFMAS *103

D, 1, floating point

reference mass

RHEAB

[@Z]

D, 2*,2, floating point

depth dependence of total Helium abundance

Default: RHEAB_i = 1.0, for all i

RHO

[@Z]

D, 5*,5, floating point

net radiative bracket

RHOPT *4, *19

D, 1, alphanumeric

a RHO selection parameter

Default: "RHOJ"

RHOWT

*13, *131

[@Z]

D, 5*,5, floating point

RHO weights

 $\mathbf{R}\mathbf{H}\mathbf{W}\mathbf{T}$

*13, *131

[@Z]

D, 5*,5, floating point

RHO weights Default: 1.0

 $\mathbf{R}\mathbf{K}$

*45

[@Z]

D, 3*,3, floating point

photoionization rate (for level KOLEV)

RKC [LR] D, 3, floating point additional photoionization parameter **RKMULT** [NSL] D, 2, floating point RK enhancement factor $\mathbf{R}\mathbf{K}\mathbf{W}$ *13, *131 [@Z]D, 3*, floating point RK-KOLEV weights RKWT*13, *131 [@Z]D, 3*, floating point RK-KOLEV weights Default: 1.0 *39, *45 \mathbf{RL} [@Z]D, 3*, 3, floating point photorecombination rate (for level KOLEV) **RQCP** *22, *93 [MR+1]D, 3, floating point = RRCP**RRCP** *22, *56 [MR]D, 3, floating point ratios of photoionization cross-sections Default: computed for Level 1 for some non-Hydrogen runs **RUNTOPOP *8** [8]B, 2, integer ion-of-the-run vs. built-in population-ion-model level correspondences, for 'population update' runs RZMD, 2*,2, floating point [@Z]metal electrons multiplier Default: $RZM_i = 1.0$, for all i R1ND, 1, floating point distance from illuminating source SCH *47 D, 4, integer partial redistribution calculation selector for Line Source Function calculations SCOW*134 [NSW] D, 2, floating point selected Continuum output wavelengths **SCTA** *55 D, 1, floating point shock temperature amplitude **SCTS** *55 D, 1, floating point shock temperature scale height

SCVA *55

F, 1, floating point

shock velocity amplitude

SCVB *55

F, 1, floating point

shock velocity parameter

SCVS *55

F, 1, floating point

shock velocity scale height

SGRAF *98

D, 4, integer

profile graphs control parameter

SHCOC

D, 1, floating point

CO chromospheric scale height

Default: 100.

SHCOP

D, 1, floating point

CO photospheric scale height

Default: 400.

 \mathbf{SIK}

[@Z]

 $H, 2^*, 2$, floating point

singly-ionized Silicon number density

Default: computed in LTE

SIN

[@Z]

H, 3*,3, floating point

Silicon-I level populations

Default: SIN_{ij} computed in LTE, for all levels j such that j > NLS

 \mathbf{SK}

[@Z]

 $H, 2^*, 2$, floating point

singly-ionized Sulphur number density

Default: computed in LTE

SMATC

D, 1, floating point

matrix samples output selection criterion

SMOOTH *49

 \mathbf{D}

RHO smoothing control parameters

Default: see Note *49

 \mathbf{SMP}

D, 1, floating point

RHO weights adjustment parameter

Default: 0.3

SN [@Z] H, 3*,3, floating point

Sulphur-I level populations

Default: SIN_{ij} computed in LTE, for all levels j such that j > NLU

SN1CC D, 1, floating point

convergence criterion for "Special N1" calculation (diffusion)

Default: 10^{-8}

SOBDMN *51 D, 1, floating point

Sobolev escape probability calculation integration control parameter

Default: 0.001

SOBDMX *51 D, 1, floating point

Sobolev escape probability calculation integration control parameter

 $Default:\ 0.01$

SOBFEQ *51 D, 1, floating point

Sobolev escape probability calculation integration control parameter

Default: 0.001

SOBOLEV *51, *82 [2] D, 5, integer

Sobolev solution limit indices

Default: (1, 1)

SRCO D, 1, floating point

scattering ratio for CO lines

Default: 0.1

STARKI D, 4, floating point

value of NE-index for Stark splitting of Hydrogen lines

Default: ISTARK

TAUCL *42 D, 1, floating point

DR parameter, PRD transitions

Default: 10^4

TAUKIN *103 [N] $D, 2^*,2$, floating point

input TAUK values

TB [@Z] D, $2^*,2$, floating point

blanketing temperature

Default: TE

TBAR

D, 1, floating point

change-over TAU-value for weight matrix calculation

Default: 0.5

TDST

[@Z]

D, 2*,2, floating point

Type-2 dust opacity calculation temperature values

TDUST

D, 1, floating point

Type-1 dust temperature

*93

Default: 200.0

TE

[@Z]

D, 2*,2, floating point

kinetic temperature

 \mathbf{TER}

[NTE]

D, 2, floating point

temperature table for input values of CE and CI

Default: 4000.0

TEX

[@Z]

 $D, 2^*, 2$, floating point

excitation temperature

Default: TE

TGLYM *67

D, 1, floating point

Lyman change-over TAU parameter

Default: 100.0

TKR

[LR]

D, 3, floating point

wavelengths for which additional photoionization values are specified

TLARGE

D, 1, floating point

 ${
m TNP}\mbox{-}{
m from}\mbox{-}{
m TNU}$ selection parameter

Default: 200.0

 \mathbf{TLIMG}

*34

D, 1, floating point

absorption contributors graph axis limit

Default: $0.0 [= \log(1.0)]$

TLTR

D, 1, floating point

limiting multiplier for TDST recalculation

Default: 1.3

TML

D, 1, floating point

large-TAU cut-off for intensity integrals

Default: 30.0

 \mathbf{TMS}

D, 1, floating point

small-TAU change-over for RT weight matrices

Default: 5.0

TOPE *8-

D, 1, integer

Continuum Plots save switch

TR

= "TRN 1"

TRFLI

D, 1, floating point

limit-interval for TR-effective calculation

Default: 1.1

TRN

*9, *102

[@Z]

D, 3*,3, floating point

radiation temperature (for a given level of the ion of the run)

Default: $TRN_{i,1} = TE_i$, $TRN_{i,j} = TRN_{i,1}$, all i, all j > 1

TS

[M]

D, 2, floating point

standard TAU table

 $Default: (0.0,\, 0.0001,\, 0.0002,\, 0.0003,\, 0.0006,\, 0.001,\, 0.002,\, 0.003,\, 0.006,\, 0.01,\\ 0.02,\, 0.03,\, 0.06,\, 0.1,\, 0.2,\, 0.3,\, 0.6,\, 1.0,\, 2.0,\, 3.0,\, 5.0,\, 7.0,\, 10.0,\, 15.0,\, 20.0,\, 30.0,\\ 50.0,\, 75.0,\, 100.0,\, 150.0,\, 200.0,\, 300.0,\, 500.0)$

TSM

D, 1, floating point

change-over TAU for mean intensity and emergent intensity calculations $Default: 10^{-4}$

TSMALL

D, 1, floating point

TNP-from-TNU selection parameter

Default: 10^{-10}

TX

D, 1, floating point

brightness temperature of illuminating source

 \mathbf{USE}

*44

B,D,F,H, 1, alphanumeric

input file designation Default: "INPUT"

17

*69, *82, *90

[@Z]

D, 2*,2, floating point

broadening velocity

VM

*82

[@Z]

D, 2*,2, floating point

mass motion velocity

VMNFE

D, 1, floating point

minimum velocity (fast electrons)

Default: 0.003

VNH *90

[NVH]

D, 1, floating point

standard table of V (as a function of HNDV) for the quiet sun Default: (15.18, 13.68, 11.92, 10.75, 9.68, 8.44, 7.81, 7.52, 6.95, 6.28, 5.52, 4.60,

3.59, 2.98, 2.20, 2.00, 1.54, 1.38, 1.18, 1.00, 0.86, 0.80, 0.68, 0.65, 0.55, 0.52,

0.63, 0.90, 1.10, 1.30, 1.46, 1.56, 1.64, 1.71, 1.76, 1.80, 1.82, 1.83)

VOITC *50

D, 1, floating point

Voigt function calculation cut-off

Default: 10^{-6}

VR *69, *82

69, *82 [@Z]

D, 2*,2, floating point

broadening velocity

 $\overline{\text{VSB}}$

*51, *82

[@Z]

D, 2*,2, floating point

Sobolev velocity Default: VXS or VM

VSMLL *71

D, 1, floating point

replacement value for divisors that equal zero (subroutine ${\tt DIVIDE})$

Default: 10^{-100}

 $\mathbf{V}\mathbf{T}$

*82

[@Z]

[N]

D, 2*, floating point

turbulent pressure velocity

 $\mathbf{V}\mathbf{X}$

*57, *82

F, 3, floating point

additional expansion velocity for emergent profile calculation

 \mathbf{VXS}

*60, *82

[@Z]

D, 2*,2, floating point

basic expansion velocity for Line Source Function calculations $% \left(1\right) =\left(1\right) \left(1$

Default: VM

WAVEMN *110

D, 1, floating point

automatic additional wavelengths limit

WAVEMX *110

D, 1, floating point

automatic additional wavelengths limit

WAVES *27

[NWV]

D, 2, floating point

additional wavelengths for continuum calculations

WBD *26

D, 1, floating point

weight for departure coefficient updating

Default: WPOP

WBDIR

D, 1, floating point

weight for results of "direct" departure coefficient calculation

Default: 1.0

WEIGHT

D, 6, floating point

weight for Statistical Equilibrium equations calculation

WEP *104

D, 1, floating point

Lyman EP-1 weighting parameter

Default: 1.0

WFB

F, 1, floating point

weight for flow broadening component velocities

Default: 0.6

WMN *131

D, 1, floating point

RHO weight adjustment parameter

Default: 0.3

WMX *131

D, 1, floating point

RHO weight adjustment parameter

Default: 0.9

WNJUNK *87

D, 1, floating point

WN-matrix "cleanup" parameter

WNU

[NSL]

D, 2, floating point

= NU, but in wavenumbers

WNUC

[NSL]

D, 2, floating point

= NUC, but in wavenumbers

WNUK

D, 1, floating point

= NUK, but in wavenumbers

WORLDLY*132

B, 1, alphanumeric

storage management dump control switch

WPOP

D, 1, floating point

weight for number densities updating

Default: WBD, or 1.0

WPRESS

D, 1, floating point

weight for adjusting NH to achieve constant pressure

Default: 1.0

WR *13

D, 4, floating point

RHO weighting parameter

Default: 1.0

 \mathbf{WRAT}

*22, *56 [MR]

D, 3, floating point

wavelengths for rates integrations

WRATMN *135

D, 1, floating point

standard rates integrations wavelengths table limit

Default: 100.

WRATMX *135

D, 1, floating point

standard rates integrations wavelengths table limit

 $Default:\ 20000.$

WRMN *131

D, 1, floating point

RHO weight adjustment parameter

Default: 0.1

WRMX *131

D, 1, floating point

RHO weight adjustment parameter

Default: 0.7

WSM

D, 1, floating point

Lyman RK-KOLEV smoothing parameter

WSN1D

D, 1, floating point

weight for Special N1 and Special NK, Diffusion

Default: 1.0

WTD

D, 1, floating point

weight for TDST recalculation

Default: 1.0

 $\mathbf{W}\mathbf{Z}$

D, 1, floating point

Z-from-TAUKIN weight

Default: 0.5

 $\mathbf{W}\mathbf{Z}\mathbf{M}$

*103

D, 1, floating point

Z weighting parameter

Default: 0.8

XC *42

DR parameter, PRD transitions

Default: 2.0

XCL *42 D, 1, floating point

 ${\rm DR}$ parameter, PRD transitions

Default: 3.5

XCOL [NCL] D, 2, floating point

table of wavelengths for each CO line, in doppler widths, for the CO-lines opacity

Default: (0.0, 0.5, 1.0, 1.5, 2.0)

 \mathbf{XCOMX}

D, 1, floating point

D, 4, floating point

width limit for each CO line, in Å, for the CO-lines opacity

Default: 3.0

XDR *42 [NDR] D, 2, floating point

DR parameter, PRD transitions

Default: (5.5, 6.0, 7.0, 8.0, 10.0, 12.0, 15.0)

XI D, 2, floating point

= XISYM

XIBLU *66 [KB] D, 2, floating point

Line Transitions frequency table, for blue side

Default: XISYM

XIBLUT *66 [KBT] D, 5, floating point

Line Transition frequency table, for blue side

Default: XISYMT

XINK [INK] D, 2, floating point

table of frequencies for which incident radiation is specified

Default: (5.948, 5.949, 7.48, 7.51, 13.16, 13.17)

XIRED *66 [KR] D, 2, floating point

Line Transitions frequency table, for red side

Default: XISYM

XIREDT *66 [KRT] D, 5, floating point

Line Transition frequency table, for red side

Default: XISYMT

XISYM *66 [KS] D, 2, floating point Line Transitions frequency table, for half of a symmetric profile

Default: (0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.1, 1.3, 1.5, 1.8, 2.1, 2.4,

2.8, 3.4, 3.9, 4.5, 6.0, 8.0, 15.0, 50.0)

XISYMT *66 [KST] D, 5, floating point

Line Transition frequency table, for half of a symmetric profile

Default: XISYM

XJFE D, 1, floating point

electron flux (fast electrons)

Default: 2.0×10^{-10}

XK *123 [KK] D, 2, floating point

Level- \mathcal{N} -to-Continuum calculation (Lyman) frequency table

Default: RRNU(KOLEV), where RRNU is computed from WRAT

XMU [LG] D, 1, floating point

MU table for GR-method weight matrix calculation

Default: (1.0, 0.8, 0.6, 0.5, 0.4, 0.3, 0.2, 0.1)

XP *42 D, 4, floating point

DR parameter, PRD transitions

Default: 2.0

XR *42 D, 4, floating point

DR parameter, PRD transitions

Default: -1.0

XQMAX D, 1, floating point

parameter for injection function integrations (fast electrons)

Default: 200.0

XRKH *95, *96 [@Z] D, 5,5*, floating point

upper-level charge-exchange data for Hydrogen

XRLH *95, *96 [@Z] D, 5,5*, floating point

upper-level charge-exchange data for Hydrogen

Y D, 1, floating point

damping parameter for frequency integrations weights (see Section 12)

Default: 0.5

YCOL

D, 1, floating point

weight matrix method control parameter for the continuum calculations required for the CO-lines opacity (see Section 12)

Default: -1.0

YCONT

D, 4, floating point

weight matrix method parameter, for Continuum calculations (see Section 12) Default: -1.0

YCR

[NCR]

D, 2, floating point

weight matrix method control parameter, for incident coronal radiation (see Section 12)

Default: -1.0

YFLUX

D, 1, floating point

damping parameter for emergent continuum flux

Default: 0.5

YH

D, 1, floating point

Helium-to-Hydrogen ratio

Default: Helium abundance (from ELE table)

YHM

[MHM]

D, 2, floating point

weight matrix method parameter, for H-minus calculation (see Section 12)

Default: -1.0

YK

[NSL]

D, 2, floating point

Hydrogen recombination parameter

YKR

[LR]

D, 3, floating point

weight matrix method parameter, for additional photoionization (see

Section 12)
Default: -1.0

 \mathbf{YL}

D, 1, floating point

weight matrix parameter, for Level- \mathcal{N} -to-Continuum source function calculation (see Section 12)

Default: -1.0

YLDT

[NDT]

D, 2, floating point

weight matrix method parameter, for Type-2 dust opacity calculation (see Section 12)

Default: -1.0

YLINE

D, 4, floating point

weight matrix method parameter, for Line Source Function (see Section 12)

Default: -1.0

YLYM

[KK]

D, 2, floating point

weight matrix parameter, for Level- \mathcal{N} -to-Continuum continuum source function calculations (see Section 12)

Default: -1.0

YPRE

D, 1, floating point

damping parameter for standard weight matrix (see Section 12)

YRATE *22

[MR+1]

D, 3, floating point

weight matrix method parameter, for rates calculations (see Section 12)

Default: -1.0

YRATS

D, 1, floating point

damping parameter for standard rates integrations wavelengths (see Section 12) Default: -1.0

YWAVE

[NWV]

D, 2, floating point

weight matrix method parameter, for additional calculations (see Section 12) Default: -1.0

 ${f Z}$

[N]

D, 2, floating point

grid of geometrical depths (main Z-table of the run)

ZALBK

[NKA]

D, 1, floating point

scattering albedo parameter for Background Line Opacities (see Section 9) Default: (Z_1, Z_N)

ZAUX

[LZA]

D,F,H, 3, floating point

auxiliary Z-table

ZECL

[NZE]

F, 2, floating point

selected Z-values for eclipse continuum calculation

ZGM

*138

[NGM]

D, 2, floating point

Z-table for DGMZ

 $Default:\ (-2000,\ -1900,\ -1800,\ -1700,\ -1600,\ -1500,\ -1400,\ -1300,\ -1200,\ -11000,\ -11000,\ -11000,\ -11000,\ -11000,\ -11000,\ -11000,\ -11000,\ -11000,\ -11000,\ -11000,\ -11000,\ -1100$

-1000, -900, -800, -700, -600, -500, -400, -300, -200, -100, -50, 0, 50

ZMASS

*103

[N]

D, 2, floating point

gas column mass

Notes

\mathbf{ZME}	[@Z]	$D, 2^*, 2$, floating point			
non-H electr	on ratio				
ZNDW *	86	D, 1, floating point			
Z-value for optional NDW-default calculation					
ZRCO		D, 1, floating point			
CO reference	e height				
Default: -50).				
ZXMIN		D, 1, floating point			
diffusion cale Default: 0.1	culation parameter	for ZION			
		*1			
		e obtained from the element tables (see Section recognizable chemical element symbol.			
		*2			
tween levels. Trelationships a the transitions "INPAIR (51	These pairs may be re preserved. For exto be specified, the 5 2 5 3 2 1 5 4)	gers u, ℓ $(u > \ell)$, which specify transitions belisted in any order, as long as the proper pair xample, if $(2,1)$, $(5,1)$, $(5,2)$, $(5,3)$ and $(5,4)$ are en the input statement might be: default for $(\mathbf{MS}, \mathbf{NS})$.			
		*3			
NAME must blanks.	not have more than	n 8 characters, and may not contain imbedded			
		*4			
	ifies the RHO optic, "RHOJ", or "RHOW"	on, and may only take on one of the following.".			
		*5			
		5.63			

Notes

When $\mathbf{JSTCN} > 0$, then PANDORA will do only background continuum calculations and emergent continuous spectrum calculations (depending on the specific options settings); this is called: a 'continuum-only' run.

The value of **JSTCN** controls which wavelengths will be included in the computations of this run.

JSTCN should be set equal to $KAW + 2 \times KOM + 4 \times KCO$, where KAW = 1 means: use 'additional wavelengths' (*i.e.* **WAVES**), KAW = 0 means: do not;

KOM=1 means: use Composite Lines Opacity wavelengths; KOM=0 means: do not:

KCO=1 means: use CO-lines opacity wavelengths; KCO=0 means: do not.

JSTCN and **JSTIN** may not both be > 0 for the same run. **JSTCN** and **NOION** may not both be > 0 for the same run.

*7

Any of the absorbers/emitters automatically included in the background opacity/emission calculations can be turned off by mentioning them in **NABS** statement(s). For this purpose, the absorbers/emitters are specified using the "index" by which they are identified in the left margin of the 'List of potential contributors to "continuum" or "background" absorption and emission.' which is part of the ATMOSPHERE printout at the beginning of the regular output from a run. For example, the following statement will cause the H Ly alpha Abs and the ${\rm H}_2^+$ opacity to be turned off: "NABS (11 9) ".

____*8

The **POPUP** switch is used to tell PANDORA whether this is a run in which the number densities computed at the end of every overall iteration must also be copied into the appropriate 'non-LTE populations' tables set aside for certain ions. The **POPUP** switch may only take on the values:

- 1) HYDROGEN, 2) CARBON, 3) SILICON, 4) HELIUM, 5) HELIUM2, 6) ALUMINUM,
- 7) MAGNESIUM, 8) IRON, 9) SODIUM, 10) CALCIUM, 11) OXYGEN, or 12) SULFUR; i.e.: "POPUP (CARBON)". A run that is not concerned with one of these should not have **POPUP** among its input statements. Moreover, runs with 'population ions' can be made without 'population updating' simply by not specifying **POPUP**.

In a 'population update' run, the values of the integer array **RUNTOPOP** specify the correspondence between the levels of the ion-of-the-run and the levels of the built-in population-ion-model. (The description of the built-in population-ion-model is printed as part of the first printout of the corresponding 'population ion' number densities and departure coefficients; note that specific options must be turned on for this, e.g. CARPRNT.) **RUNTOPUP**_i = j means that level j of the ion-of-the-run corresponds to level i of the built-in population ion model. If k is the lowest level of the built-in population-ion-model to which no level of the ion-of-the-run corresponds, then **RUNTOPOP**_{ℓ} = $0, k < \ell \le$ LIMDAT, is re-

Notes

quired. (Note that the default values are $\mathbf{RUNTOPOP}_i = 0, 1 \le i \le \text{LIMDAT.}$)

Input tables of **TRN** may be specified in abbreviated forms: either

- (a) **TR** (**I** $k x_k x_{k+1} x_{k+2} \dots x_m$),
- *i.e.* "TR (I 12 3600. 3700. 3750. 3800.) ", or
- (b) **TRN** j (I $k x_k x_{k+1} x_{k+2} \dots x_m$),
- i.e. "TRN 2 (I 12 3600. 3700. 3750. 3800.) "

In both these forms, several elements of an array, (beginning, here, with the 12. one), are set equal to the floating point numbers given.

Case (a) tells PANDORA to do the following (after **GO** has been read):

to set $TR_i = x_k$, $1 \le i \le k$, to leave $TR_i = x_i$, $k+1 \le i \le m$, as specified in the input statement, and to set $TR_i = TE_i$, $m+1 \le i \le N$.

Case (b) is equivalent to (a) when j = 1; otherwise, it specifies the j'th TRN table.

The rationale for this procedure derives from the structure of a typical TRN table, as follows: the initial elements of the table are equal to some constant value, then there is a variation extending over several values, until, finally, the values of TRN are equal to the values of TE at the corresponding interior depths. Thus the abbreviated input form specifies the index of the last of the constant values, that constant itself, and then the set of values which differ from TE.

Note: This abbreviated input form may only be used when the TRN table is specified with respect to the main depth table of the run; it may not be used when the TRN table is specified with respect to a **ZAUX** (auxiliary depth) table.



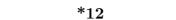
After **GO** has been read, PANDORA examines the values of $\mathbf{KPC}^{u,\ell}$ for every radiative transition (u,ℓ) . If all the values of $\mathbf{KPC}^{u,\ell}$ are =0 (normal default), then it sets $\mathbf{KPC}^{u,\ell} = \mathbf{KPCR}_i^{u,\ell} \times \mathbf{KPC}_i^{MS,NS}$, $1 \leq i \leq N$, where $(\mathbf{MS,NS})$ is the reference transition. After this process is finished, $\mathbf{KPC}_i^{u,\ell} = 0$ can only come about because $\mathbf{KPC}_i^{MS,NS} = 0$ (if there were no explicit input values $\neq 0$), or, for $i,j \neq MS,NS$, because either $\mathbf{KPC}_i^{MS,NS} = 0$, or because $\mathbf{KPCR}^{u,\ell} = 0$. Those transitions for which nonzero input values of continuous opacity were obtained by this procedure, will retain those values for the first overall iteration. For those transitions for which no nonzero values of continuous opacity could be obtained, PANDORA will compute them. (Normally, PANDORA computes opac-

Notes

ity values for every radiative transition in every overall iteration.)



When **NOION** = 1 (*i.e.* if the option DOION is off), then no ion-related calculations will be done. **JSTCN** and **NOION** may not both be > 0 for the same run. See also Note 84.



KONFORM controls the format of the printing of detailed contributions to the background opacity and the absorption source function (*i.e.* the detailed printouts of 'absorbers' and 'emitters').

KONFORM = 1 means: print their absolute values, using Fortran E-format conversion;

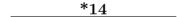
 $\mathbf{KONFORM} = 2$ means: print them as fractions of the total, using Fortran F-format conversion.



 $X_i^{s+1}=(1-W_i)\times X_i^{new}+W_i\times X_i^s,\ 1\leq i\leq N,$ where X stands for RHO; or $X_i^{s+1}=[(X_i^{new})^{(1-W_i)}]\times [(X_i^s)^{W_i}],\ 1\leq i\leq N,$ where X stands for RK-KOLEV (Lyman).

The values of X_i for iteration s + 1 will be obtained, in the manner shown, from the values of X_i used during iteration s and the *new* values of X_i calculated at the end of iteration s. The values of W_i (which may all be equal to some constant) are obtained from WRHO, **WR**, **WRLY**, and **WTW**_j as described in the writeup [7/3/72], (WRHO is continually recomputed as the calculation proceeds), or from **RHOWT**_i or **RKW**_i, respectively, as described in the writeup [74 Oct 23].

Important: Note 13 is now obsolete; see Note 131.



BLCSW^{u,ℓ} tells which components of DP to use for the Line Source Function calculation for transitions (u,ℓ) . Its input value should be established according to $BLCSW = SRD + 2 \times SVW + 4 \times SSK + 8 \times SRS + 16 \times SIC$. Here SRD = 1 if radiative broadening should be used, = 0 if not; SVW, SSK, SRS, and SIC similarly control van der Waals, Stark, resonance, and ion colli-

Notes

sion broadening, respectively. (*Note*: ion collision broadening is used for Hydrogen transitions above level 5 only.) In the ATOM printout, the values of SRD, SVW, SSK, SRS, and SIC are shown as a string of digits (*i.e.* as a binary number) in order from right to left.

70.7	r		
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*15___

 $X_i^{s+1} = \mathbf{HSEC} \times X_i^{new} + (1 - \mathbf{HSEC}) \times X_i^s$, $1 \le i \le N$, where X stands for either NE or NH.

When the option HSE is on, the X_i for overall iteration s+1 will be obtained, in the manner shown, from the X_i used during iteration s and the new values of X_i calculated at the end of overall iteration s.

*16

LSFBOC^{u,ℓ} and **OML**^{u,ℓ} control whether any of the 'Line Background' opacities (see Section 9) are allowed as potential contributors to the total background (or "continuum") opacity at wavelength(s) pertaining to transition (u,ℓ) . If **LSFBOC** = 0 then all these 'Line Background' opacities will be suppressed; if **LSFBOC** = 1 then the appropriate one, multiplied by **OML**, will be used. By default, all **LSFBOC** = 0 and all **OML** = 1.

*17

If the value of $\mathbf{PROF}^{u,\ell} = 0$, then no emergent intensity nor flux profiles will be computed for transition (u,ℓ) . If any value of $\mathbf{PROF}^{u,\ell}$ is > 0, then $\mathbf{LF} > 0$ is required. (A flux profile will not be computed if $\mathbf{LF} = 1$; see also Note 24.) Line profile intensity and flux values are computed for tables of $\Delta\lambda$ values which are derived for frequency (XI) values; see Section 18, Frequency Tables, for additional information.

*18

 $\mathbf{OLL}^{u,\ell}$ multiplies the values of $\mathrm{GTN}^{u,\ell}$. $(\mathrm{GTN}_i^{u,\ell}$ multiplies the line absorption profile $\phi_i^{u,\ell}$ in the equation for the monochromatic total opacity at the various frequency points of transition (u,ℓ) .)

The RHO selection parameters:

RHOPT -

Values of RHO_i^{u,\ell} are calculated three different ways:

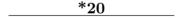
- as part of the Line Source Function calculation (RHOS);
- from S, S*, RHOS and CWJ (RHOJ); and
- by combining RHOS and RHOJ (RHOW). (See also the explanation printed with the RHO AND RBD section of the normal output.) The value of **RHOPT** tells which of these is to be chosen as the final $\mathrm{RHO}_i^{u,\ell}$, to be used in subsequent iterations.

NWRHO, WMN and WMX -

At the end of every iteration s, the current values of CHECK_i^j are compared to the ones from the previous iteration s-1, for $1 \leq i \leq N$ and $3 \leq j \leq NL$. A counter K is initialized to zero. Whenever: $CC = |\mathrm{CHECK}_i^j - 1| > 0.002$ and $OC = |\mathrm{CHECK}_{i-1}^j - 1| > 0.002$ and $OC/CC \leq 0$, then K will be increased by 1. All values of CHECK_i^j will be tested to determine K. If $K > \mathbf{NWRHO}$ then, if WRHO $< \mathbf{WMX}$, WRHO will be increased by 0.1. If $K \leq \mathbf{NWRHO}$, then, if WRHO $> \mathbf{WMN}$, WRHO will be decreased by 0.1. (If WRHO $< \mathbf{WMN}$ or WRHO $\geq \mathbf{WMX}$, then WRHO will remain unchanged.) This new value of WRHO will then be used in the next iteration, as specified in Note 13.

CHOP, CWR, ILI, NIL, CHLIM, and option RHOWOPT –

The significance of these parameters is explained in the text accompanying the RHO AND RBD printout (when option RHBPRNT is on). (If such a printout happens not to be immediately at hand, it won't hurt to set up a one-iteration run using the automatic defaults.)



If the option ISCRS is on (i.e. if **ISCRS** = 0), then 'scratch I/O' will be done 'in memory' to the extent possible (i.e. depending on the amount of memory reserved for the MEMOIR routines). When memory is full, scratch I/O will overflow to the temporary scratch disk file (logical unit 1, see Section 7). (For some runs, scratch I/O can be accommodated entirely in memory, and no temporary scratch disk file will be required; in other runs, the size of the temporary scratch disk file will be reduced.) This 'in-memory scratch I/O mode' may be particularly benefi-

Notes

cial when PANDORA is run on systems with real memory so large that no hard page faults occur.

If the option ISCRS is off (*i.e.* if ISCRS = 1), then 'in-memory scratch I/O' is not allowed; all scratch I/O will use the temporary scratch disk file. See also Note 84.

METEP specifies the method for computing EP1 and EP2 in the Level- \mathcal{N} -to-Continuum (Lyman) transfer calculation.

METEP=0 means: NOVA-like method (writeup dated 06/04/68);

METEP=1 means: COMPLEX/UPPER-like method (writeup dated 04/12/90);

METEP=2 means: COMPLEX/LOWER-like method (writeup dated 06/22/76);

METEP=3 means: CHAIN-like method (writeup dated 11/24/76).

(The values of **METEP** are analogous to those of **METSE**; see Note 35.)



For a particular energy level j, \mathbf{WRAT}^j specifies a set of wavelength values, \mathbf{RRCP}^j a tabular function of these wavelength values, and \mathbf{YRATE}^j a set of method control parameters (see Section 12) for Continuum Source Function calculations at these wavelengths. We have \mathbf{WRAT}_m^j , \mathbf{RRCP}_m^j , and \mathbf{YRATE}_m^j , $1 \le m \le \mathbf{MR}^j + 1$. Since the value of \mathbf{WRAT}_1^j is obtained from $(\mathbf{NUC}^j - \mathbf{NU}^j)$, this value need not (actually: cannot) be input; and since \mathbf{RRCP}_1^j usually = 1.0, this value normally need not be input. Thus, for every level for which $\mathbf{MR}^j > 0$, the input must contain specifications of the values of \mathbf{WRAT}_m^j and \mathbf{RRCP}_m^j , $2 \le m \le \mathbf{MR}^j + 1$. On the other hand, all values of \mathbf{YRATE}_m^j can (actually: must) be input. Thus, the input statements for \mathbf{WRAT} and \mathbf{RRCP} are different from those for \mathbf{YRATE} . For example, if we have:

m	WRAT_m^2	RRCP_m^2	$YRATE_m^2$
1	(3612.0)	(1.0)	-1.0
2	3575.0	0.99	1.0
3	3540.0	0.97	0.9

the input statements might be:

"WRAT 2 ($3575.\ 3540.$) ",

"RRCP 2 (0.99, 0.97)",

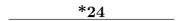
"YRATE 2 ($-1.0 \ 1.0 \ 0.9$) ".

However, there are infrequent occasions when \mathbf{RRCP}_1^j should not = 1.0. In such a case, such a value can be input by referring to that array under another name, namely \mathbf{RQCP} , for which the first value can (actually: must) be input (as with \mathbf{YRATE}). Thus if, in the above example, $\mathbf{RRCP}_1^2 = 1.2$ is wanted, the input statements might be:

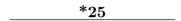
Notes

```
"WRAT 2 ( 3575. 3540. ) ",
"RQCP 2 ( 1.2 .99, .97 ) ",
"YRATE 2 ( -1.0 1.0 0.9 ) ".
```

OUTPUT can take on the values: MERGE, SPLIT. See Section 7, the part headed "**Output files**".



The MU table (for intensity) must be a proper subset of the MUF table (for flux); thus it is required that $\mathbf{L} \leq \mathbf{LF}$ and that, for every m, $\mathbf{MU}_m = \mathbf{MUF}_n$, some n. Both MU and MUF must be in order of decreasing values.

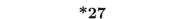


CE is used in the calculations of the collisional transition rates, which normally depend on NE. However, if some input value of \mathbf{CE}^j is negative, then its absolute value will be used, and the corresponding rate calculation for level j will use NH in place of NE.



WPOP is used for the iterative calculation of number densities, as follows: $P^{i+1} = 10^{[W \times \log(P^{new}) + (1-W) \times \log(P^i)]}$, where W stands for **WPOP** and P stands for the level populations or the ionized number density computed at the end of an overall iteration. When the POPUP switch is on, the values of P^{i+1} for overall iteration i+1 will be obtained, in the manner shown, from the P^i available at the start of iteration i and the P^{new} computed during iteration i.

WBD is used similarly for departure coefficients.



Any values of \mathbf{WAVES}_k may be < 0.0, and only $|\mathbf{WAVES}_k|$ will be used, both for the 'additional' background continuum calculations and the emergent continuous spectrum calculations. Moreover, when $\mathbf{WAVES}_k < 0.0$, then the Continuum Eclipse Intensities for $|\mathbf{WAVES}_k|$ will also be computed (provided the option ECLIPSE is on).

These input statements are not intended for general use. They provide emergency means for changing the built-in contents of the population-ion-model data tables. (These data are printed the first time that the values of number density and departure coefficient for the 'population update ion' are printed.) The preferred way to change these data is for me to change the program.

The statements have the following forms:

POPION k j (V),

where k is the 'population update ion' number (as in Note 8); V is a simple array specifying all or some of the elements of data table j; and j designates one of the population-ion-model data tables, as follows: j=1 for XLMTHR, threshhold wavelength (floating point), j=2 for CCPLEV, coefficient CCP (floating point), j=3 for NPTABL, LM-table length (integer), j=4 for SCPLEV, exponent SCP (floating point), j=5 for PILEVL, statistical weight (floating point), j=6 for LLABEL, term designation (alphanumeric, ≤ 16 characters, embedded blanks not permitted).

POPXLM k ℓ (V),

where k and V are as for **POPION** above, and ℓ designates a level of the population-ion-model. This statement provides values for one of the LM tables.

POPRCP $k ext{ } \ell ext{ } (V),$

which is like **POPXLM**, but provides values for one of the RCP tables.

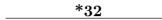
*29

The size limits on NAB, NCL, NMT, NSL, NVX and the total number of Composite Lines Opacity wavelengths (see Section 3, Notes) are for programming convenience; to enlarge them requires changing the source code.

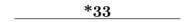
*30

When detailed PRD results are printed, the amount of output can be controlled as follows: data for frequency value XI = 0 are printed, and for every \mathbf{IPRDF}^{th} one from there; data for the first Z value are printed, and for every \mathbf{IPRDD}^{th} one thereafter.

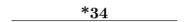
 $\mathbf{A}^{u,\ell}$ can be greater than or equal to zero. If zero, then there is no line transition between levels u and ℓ ; if greater than zero, then there is. The input parameter $\mathbf{KTRANS}^{u,\ell}$ (see Note 33) further specifies the type of transition. Line Source Functions are computed iteratively for radiative transitions, and only once (from the final iterated results) for passive transitions.



The default values of \mathbf{ND}_i^j , $1 \leq i \leq N$, $1 \leq j \leq NL$, are zero, unless this is a run with the POPUP switch on, in which case the input population data, or the LTE population data computed before the first overall iteration, will be used as the defaults for \mathbf{ND}_i^j .



KTRANS^{u,ℓ} is used only when $\mathbf{A}^{u,\ell} > 0$, and describes that transition. It may take on the values: "RADIATIVE", "PASSIVE", "THICK, "THIN", or "2-PHOTON".



The ordinates controlled by the options OPAGRAF and EMIGRAF increase logarithmically (base 10) upwards from **BLIMG** to **TLIMG**.

*35

METSE^{u,ℓ} selects the method of computing the statistical equilibrium equations (*i.e.* the values of PE^{u,ℓ} and FE^{u,ℓ}) for transition (u,ℓ).

 $\mathbf{METSE}^{u,\ell} = 0 \text{ means: NOVA};$

 $\mathbf{METSE}^{u,\ell} = 1 \text{ means: COMPLEX/upper;}$

 $\mathbf{METSE}^{u,\ell} = 2 \text{ means: COMPLEX/lower;}$

 $\mathbf{METSE}^{u,\ell} = 3 \text{ means: CHAIN;}$ $\mathbf{METSE}^{u,\ell} = 4 \text{ means: VAMOS.}$

(Except for VAMOS, the values of **METSE** are analogous to those of **METEP**; see Note 21.) Suggestions for choosing **METSE** are given in the printout section "LINE (U/L)." The default value of **METSE**^{u,ℓ} = **METSEDW** if $\ell = 1$, and =

METSEDG otherwise.

LSFFDB^{u,ℓ} = 0 means: use 'constant background' for the Line Source Function calculation (*i.e.* use line-core background opacity and source function for all line integration frequencies). **LSFFDB**^{u,ℓ} = 1 means: use 'varying background' for the Line Source Function calculation (*i.e.* compute background opacity and source function explicitly at all line integration frequencies, as in a PRD solution). FDB solutions can only be calculated for radiative transitions (*i.e.* **KTRANS**^{u,ℓ} = "RADIATIVE") using the 'full' solution (*i.e.* **LSFTYP**^{u,ℓ} = 0). *Note:* **LSFFDB** is set = 1 automatically when PRD is used (see Note 47).

*37

MODLAB (up to 8 characters long) is an 'atmospheric model name' used for the MODEL DATA section of the normal output, and for the 'performance data archive record' (in file 28; set Section 7).

*38

The PANDORA output includes many printed graphs as functions of depth. The abscissae of the graphs are established under control of input parameters **IZOPT**, **NGRL** and **NGRR**, as follows:

IZOPT = 1 means: the abscissa is depth index i, $LG \le i \le MG$;

IZOPT = 2 means: the abscissa is Z_i , $LG \le i \le MG$;

IZOPT = 3 means: the abscissa is $\log(|Z_i|)$, $LG \leq i \leq MG$, but excluding Z = 0, (moreover, if Z_i changes sign in the range of interest, proceed as if **IZOPT** = 1);

IZOPT = 4 means: the abscissa is $\log(TAU_i)$, $LG \leq i \leq MG$.

Here LG and MG are determined as follows: if $\mathbf{NGRL} \leq 0$, then LG = 1; if

NGRL > 0, then LG = NGRL, but the limit $LG \leq (N-1)$ is enforced; if

NGRR ≤ 0 , then MG = N; if **NGRR** > 0, then MG =**NGRR**, but the limit $MG \leq N$ is enforced.

For some graphs, LG and MG are also controlled by the value of the input parameter **JZOPT**, as follows:

JZOPT = 1 means: use the above procedure controlled by IZOPT;

JZOPT = 0 means: LG is set to the greatest value of i such that $TAU_i \leq 10^{-4}$ (LG > 1 if **IZOPT** = 4), and MG is set to the smallest value of i such that

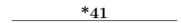
 $TAU_i \ge 10^3$.

Notes	
*39	

The selector **IRLS1** is used to select RLA (**IRLS1** = 1) or RLB (**IRLS1** = 2) for RL^j , j = KOLEV; **IRLSN** is used similarly for RL^j , $j \neq \text{KOLEV}$.



When the option JSTIN is on (i.e. if **JSTIN** > 0), then PANDORA will just read all the input, print it, and stop; this is called an 'input-only' run. See also Note 84.



KHFFS controls whether H free-free is part of the subtotal labelled 'Total Hydrogen' in the cooling rate calculation of a Hydrogen run. **KHFFS** = 1 means that it is, **KHFFS** = 0 means that it is not, part of that subtotal.

KOOLSUM controls which components are added to 'Total Hydrogen' to compute the grand total labelled 'Total Cooling Rate' in a Hydrogen run.

KOOLSUM should be set equal to $K1 + 2 \times K2 + 4 \times K3 + 8 \times K4 + 16 \times K5$, where

K1 = 1 means: add H-minus, K1 = 0 means: do not add H-minus;

K2 = 1 means: add conduction, K2 = 0 means: do not add conduction;

K3 = 1 means: add composite lines, K3 = 0 means: do not add composite lines;

K4 = 1 means: add X-ray, K4 = 0 means: do not add X-ray;

K5 = 1 means: add CO-lines, K5 = 0 means: do not add CO-lines.

*42

See Section 15, Partial Redistribution.

*43

BDOPT specifies the BD option, and may take on one of the following values: "BDJ", "BDR", or "BDQ" (see explanation in RHO AND RBD section of normal printout).

PANDORA can read input from several files. The parameter **USE** specifies which one of these files to use; it can take on any one of the following values: "ATOM", "INPUT", "MODEL", "RESTART" or "GENERAL".

After a **USE** statement has been read, the next input statement(s) will be read from the file designated by the last **USE** statement. Specifications to read from any file may be arbitrarily intermixed among the input statements. The first occurrence of **USE** must be in INPUT (i.e. file 03, see Section 7).

When "USE (GENERAL) " occurs, reading will continue from the file defined by the last preceding ${\bf FILE}$ statement. Thus, at least one ${\bf FILE}$ statement must precede the first occurrence of "USE (GENERAL) ".

The **FILE** statement specifies two parameters, k and f, in that order; for example, "FILE (0 FILESPEC)". f is alphanumeric (\leq 60 characters, embedded blanks not permitted); it is the "complete" file specification of a file to be read, i.e., whatever the operating system requires under the current circumstances to identify the file uniquely, in other words, f is used as the file-name specification with the FILE keyword in a Fortran 'open' statement. k (integer) is a switch: when k=1, a message containing the value of f will be printed on in the 'message printout file' (i.e., file 16, see Section 7) whenever "USE (GENERAL) "occurs; when k=0, no message will be printed.

*45

IRKCOMP is an array of switches specifying for which levels RK should be computed in the Rates calculation of the first iteration. **IRKCOMP**^j = 1 means: compute RK^{j} ; **IRKCOMP**^j = 0 means: do not compute RK^{j} (in this case, presumably, RK^{j} was supplied in the input of the run). **IRLCOMP**, analogously, concerns RL.

*46

If a set of JNU values for partial redistribution (PRD) calculations has been provided in a file on unit 09, then PANDORA can be made to read them by setting JNUNC = 1. These JNU values pertain to particular values of Z and XI; if necessary, these data will be interpolated to the values of Z_i , $1 \le i \le N$, and of XI_k , $1 \le k \le K$, currently in use.

For general background, see Section 15.

 $\mathbf{SCH}^{u,\ell} = 0$ means: do not include partial redistribution (PRD) calculations for line (u,ℓ) ;

 $\mathbf{SCH}^{u,\ell} = 1$ means: do include PRD calculations for line (u,ℓ) .

Note: Only $\mathbf{SCH}^{u,\ell} = 0$ is allowed when $\mathbf{DIRECT}^{u,\ell} = 1$.

Note: PRD solutions are only calculated for radiative transitions, *i.e.* those with $\mathbf{KTRANS}^{u,\ell} = \text{``RADIATIVE''}$.

Note: When PRD is requested for line (u, ℓ) , then **LSFFDB**^{u, ℓ} is set = 1 automatically.

Note: In a stationary plane-parallel atmosphere, a single ray (i.e. the normal) is traced; in a spherical and/or expanding atmosphere, many rays are traced. The number of frequency values used must be less than 1000. Moreover, the product of the number of frequency values used (see also Note 66) times the number of depth points probably should not be larger than 10000, except for good reason.



LSFTYP^{u,ℓ} is the Line Source Function solution method selection selector, used as follows:

LSFTYP^{u,ℓ} = 0 means: do a 'full Line Source Function solution', computing the line source function using frequency/angle sums and a final grand matrix, and then RHO and JBAR from that S;

LSFTYP^{u,ℓ} = 1 means: compute the line source function 'directly' from the number densities of levels u and ℓ , do frequency/angle sums, then compute RHO from those sums and S, and then JBAR;

LSFTYP^{u,ℓ} = 2 means: compute the line source function from the number densities of levels u and ℓ , compute RHO with the 'escape probability approximation', and then JBAR from them. (See also Note 51.)

'Direct' solutions are only calculated for radiative transitions, *i.e.* $\mathbf{KTRANS}^{u,\ell}$ = "RADIATIVE".

Note: If transition (u, ℓ) is a passive transition, or if the Line Flux Distribution calculation has been requested for it, then the value of **LSFTYP**^{u,ℓ} will automatically be forced = 1!

Note: If $TAU_2^{u,\ell} > \mathbf{ESCTAU}$, then the 'static' escape probability approximation is used for transition (u,ℓ) , regardless of the value of $\mathbf{LSFTYP}^{u,\ell}$.

The statement **SMOOTH** u ℓ (q) (e.g. "SMOOTH 3 1 (ILS 17 WSM 0.5)") is used for the parameters governing smoothing of the RHO values of transition (u,ℓ) . q consists of pairs of input fields of the form "A v", where A is an alphanumeric identification field whose value may be "WSM", "IFS" or "ILS", and v is a numerical field, which must be floating point if it follows WSM, and integer otherwise. WSM is the smoothing weight (=0.0 means: no smoothing; 0.0 is the default). IFS and ILS are limiting indices such that smoothing is done only for $RHO_i^{u,\ell}$, $1 \leq IFS \leq i \leq ILS \leq N$; (defaults are: IFS =1 and ILS =N).

*50

The Voigt profile may be computed by one of three subroutines, as specified by the input parameter **IVOIT**.

IVOIT = 1 selects George Rybicki's method; this is the most precise routine but also the slowest, as it takes about 12 times longer than the high-speed routine.

IVOIT = 2 selects S. R. Drayson's method, which takes about 2 times longer than the high-speed routine; its relative difference from Rybicki's routine is generally below the seventh significant figure, but sometimes in the fourth significant figure.

IVOIT = 3 selects Eric Peytremann's method, which is the high-speed routine; it has a relative difference from Rybicki's routine that is generally less than 0.001, but sometimes as large as 0.05.

If the value V = Voigt(x, a) must be computed immediately after the value V' = Voigt(x', a') has been computed, then, if both x = x' and a = a' to relative accuracy **VOITC**, V = V' will be used (to save time).

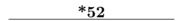
Note: If **IHSSW** = 1 and any value of **CSTARK**^{u,ℓ} = 1 (indicating that a convolved Stark profile should be computed) in a Hydrogen run, then PANDORA will set **IVOIT** = 3 and **NVOIT** = 1.

The **SOBOLEV** statement specifies a particular transition (u, ℓ) , and provides an array of two indices: the first of these is $ISB1^{u,\ell}$, and the second of these is $ISB2^{u,\ell}$.

The 'escape probability' solution for transition (u, ℓ) (i.e. **LSFTYP**^{u, ℓ} = 2) comes in two flavors: 'static' and 'Sobolev'. The static solution is used by default. If $ISB1^{u,\ell} > 1$, the Sobolev solution will be used for depths i, $1 \le i \le ISB1^{u,\ell}$; the static solution will be used for the depths i, $ISB2^{u,\ell} \le i \le N$; and a linear transition from one to the other for depths i, $ISB1^{u,\ell} < i < ISB2^{u,\ell}$.

A table of velocity values, **VSB**, is needed for the Sobolev calculation (see Section 16, Velocities).

The integral needed for the Sobolev solution is computed by trapezoidal rule using an interval refinement procedure which seeks to achieve a piecewise-linear approximation to the run of the integrand, with a specified tolerance. Three parameters control this interval refinement process: **SOBDMN** is the smallest interval size needed (*i.e.* intervals need not be reduced further than **SOBDMN**); **SOB-DMX** is the maximum acceptable interval size (*i.e.* intervals must be reduced to a size smaller than **SOBDMX**); **SOBFEQ** is the tolerance to which interpolated and actual values of the integrand must agree (*i.e.* these two quantities are computed at the midpoint of the current interval, and if they do not agree to this tolerance, then the interval must be reduced further).



IPPOD controls absorption/emission calculation debug dumps at all wavelengths for all 'population update ions'; **IPPOD** = 0 for nothing, **IPPOD** = 1 for absorption, **IPPOD** = 2 for emission, **IPPOD** = 3 for both. Printout occurs for every Z_i such that mod[i, LDINT] = 0.



'Level designations' are alphanumeric labels consisting of up to 8 (non-blank) characters, which will be printed with the levels data as part of the ATOM print-out.

The **LEVDES** statement DOES NOT conform to the standard PANDORA input conventions. It has the form:

"LEVDES (label1 label2) ". Exactly ${f NSL}$ labels must be provided.

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Detailed printout of transition terms (*i.e.* 'A*RHO' and 'Term added to upward C') is controlled by **LDINT** and **LDTYP**. (Of course, option ARHODMP must be on.)

LDTYP specifies the context from which printout is wanted:

LDTYP= 1 means: statistical equilibrium calculation;

LDTYP = 2 means: b-ratio calculation;

LDTYP = 3 means: both.

LDINT specifies the depth points for which printout is wanted:

 $\mathbf{LDINT} > 0$ means: print every \mathbf{LDINTH} 'th depth point, beginning with the first point;

LDINT < 0 means: print for depth $\# |\mathbf{LDINT}|$ only;

LDINT= 0 means: no printout.

In the same way, **LDINT** specifies the interval between depth points for the printouts controlled by the options EPDMP and SEBUG, and by **IPPOD** (see Note 52).



A simple simulation of a shock wave can be obtained by specifying the shock's velocity and temperature perturbation. The shock velocity is further treated in Section 16. The temperature perturbation is computed from input parameters and then added to the input values of \mathbf{TE} to obtain the TE_i actually used in the run:

$$TE_i^{used} = \mathbf{TE}_i^{input} + DTE_i$$
,

where $DTE_i = 0$ for $i < \mathbf{JSSV}$ but

$$DTE_i = \mathbf{SCTA} \exp[(\mathbf{Z_{JSSV}} - \mathbf{Z}_i)/\mathbf{SCTA}].$$

Here **JSSV** is the depth index of the shock's location, **SCTA** is the amplitude of the temperature perturbation, and **SCTS** is the temperature scale height.



 $\mathbf{CP}^{NSL+1} > 0.0$ is the signal that the K-shell photoionization effect is to be computed. If \mathbf{MR}^{NSL+1} is then set $\neq 0$ but, say, equal to IKS, then values of

 \mathbf{RRCP}_m^{NSL+1} , $1 \leq m \leq IKS$ must be provided (as for the other levels), as well as IKS+1 values of \mathbf{WRAT} (see also Note 22). Note that \mathbf{WRAT} input for the K-shell differs from that of the other levels in that the wavelength of the head of that continuum must be specified explicitly.

VX values must be specified as functions of **Z** (the main depth-table of the run). Extra(inter)polation involving **ZAUX** tables has not been provided for **VX**.

*58

If the value of $\mathbf{ECLI}^{u,\ell}$ is > 0, then Eclipse emergent line intensity and flux profiles will be computed for transition (u,ℓ) , but only if this is a transition for which a full-profile integration is done.

*59

Detailed dump printouts from the Line Source Function calculations performed in subroutine PERSEUS can be obtained using the options PERDMP0, PERDMP1, PERDMP2 and PERDMP3.

The 'frequency sums' (subroutine DIANA) or the 'frequency/angle sums' (subroutine ORION) accumulate the contributions from the 'frequency data blocks' or the 'frequency/angle data blocks'. The contents of these data blocks will be printed when the option PERDMP0 is on.

WN matrices of each data block, and the results of computing the above sums, will be printed when the option PERDMP1 is on.

All terms and intermediates for these sums at selected depths will be printed when the option PERDMP2 is on.

PRD data arrays will be printed when the option PERDMP3 is on.

The data blocks are identified by the value of the index IND, whose values range from 1 to K, or from 1 to $NR \times K$, where NR is the total number of rays, and K is the number of entries in the XI table, as explained in Note 66, below. Only data for $\mathbf{IPR01} \leq IND \leq \mathbf{IPR02}$ will be dumped by PERDMP0, PERDMP1, PERDMP2 and/or PERDMP3. Moreover, only the details for the depths $\mathbf{IPR03} \leq i \leq \mathbf{IPR04}$ will be dumped by PERDMP2.

These dump printouts will be provided only for transition (MS,NS).

*60

PANDORA can be instructed to compute an expanding atmosphere by turning the option EXPAND on. When EXPAND is on, then the velocity table **VXS** is

used; see Section 16, Velocities.

PART is the partition function of the next higher stage of ionization of the ion of the run, and is a constant.

If PART > 0.0, then all values of the depth-dependent partition function table will be set equal to it.

If $PART \leq 0.0$, then values of the depth-dependent partition function of the ion of the run can be obtained as follows:

If the option PARTVAR is off, then, if the appropriate value of U2 can be located in the element data tables (see Section 10), that will be used; if not, the run will stopped.

If the option PARTVAR is on, then PANDORA attempts to compute the values of the depth-dependent partition function with the subroutines incorporating the 'Hamburg' data. If this is unsuccessful, then the run will be stopped.

Note: Therefore, to obtain truly depth-varying entries in the partition function table, the option PARTVAR must be on, and the value of **PART** must not be greater than 0.0.



The set of shell rays, and the associated weight matrices, for a spherical atmosphere, are regulated by **NTAN** and **MSKIP**. The value of **NTAN** must be > 0, that of **MSKIP** must be 0, 1, or 3.

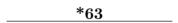
Rays will be sent tangent to every \mathbf{NTAN}^{th} shell (= depth), beginning with the innermost one (i.e. Z_N), and going out as far as possible. (The option TANG also plays a role here.)

The value of MSKIP matters only when NTAN = 1. In that case,

when $\mathbf{MSKIP} = 0$, then the weight matrices for every shell ray will be computed directly;

when $\mathbf{MSKIP} = 1$, then only weight matrices for every 2^{nd} shell ray will be computed directly, while the others will be obtained by interpolation;

when $\mathbf{MSKIP} = 3$, then only weight matrices for every 4^{th} shell ray will be computed directly, while the others will be obtained by interpolation.



IRTIS controls extra(inter)polation of the input table of incident radiation.

 $\mathbf{IRTIS} = 1 \text{ means: linear in XINK, linear in FINK;}$

IRTIS = 2 means: linear in XINK, linear in log(FINK);

IRTIS = 3 means: linear in log(XINK), linear in log(FINK).

NHTSW controls the calculation of the correction to the abundance of atomic Hydrogen due to the possible presence of H_2 molecules.

NHTSW = 0 means: do not compute the H2 abundance correction;

NHTSW = 1 means: compute the H2 abundance according to Kurucz (1970);

 $\mathbf{NHTSW} = 2$ means: compute the H2 abundance according to Tsuji;

NHTSW = 3 means: compute the H2 abundance according to Kurucz (1985).

*65

Detailed dump printouts from the Continuum Calculations (intended to help with handchecks) can be obtained by means of various options and input switches. Such printouts will only be provided for wavelengths listed in the input table \mathbf{DWAVE} , of length \mathbf{NDV} , except when $\mathbf{DWAVE}_1 = 0.0$, in which case such printouts will be provided for all wavelengths. When values of \mathbf{DWAVE} are provided they must match to 8 figures or more the values of the Continuum Calculation wavelengths for which dumps are wanted.



See Section 18, Frequency Tables, for more information about this input parameter. **See also** the *Note* at the end of Note 47.

*67

The "Lyman" source function can be calculated in three ways:

- 1) using the coupled "Lyman" continuum equations, Case A;
- 2) using the large-depth, saturation, or generalized on-the-spot approximation,

Case B (see: Avrett and Loeser 1988, Ap.J., 331, 221, Appendix B); or

3) using Case A for depths 1 through η (if any), and Case B for depths $\eta + 1$ to N (if any); this is Case C, the 'normal' procedure.

(Note that $\eta = N$ means: Case A throughout; $\eta = 0$ means: Case B throughout.) PANDORA computes the value of η as follows: it finds smallest index k for which both $TAUK_k > \mathbf{TGLYM}$ and $(EP1_k)^2 \times TAUK_k \geq \mathbf{EXLYM}$. (If it finds no such index, then k = N.) It then sets $\eta = k$ unless: (a) if $\mathbf{LN} \leq 1$, it sets $\eta = 0$; (b) if $k \leq \mathbf{LN}$, it sets $\eta = 0$; or (c) if $TAUK_2 \geq 10$, it sets $\eta = 0$.

$\mathbf{TGLYM},\,\mathbf{EXLYM}$ and \mathbf{LN} are input parameters.

 $Special\ cases:$

- 1) When the option SPHERE is on, η is set = N;
- 2) when the option SPHERE is off but the option FINITE is on, η is set = N.

LSFGC controls the format of all the Line Source Function graphs.

When LSFGC = 1, then the x-axis is **Z**-index;

when **LSFGC**= 2, then the x-axis is \mathbf{Z}_i ;

when **LSFGC**= 3, then two graphs will be provided, one of each format.

*69

Use of broadening velocity (= microturbulent velocity) depends on the option VSWITCH. When the option VSWITCH is off, then the broadening velocity is isotropic and is specified by the input table \mathbf{V} . When the option VSWITCH is on, then the broadening is anisotropic: the input values of \mathbf{V} are the tangential component, and the input values of $\mathbf{V}\mathbf{R}$ are the radial component. See Section 16, Velocities.



The input value of **IFXDS** should = $8 \times ICF + 4 \times ICM + 2 \times IFD + IFX$.

To print flux tables, use IFX = 1, to omit them, use IFX = 0.

To print flux derivative tables use IFD = 1, to omit them, use IFD = 0.

To print cumulative derivative tables, use ICM = 1, to omit them, use ICM = 0.

To print quadratic coefficients, use ICF = 1, to omit them, use ICF = 0.

The default is IFXDS = 0 (*i.e.* no details at all are printed.)

*71

Many quotient calculations are done in subroutine DIVIDE, which checks for denominator = 0.0. **VSMLL** is used in place of such vanished divisors. DIVIDE will print various error messages, depending on the value of the control switch **IPZER**. When **IPZER** = 0, no messages are printed; when **IPZER** = 1, a message will be printed every time 'A/0' occurs; when **IPZER** = 2, a message will be printed every time '0/0' occurs; **IPZER** = 3 enables both messages.

*72

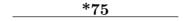
When $\mathbf{LFLUX}^{u,\ell} = 1$, then the Line Flux Distribution and the Radiative Force

for transition (u, ℓ) will be computed. The option LFDPRNT affects the amount of printout. Dump output (for transition [MS,NS]) is controlled by IHDMP.

The 'HI/BYE' system, and the control parameters for it, are intended as debugging aids for me as program developer. 'HI/BYE' is not intended for use in regular production runs.



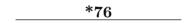
When the option IRUNT is on (*i.e.* when IRUNT = 1), then more extensive execution performance data and program version description data will be printed than when the option IRUNT is off (*i.e.* when IRUNT = 0 (the default)). It should not be necessary to use IRUNT = 1 in regular production runs.



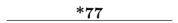
The 'banner' pages at the start of the printout file (see Section 3) display 'giant' characters that are themselves composed (in 'dot-matrix' fashion) of individual print characters. The value of **NARB** tells how many such pages to print, the value of **KARB** selects the print character(s) used for this purpose.

 $\mathbf{KARB} = 1$ means: use "\$" to represent the giant character.

KARB = -1 means: use "O" over "X" over "+" (this of course works only with processing systems which fully implement traditional 'Fortran carriage control'). **NARB** may assume the values 0, 1, or 2.



In many runs, the sets of 'Composite Lines Opacity' wavelengths and 'CO-lines Opacity' wavelengths are added automatically to the list of wavelengths for which continuum calculations are done. If any value of **DELWAVE**_i, $1 \le i \le NWS$, equals (to one part in 10^{10}) a wavelength in one of these two sets, then that wavelength value will be deleted from the list of wavelengths for which continuum calculations are done. (These counterparts to the 'additional' wavelengths are therefore called 'subtractional' wavelengths.)

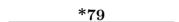


See also the note regarding maximum counter values, and order of occurrence

among the input, at the end of Section 3. See also Note 29.

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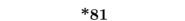
DOPROF is an alternate form of the **PROF** statement; it contains pairs of transition indices, like the **INPAIR** statement (see Note 2). The occurrence of the index pair u, ℓ in **DOPROF** causes the program to set **PROF**^{u,ℓ} = 1.



DOFLUX is an alternate form of the **LFLUX** statement; it contains pairs of transition indices, like the **INPAIR** statement (see Note 2). The occurrence of the index pair u, ℓ in **DOFLUX** causes the program to set **LFLUX**^{u, ℓ} = 1.

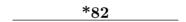


DOFDB is an alternate form of the **LSFFDB** statement; it contains pairs of transition indices, like the **INPAIR** statement (see Note 2). The occurrence of the index pair u, ℓ in **DOFDB** causes the program to set **LSFFDB**^{u,ℓ} = 1.



DOSFPRNT is an alternate form of the **LSFPRINT** statement; it contains pairs of transition indices, like the **INPAIR** statement (see Note 2). The occurrence of the index pair u, ℓ in **DOSFPRNT** causes the program to set **LSFPRINT**^{u,ℓ} = 1.

Note: **LSFPRINT**^{u,ℓ} and option LSFPRNT are different beasties, but they work together.



See Section 16, Velocities, for more information about this input parameter.

*83

When **MTHEI** = 0, then exponential integrals are computed using Cooley's routine, which gives about 8 figures for the first exponential integral; higher orders are computed with the recursion relation which rapidly loses precision for increasing orders. See Avrett & Loeser, SAO Special Report No. **303**, 1969.

When MTHEI = 1, then exponential integrals are computed using a routine published by Press and Teukolsky. This routine has been set up to deliver about 14 figures for all orders; it is slower than Cooley's routine. See Press & Teukolsky, Computers in Physics, Sep/Oct 1988.

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*21	

The switches ISCRS, NOION, NVOIT, IXSTA, JBDNC, JSTIN, IRPUN, IRUNT and TOPE are alternate forms of the options ISCRS, DOION, NVOIT, IXSTA, JBDNC, JSTIN, RABDAT, IRUNT and TOPE, respectively. The program will set their *default* values to agree with the status of the corresponding options.



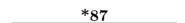
Subroutine EDITH is used in various context to edit values ≤ 0 out of various computed tables; it is set up to print error messages to report what it did. For each editing context k, a separate count of error messages, $KERM_k$, is kept. The value of the input parameter **NERM** controls the printing of error messages: when **NERM** = 0, then no error messages are printed;

when **NERM** > 0, then error messages from context k are printed as long as $KERM_k \leq \mathbf{NERM}$;

when NERM < 0, then all error messages are printed, but greatly abbreviated.



If $\mathbf{ZNDW} \neq 0$, then \mathbf{NDW} will be set equal to i, where $\min(|Z_i - ZNDW|)$, $1 \leq i \leq N$. If $\mathbf{ZNDW} = 0$, then, if $\mathbf{NDW} < 1$ or $\mathbf{NDW} > N$, \mathbf{NDW} will be set equal to N/2.



As the final step in constructing WN-matrices (which are used in source function calculations), the computed matrix is scanned and every element whose absolute value is less than \mathbf{WNJUNK} is set = 0.



LODCG and **NODCG** are parameters controlling the depth range for diffusion graphs (no graphs appear when **NODCG** = 0). Various parameters are plotted as functions of \mathbf{Z} , for the range \mathbf{Z}_I to \mathbf{Z}_J .

When LODCG< 0, then I = 1; when LODCG> 0, then I = LODCG.

When $\mathbf{NODCG} < 0$, then J = K; when $\mathbf{NODCG} > 0$, then $J = \mathbf{NODCG}$ or K, whichever is less. K is the smallest depth index such that $\mathbf{TE}_K < 9000$.

d-coefficients are computed for the diffusion calculations.

When IDFDM = 0, the "original" method is used;

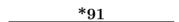
when IDFDM = 1, an "improved," more complete method is used.

When options AMDDMP and/or GNVDMP are on, then the d-coefficients will be printed for depth i; when $\mathbf{IDFDI} > 0$, then $i = \mathbf{IDFDI}$, but when no value of \mathbf{IDFDI} is input, then $i = \mathbf{N}/4$.

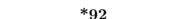


If the input values of $\mathbf{V}_i = 0, 1 \leq i \leq \mathbf{N}$, then, if $\mathbf{NVH} > 0$, "default" values of \mathbf{V}_i will be computed from $\mathbf{VNH}_j, 1 \leq j \leq \mathbf{NVH}$. Here \mathbf{VNH} is a velocity table appropriate for the quiet Sun, and is specified as a function of Hydrogen density, \mathbf{HNDV} . Values of \mathbf{V}_i corresponding to the input values of \mathbf{NH}_i are obtained by interpolation from the tables \mathbf{HNDV}_j and \mathbf{VNH}_j ; the logarithms of \mathbf{NH}_i and \mathbf{HNDV}_j are used for this purpose.

IMPORTANT: if $V_i = 0$ is intended, then **NVH** must be set = 0 explicitly in the input, since the default value of **NVH** > 0.



CIJADD uses special cases of Statement Forms 5* and 5, in that $u > \ell$ is not required – rather, all combinations $u \neq \ell$ are accepted.



ASMCR and NIASM are parameters used in sequential smoothing; see write-ups [89 Dec 22] and [92 Jan 29]. The smoothing used here is based on the following principle. Consider the sequence of graphical points representing the values of a function. If the function varies smoothly, a given point usually lies within the triangle defined by the two lines through the pair of points on either side and the line through the point on either side, provided the two lines intersect within the given interval. If the given point falls outside, it is moved to the boundary of this triangle; if the given point lies within this triangle, it is left unchanged. Smoothing consists of a repeated search for the most deviant point, and then

changing it if necessary. Then this edited sequence is searched for the most deviant point; and so on. The search is repeated at most $\mathbf{NIASM} \times n$ times, where n is the number of points in the sequence. However, the process stops after the first time that the relative change applied to the most deviant point is less than \mathbf{ASMCR} .

See Section 19, Atomic Models, for more information about this input parameter.

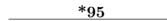
*94

NLPAIR is a list of integers (n_j, ℓ_j) , $1 \le j \le \mathbf{NL}$, such that n_j is the principal quantum number of level j and ℓ_j is the rotational quantum number of level j of the model of the ion-of-the-run. For example, $(n_{22}, \ell_{22}) = (5, 3)$ means the for level 22 the principal quantum number n = 5 and the rotational quantum number $\ell = 3$.

The value $\ell_j = -1$ is meaningful; this means that level j is a synthetic level obtained by combining all of the sublevels characterized by the same value of n but different values of ℓ .

When $\ell_j = -1$, then n_j must be > 0. For Hydrogen, default values of (n_j, ℓ_j) are provided: $n_j = j$ and $\ell_j = -1$.

In the **NLPAIR** statement, the (n, ℓ) pairs should be specified in level sequence, beginning with level 1.



The "upper-level charge-exchange" calculation is enabled when option CHEXUP is on and this is a run with Hydrogen, or with a "charge-exchange" ion. The list of eligible "charge-exchange" ions is built into PANDORA; it consists of: He-I, C-I, N-I, O-I, Na-I, Mg-I, Al-I, Si-I, S-I, and

Ca-I, in that order. A particular "charge-exchange" ion is internally known to PANDORA by the value of MCX, $1 \le MCX \le 10$, *i.e.* by the index of that ion in the above list.

In a run other than Hydrogen in which "upper-level charge-exchange" is enabled, only a subset of levels, namely "levels affected by charge-exchange" a.k.a. "CX-levels," is affected. Any level j of the model of the ion-of-the-run whose rotational quantum number $\ell_j \neq 0, 1, 2$ is a CX-level, but only if that level's principal quantum number $n_j > \ell_j$. Such runs produce the output tables **XRKH** and **XRLH** for use in Hydrogen upper-level charge-exchange runs.

In a Hydrogen run with "upper-level charge-exchange," all levels j, $j \geq 4$, are CX-levels. Such runs make use of various input sets of **XRKH** and **XRLH** produced by upper-level charge-exchange calculations with other elements.

The arrays $\mathbf{XRKH}_{i}^{k,n}$ and $\mathbf{XRLH}_{i}^{k,n}$ are input for the upper-level charge exchange calculation (option CHEXUP on) in Hydrogen runs.

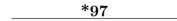
The superscript k, $1 \le k \le 10$, designates a particular charge-exchange element (see also Note 95); the superscript n, $1 \le n \le \mathbf{NL}$, designates the affected level of the Hydrogen ion model. (In the case of Hydrogen, the level number is numerically equal to the principal quantum number of that level.) The indices k and n appear in that order in an **XRKH** or **XRLH** input statements; for example:

"XRKH 4 6 (. . . .) "

which are data from a Mg-I run for level 4 of the Hydrogen ion model; or: "XRLH 14 2 (.) "

which are data from a C-I run for level 14 of the Hydrogen ion model.

Note: values of n must not be greater than NL.



 $\mathbf{RCHX}^{n,\ell}$ is a parameter used for the upper-level charge-exchange calculation (option CHEXUP on). The value of $\mathbf{RCHX}^{n,\ell}$ is used for all those levels of the model of the ion-of-the-run for which the principal quantum number is n and the rotational quantum number is ℓ . The indices n and ℓ appear in that order in the \mathbf{RCHX} input statement; for example:

"RCHX 4 3 (1.23) " which sets $\mathbf{RCHX}^{4,3} = 1.23$.

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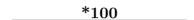
The emergent line profile graphs for transition (u, ℓ) (option INTGRAF) can be controlled with **PROGLI**^{u,ℓ}, which controls the limits of the wavelength axis, and with **SGRAF**^{u,ℓ}, which applies to 'blended' lines.

When $\mathbf{PROGLI}^{u,\ell} = 0$ (the default), then the x-axis spans the entire $\Delta \lambda$ range. When $\mathbf{PROGLI}^{u,\ell} > 0$, then the x-axis extends from the core out to \mathbf{PROGLI} . When $\mathbf{PROGLI}^{u,\ell} < 0$, then the x-axis extends from the core out to that point where successive intensity values differ relatively by less than $|\mathbf{PROGLI}|$. (If there are several such points, the point with the largest $\Delta \lambda$ value is used.) If transition (u,ℓ) is a blended line then,

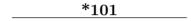
when $\mathbf{SGRAF}^{u,\ell} = 1$, separate graphs are provided for each component;

when $\mathbf{SGRAF}^{u,\ell} = 0$, only a single, composite graph is provided.

ISMSW provides additional control over the format of Iterative Summaries. When $\mathbf{ISMSW} = 0$, then the format is controlled by option SUMGRAF. When $\mathbf{ISMSW} > 0$, then the summaries will be provided in both formats.



Regardless of the setting of option RATEPRNT, a 'minimal' RATES calculation printout is provided when the input value of **IRATE** is a valid depth index. In that case, values of QU, QS, GM, RK, RL and CK for all levels, and of CIJ and PIJ for all transitions, will be printed, for that depth only.



ICDIT specifies the classes of continuum wavelengths for which dI/dh analyses will be printed when option DIDHC is on.

ICDIT= 1 means: for all 'additional' wavelengths;

ICDIT= 2 means: for the line center wavelengths of those transitions for which a Line Source Function calculation printout was provided;

ICDIT = 3 means: 1 and 2.

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The photorecombination rates \mathbf{RL} and photoionization rates \mathbf{RK} can be computed either by detailed integration of the continuum radiation field, or from specified runs of radiation temperatures (input tables of \mathbf{TRN}_i). These alternatives are controlled by option USETRIN.

When USETRIN is on, then the computed values of $\mathbf{R}\mathbf{K}_i^{\ell}$, $1 \leq i \leq \mathbf{N}, 1 \leq \ell \leq \mathbf{NSL}$, can be manipulated by means of the factor HJ_i , the photoionization rates multiplier. Values of $HJ_i = 1$ by default; however, if appropriate input values of **JH1** and **JH2** are provided, then various specific runs of HJ_i are constructed such that HJ = 0.5 near the surface and HL = 1.0 at depth, with an intermediate transition region defined by depth indices **JH1** and **JH2**. This is also explained in a note following the ATMOSPHERE printout.

When full continuum integrations are done (option USETRIN off), PANDORA also computes "effective radiation temperatures"—i.e., those values of radiation

temperature which yield the same values of $\mathbf{R}\mathbf{K}_i^\ell$ as the full integrations did. These computed $\mathbf{T}\mathbf{R}\mathbf{N}_i^\ell$ values are included in output file F0R020 (see Section 8), and can be used as input for a subsequent restart run with option USETRIN on.

PANDORA can be requested to adjust the values of **Z** so that certain constraints are satisfied: 1) that each value of the computed mass table be equal to the corresponding value of an input mass table (for this case option HSE must be on), or 2) that each value of a computed TAUK table (continuum optical depth at a specific wavelength) be equal to the corresponding value of an input TAUK table. What happens in such runs is that a particular relationship between **TE** and mass, or between **TE** and TAUK, is intended, and PANDORA tries to make sure—by adjusting the **Z** values—that its computed mass or continuum optical depth values come as close as possible to the specified ones. Like so much else in PANDORA, these 'Z-recalculation' procedures require several iterations to give good results.

(In principle, atmospheric parameters can be specified not only on a grid of Z-values, but also on grids of other quantities, such as mass or optical depth. We did not think to allow for such flexibility during the early years of PANDORA development, and internally PANDORA is solidly based on a grid of geometric depth values. Thus—to allow the user the convenience of working with fixed sets of mass or optical depth values—the program must establish the corresponding geometrical depth values in order to function at all.)

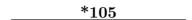
When such 'Z-recalculation' is requested, this will be done whenever appropriate as the calculations proceed.

The final recomputed **Z** table is included in output file fort.20 (see Section 8), and can then be used to replace the previous **Z** table of that atmospheric model.

- 1) To specify an input mass table, use the input parameters \mathbf{ZMASS} and \mathbf{RFMAS} ; these define the 'input' mass table: $MASS_i = \mathbf{ZMASS}_i + \mathbf{RFMAS}$. This Z-recalculation procedure will be done whenever the input values of \mathbf{ZMASS}_i do not all = 0. It is possible that overcorrections computed during early iterations of this process can cause things to go awry, and a weighting step has been included to keep things under control. Thus, in the current iteration, the final new \mathbf{Z} values = $\mathbf{WZM} \times (\text{newly-computed Z}) + (1 \mathbf{WZM}) \times (\text{final Z})$ from previous iteration).
- 2) The other Z-recalculation procedure will be done whenever the input values of \mathbf{TAUKIN}_i do not all = 0; a value of \mathbf{PZERO} (surface pressure) may need to be specified; the value of \mathbf{REFLM} (the specific wavelength) can also be specified.



The meanings of LMA, LMB, LME, LMF, LMR, LMT, WEP, and of options ENL and ENL2, are explained in detail in the text included in the LEVEL 1 TO K (*i.e.*, "Lyman") printout.

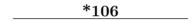


When transition (u, ℓ) is designated as a blend of component lines, then $\mathbf{LDL}^{u,\ell}$ input values of the displacements $\mathbf{DDL}^{u,\ell}$ and of the relative line strengths $\mathbf{CDL}^{u,\ell}$ must be provided for that line. The units of \mathbf{DDL} are Angstroms; however, if it is more convenient to specify displacements in units of wavenumbers $(/\mathrm{cm})$, then the alternate input parameter $\mathbf{DWN}^{u,\ell}$ may be used. The sum of the values of $\mathbf{CDL}^{u,\ell}$ should be 1. Furthermore, $\mathbf{LDL}^{u,\ell}$ input values of $\mathbf{CRD}^{u,\ell}$, of $\mathbf{CVW}^{u,\ell}$, and of $\mathbf{CSK}^{u,\ell}$ must also be provided (zeroes will be used otherwise).

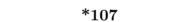
For blended line transition (u, ℓ) , the line profile function is calculated as

$$PHI_i = \sum_{L=1}^{LDL} \mathbf{CDL}^L PHI_i^L$$

where each set PHI^{L} is displaced (in wavelength or in wavenumber) as specified.



Details of a Hydrogen Stark broadening convolved profile calculation for the (MS,NS) transition are printed for the IHSDP'th depth point and for the IHSDD'th frequency value, when option ANALYSIS is on.



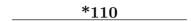
Input parameter IHSSW overrides all CSTARK $^{u,\ell}$.

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When option AMDIFF is on and option VELS is off, then PANDORA will automatically set $\mathbf{NVX} = 1$. See Section 16, Velocities.

When NCB > 0 (*i.e.* when CO-lines wavelength bands are specified):

- 1) if $\mathbf{NCL} = 0$, then no CO-related wavelengths will be added to the list of wavelengths for which continuum calculations are done;
- 2) if $\mathbf{NCL} = 1$, then $\mathbf{XCOL}_1 = 0$ is assumed, and only CO-line core wavelengths and the specified band limits will be added to the list of wavelengths for which continuum calculations are done.



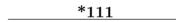
If **WAVEMN** > 0 and **WAVEMX** > **WAVEMN**, then PANDORA attempts to use built-in procedures to add more additional wavelengths to the table **WAVES**_i, $1 \le i \le NWV$, as follows.

If **NWV** > 0 and there is an index I, I < **NWV**, such that **WAVES**_i = 0 for all I < $i \le NWV$, then:

1) all standard rates integration wavelengths λ^c falling in the range **WAVEMN** $\leq \lambda^c \leq \text{WAVEMX}$, will replace such zeroes (working systematically upwards from i = I + 1).

If thereafter it is still the case that there is an index I, I < **NWV**, such that $\mathbf{WAVES}_i = 0$ for all I < $i \leq \mathbf{NWV}$, then:

2) those remaining zeroes will be replaced by values λ^a such that **WAVEMN** $\leq \lambda^a \leq$ **WAVEMX**; these λ^a will be equi-spaced in the log.



The input switch **IXNCS** (default =1) allows reversion to the "old" method of calculating default values of **CE** and **CI** in Hydrogen runs (see Section 19). "Old" method (**IXNCS** = 0): if no input values of **CE** or **CI** (as tabulated functions of **TER**) are given, then default tables are computed (using the method specified) and listed in the ATOM printout. These calculations do not take the "lowering of the ionization potential" into account. Whenever particular values of $\mathbf{CE}_i^{u,\ell}$ or \mathbf{CI}_i^j as functions of temperature are needed during the calculations, then they will be obtained from these tables by interpolation.

"New" method (**IXNCS** = 1): if no input values of **CE** or **CI** (as tabulated functions of **TER**) are given, then particular values of $\mathbf{CE}_i^{u,\ell}$ or \mathbf{CI}_i^j as functions of temperature and charged particle density will be computed as needed during the

calculations; values pertaining to **TER** and a reference value of charged particle density (note input parameter **IRFNC**) appear in the ATOM printout as sample values only. (This only makes sense if the method of Johnson, or of Vriens and Smeets, is specified; or if no set of **TER** values yields acceptable interpolated results.)

The statement COLINES (q) (e.g. "COLINES (KROT 15 RC1213 17.) ") is used for parameters controlling the CO-lines calculations. q consists of pairs of input fields of the form "A v", where A is an alphanumeric input field whose value may be "JFUND", "KFUND", "JOVER", "KOVER", "JSECN", "KSECN", "JROT", "KROT", "ISOSLCT", "METHCOF", "METHCOW", or "RC1213", and v is a numeric field, which must be floating point if it follows RC1213, and integer otherwise. Here: JFUND ... KROT specify maximum values of the quantum numbers j and ν , as follows:

JFUND is the maximum value of j for fundamental lines (default = 111); KFUND is the maximum value of ν for fundamental lines (default = 20); JOVER is the maximum value of j for first overtone lines (default = 111); KOVER is the maximum value of ν for first overtone lines (default = 13); JSECN is the maximum value of j for second overtone lines (default = 111); KSECN is the maximum value of ν for second overtone lines (default = 12); JROT is the maximum value of j for rotational lines (default = 53); KROT is the maximum value of ν for rotational lines (default = 21); ISOSLCT selects the isotope; = 1 means: use ^{12}CO , = 2 means: use ^{13}CO ,

= 3 means: use both (default = 3);METHCOF selects the method for computing f-values;

- = 1 means: use Chackerian and Tipping, = 2 means: use new Chackerian data,
- = 3 means: use Goorvitch, 1994 (default = 3);

METHCOW selects the method for computing energies (wavelengths);

- = 1 means: use Farrenq et al., = 2 means: use Coxon and Hajigeorgiou,
- = 3 means: use Goorvitch, 1994 (default = 3);

RC1213 is the isotopic abundance ratio ${}^{12}CO/{}^{13}CO$ (default = 90).

Notes:

The input values of the maximum quantum numbers JFUND ... KROT cannot be set larger than their respective default values.

JFUND = 0 and/or KFUND = 0 means: do not include any fundamental lines.

JOVER = 0 and/or KOVER = 0 means: do not include any first overtone lines.

JSECN = 0 and/or KSECN = 0 means: do not include any second overtone lines.

JROT = 0 and/or KROT = 0 means: do not include any rotational lines.

IPEX controls debug printout intended to be useful for program development only. **IPEX** = -1 will generate a flood of printout; **IPEX** = k, where k is one of several integers > 0, will generate selected printouts only.

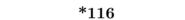


LOGAS > 0 turns on the "location analysis graph" of the emergent line profile calculation, and selects the type of abscissa: = 1 for $\Delta\lambda$ -index or wavenumber-index, =2 for $\Delta\lambda$ -value or wavenumber-value. (Option WAVENUMB controls whether wavelength or wavenumber is used.)



Debug output from the calculation of CI (in Hydrogen runs using AR, VORONOV, VS, or JOHNSON) can be obtained by setting $\mathbf{JDMCI} = [(1000 \times i) + j], \ 1 \le i \le \mathbf{N}, 1 \le j \le \mathbf{NL}$, where i is a depth index and j is a level index. When i = 0, then output is provided for level j at all depths; when j = 0, then output is provided at depth i for all levels.

Debug output from the calculation of CE (in Hydrogen runs using VS or JOHNSON) can be obtained by setting **JDMCE** = $[1000 \times (100 \times u + \ell) + i]$, $1 \le i \le \mathbf{N}$, where i is a depth index and (u, ℓ) are transition indices, $u > \ell$. When i = 0, then output is provided for transition (u, ℓ) at all depths; when the transition indices are (0, 0), then output is provided at depth i for all transitions.



When $\mathbf{NGNV} > 0$, then GNV^{ℓ} , $\mathbf{NGNV} \leq \ell \leq \mathbf{NL}$ will be suppressed (i.e. set = 0) in the diffusion calculations.

 CQM_i occurs in the equation of the scattering albedo of the 'Line Background' opacities (see Section 9).

If input parameter $\mathbf{CQM} > 0$, then PANDORA uses $\mathbf{CQM}_i = \mathbf{CQM}$, $1 \le i \le \mathbf{N}$. If input parameter $\mathbf{CQM} \le 0$, then PANDORA expects to find the tables \mathbf{CQT}_k , \mathbf{CQA}_k , $1 \le k \le \mathbf{NCQ}$, which specify CQM as a tabulated function of temperature. PANDORA interpolates in $\log[\mathbf{CQA}(\mathbf{CQT})]$ to obtain $\mathbf{CQM}_i = \mathbf{CQA}(\mathbf{TE}_i)$, $1 \le i \le \mathbf{N}$.

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 $\mathbf{KRATE}^{u,\ell}$ controls the formulation of certain terms in the statistical equilibrium equations:

KRATE^{u,ℓ} = 1 means: use net-rate (computed from ρ); **KRATE**^{u,ℓ} = 2 means: use single-rate (computed from \bar{J}).

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First derivatives of various quantities need to be computed for the diffusion calculations (option AMDIFF). The input parameter **KDIFD1** selects one of several methods:

 $\mathbf{KDIFD1} = 1$ means: compute the slope at the given point as the slope of the straight line through the two bracketing points.

KDIFD1 = 2 means: first apply "sequential smoothing" to the table of values; then compute the slope at the given point as the average of two slopes: the slope of the straight line through the given point and the adjacent point on the left, and the slope of the straight line through the given point and the adjacent point on the right.

KDIFD1 = 3 means: first apply "improved sequential smoothing with irregular point spacing" to the table of values; then compute the slope at the given point from the cubic spline fitted to all the points.

KDIFD1 = 4 means: compute the slope at the given point as the average of two slopes: the slope of the straight line through the given point and the adjacent point on the left, and the slope of the straight line through the given point and the adjacent point on the right (i.e., like **KDIFD1** = 2 but without smoothing). The default value is **KDIFD1** = 1.

If any nonzero values of \mathbf{RABDL}_i were input, then \mathbf{RABD}_i will be set equal to antilog (\mathbf{RABDL}_i), all i. Otherwise, if any nonzero values of \mathbf{RABD}_i were input, then those input values will be used. Otherwise, \mathbf{RABD}_i will be set equal to 1.0, all i.



The detailed dump printout for the calculation of S-from-Number-Densities is controlled by **ISNDD**. When **ISNDD** = 0, then no dump ever appears; when $\mathbf{ISNDD} = 1$, then a dump appears for every such calculation; when $\mathbf{ISNDD} = 2$, then a dump appears only if an error occurred during the calculation.

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The 'Special N1' calculation (part of the "Diffusion Calculation" when option AMDN1 is on) can be done in various ways; the choice of method is controlled by input parameters **N1MET**, **KDIAG**, **I4DFM**, **I4DEQ**, **I4DIO**, **KBNDS** and **KDAMP**. (A more detailed explanation of these parameters appears in sections INPUT and DIFFUSION of the main output file.)

When $\mathbf{N1MET} = 1$, use the exponential method (if possible, otherwise, a diagonal method); when $\mathbf{N1MET} = 1$, use the diagonal method specified by \mathbf{KDIAG} ; when $\mathbf{N1MET} = 3$, use the simultaneous method (for He-I or He-II only).

KDIAG = 3, 4, or 5 selects the 3-diagonal, 4-diagonal, or 5-diagonal method, respectively. Additional controls are needed for the 4-diagonal method: $\mathbf{I4DIO} = 1$ specifies the inward version, and $\mathbf{I4DIO} = 2$ the outward version (in the staionary case); $\mathbf{I4DEQ} = 0$, 1, or 2 specifies the "original," "method-1," or "method-2" equations, respectively; when $\mathbf{I4DEQ} = 1$, use the results from the Z-formulation, when $\mathbf{I4DEQ} = 2$, use the results from the ζ -formulation.

KDAMP = 0 means: use the raw matrix solution, whereas **KDAMP** = 1 means: use the damped matrix solution (obtained by a weighted moving 3-point average), for the three-diagonal, five-diagonal, or simultaneous method.

 $\mathbf{KBNDS} = 1$ means: use equations incorporating relevant boundary conditions, = 0 means: do not.

If not input values of the "Lyman" calculation tables $\mathbf{X}\mathbf{K}_i$, $\mathbf{G}\mathbf{K}_i$, $1 \leq i \leq \mathbf{K}\mathbf{K}$ are specified, then defaults are provided from the rates integration data tables $RRNU_i^{\mathbf{KOLEV}}$, $\mathbf{RRCP}_i^{\mathbf{KOLEV}}$, $1 \leq i \leq \mathbf{MR}^{\mathbf{KOLEV}}$. If $\mathbf{MR}^{\mathbf{KOLEV}} > \mathbf{K}\mathbf{K}$, then only the first $\mathbf{K}\mathbf{K}$ values of RRNU and \mathbf{RRCP} are copied into $\mathbf{X}\mathbf{K}$ and $\mathbf{G}\mathbf{K}$, respectively; if $\mathbf{K}\mathbf{K} > \mathbf{MR}^{\mathbf{KOLEV}}$, then RRNU and \mathbf{RRCP} are copied into the first $\mathbf{K}\mathbf{K}$ elements of $\mathbf{X}\mathbf{K}$ and $\mathbf{G}\mathbf{K}$, respectively, while the rest of those tables will be left undisturbed.

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The "Diffusion Calculations" (options AMDIFF and VELGRAD) compute tables of $GNVL_i^{\ell}$, $1 \leq i \leq \mathbf{N}$, $1 \leq \ell \leq \mathbf{NL}$. At times the raw computed values of these tables should not all be used; instead, they should be set =0 at some depths. A table of GRF_i values ('GNVL reduction factor') has been introduced for this purpose; GRF_i multiplies the raw values to produce the final values of $GNVL_i^{\ell}$. The values, and the use, of GRF_i , are controlled by input parameters **KDIFGS**, **KDIFGA**, and **KDIFGB**.

The GRF_i table is established as follows: $GRF_i = 1, 1 \le i \le \mathbf{KDIFGA}$; $GRF_i = (\mathbf{KDIFGB} - i)/(\mathbf{KDIFGB} - \mathbf{KDIFGA})$, $\mathbf{KDIFGA} < i < \mathbf{KDIFGB}$; $GRF_i = 0$, $\mathbf{KDIFGB} \le i \le \mathbf{N}$.

When **KDIFGS** = 0, then GRF_i is not used (and the raw values become the final values); when **KDIFGS** = 2, then all values of $GNVL_i^{\ell}$, $1 \leq \ell \leq NL$ are multiplied by GRF_i ; when **KDIFGS** = 1, then only values of $GNVL_i^1$ are multiplied by GRF_i .

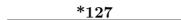
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IPDEE and **NEFDF** are related to the calculation of the d-coefficients that are used in the diffusion calculation (the relavant routines are minor adaptations of code written and provided by Juan Fontenla). The d-coefficient-calculation needs values of the electron density; when $\mathbf{NEFDF} = 1$, then internally-computed values of electron density are used, when $\mathbf{NEFDF} = 2$, then the program-wide \mathbf{NE} -table is used.

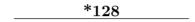
A schematic graph of the computed d-coefficients is always printed; the complete set of values will be printed, in addition, when $\mathbf{IPDEE} = 1$.



The table $beta_i$ (the He II number density) used in the diffusion calculations can be computed in different ways, controlled by **IBETSW**. When **IBETSW** = 0, then $beta_i = \frac{1}{2}(HEK_i + HE21_i)$; when **IBETSW** = 1, then $beta_i = HEK_i$; when **IBETSW** = 2, then $beta_i = HE21_i$.



The array DIJ is one of the aids that are calculated, printed, and plotted for analyzing the effects of diffusion. When $\mathbf{IPDIJ} = 0$, then the entire array will be printed; when $\mathbf{IPDIJ} = 1$, then only an abbreviated analysis of DIJ will be printed.



KB1WA and **KB1WB** are depth indices that control the generation of B1-weights in the same way that **KDIFGA** and **KDIFGB** control the generation of values of GRF_i (see Note 121).



The input switch **KANTNU** controls the summary printout of all TNU tables of a radiative transition. (The default is **KANTNU** = 0.)

KANTNU = 0 means: none;

KANTNU = 1 means: for all transitions with LSFPRINT = 1;

 $\mathbf{KANTNU} = 2$ means: for all transitions when option LSFPRNT is on; $\mathbf{KANTNU} = 3$ means: for all transitions when option LSFGRAF is on;

KANTNU = 4 means: for all transitions.

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The ORIGINS printout, and/or the CONTRIBUTORS printout, part of the spectrum analysis aids, can be restricted to a specified range of wavelengths (or of wavenumbers when option WAVENUMB is on). **CORMIN**, when > 0, is the minimum value, and **CORMAX**, when > 0, is the maximum value of wavelength (or of wavenumber, as the case may be).

 $X_i^{s+1} = W_i \times X_i^{new} + (1 - W_i) \times X_i^s$, $1 \le i \le N$, where X stands for RHO^{u,ℓ} and W syands for RHWT^{u,ℓ}; or

 $X_i^{s+1} = [(X_i^{new})^{W_i}] \times [(X_i^s)^{(1-W_i)}], \ 1 \leq i \leq N, \text{ where } X \text{ stands for RK}^{KOLEV}$ and W stands for RKWT, as used in the Lyman calculation.

The values of X_i for iteration s + 1 will be obtained, in the manner shown, from the values of X_i used during iteration s and the new values of X_i calculated at the end of iteration s.

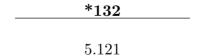
The first equation above illustrates *linear* weighting, while the second illustrates *logarithmic* weighting. Logarithmic weighting is always used for RK^{KOLEV} ; logarithmic weighting can also be used for $RHO^{u,\ell}$, depending on option WATESTR.

The values of \mathbf{RHWT}_i and \mathbf{RKWT}_i may vary with depth index i, or may be constants. They are updated in every iteration as described in the writeup [74 Oct 23]. The procedure for updating these weights uses input parameters \mathbf{INCH} , \mathbf{WRMN} , and \mathbf{WRMX} .

Note: RHO and RK weighting used to be done differently, using different input parameters and input tables (see Note 13). The former input quantities NTW, TAW, WTW, NWRHO, WRLY, and WRHO are no longer recognized by the program and must be removed from old files. The former input quantities WMN, WMX, RHOWT, and RKW are no longer used, however, the program continues to recognize them and uses their values to compute related values of **WRMX**, **WRMN**, **RHWT**, and **RKWT**, according to:

$$\mathbf{WRMX} = 1 - WMN,$$
 $\mathbf{WRMN} = 1 - WMX,$ $\mathbf{RHWT} = 1 - RHOWT,$ and $\mathbf{RKWT} = 1 - RKW.$

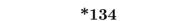
Messages are written to the output file whenever these conversions are done. It is best to remove **WMN** and **WMX** from the input (using the above conversions). **RHOWT** and **RKW** tend to occur in the restart files written by old versions of the program; the program now writes **RHWT** and **RKWT** to these files. Thus, the old quantities will normally be encountered only when an old run is restarted with the current program, so that the automatic conversion described here needs to be done only once.



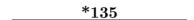
The switch **WORLDLY** can take on the values SCREEN or DISK; it controls the storage-management-system dump (which uses file fort.97 when **WORLDLY** = DISK). I use this to check the source code; it is not intended for general use.

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In the ATMOSPHERE and ATOM printout sections, parameter values = 0 are nomally printed as blanks. If the user prefers to see printed 0's, then the input parameters **JZATMO** and/or **JZATOM** may be set = 1.



As explained in Section 11, output from the Continuum Calculations at various wavelengths is controlled by various OPTIONS pertaining to the various wavelength types (for example, output will be produced for all Additional Continuum Wavelengths, **WAVES**, when option ADDCOPR is on). However, even if no wavelength-type OPTIONS are on, output will be produced for every wavelength specified in the table **SCOW**, of length **NSW**. For this purpose, a value of **SCOW** must match the value of an actual Continuum Calculation wavelength to at least 8 figures (note that a list of all Continuum Calculation wavelengths appears in the WAVELENGTHS section near the end of the PANDORA printout).



When option USEWTAB is on, the "standard rates integrations wavelengths" table is added to the list of wavelengths for which continuum calculations are done. (This "standard" table contains values bracketing all the absorption edges contained in the built-in ion models and tries to capture, for integration purposes, all the lines included among the background opacity contributors.) Only that portion of the "standard" table falling between the limits **WRATMN** and **WRATMX** will be used.

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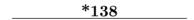
Ionization and excitation rates always include the effects of collisions with electrons; the rates due to collisions with neutral Hydrogen are always computed (and printed if the options RATEPRNT and COLHPRNT are both on), but are used only if the input switch $\mathbf{ICHSW} = 1$. Rates due to collisions with Hydrogen, however, are computed only for those levels of the ion-of-the-run whose corresponding value of the input array $\mathbf{LCH}^j > 0$, $1 \le j \le \mathbf{NSL}$. $\mathbf{LCH}^1 = 0$ by definition; but a negative value of \mathbf{LCH}^1 can be specified and will be used as a special code, as described below.

Ionization rates due to collisions with Hydrogen are computed using the formulation of B. Kaulakys, 1985, J.Phys.B, 18, L167.

Kaulakys' formulation is also used to compute the effects of collisions with Hydrogen on the collisonial excitation rates for all those transitions (u,ℓ) for which both \mathbf{LCH}^u and $\mathbf{LCH}^\ell > 0$. A second set of collisional ionization rates is then computed from H. W. Drawin, 1969, Z.Physik, **225**, 483 for all transitions to and from those lower levels whose index $\leq |\mathbf{LCH}^1|$. (For an A = 0 transition the Drawin rate is zero, and the Drawin rates for transitions whose lower level index = 1 are zero if $\mathbf{LCH}^1 = 0$. Such Drawin rates then replace the corresponding Kaulakys transitional rates that had already been computed.



The Hydrogen Lyman lines background opacity parameters are explained in Section 21, and in section INPUT of PANDORA's regular output file.



If no input values of \mathbf{DGM} are specified, and if $\mathbf{NGM} = 0$ has been specified explicitly, then $\mathbf{DGM}_i = 1$, $1 \leq i \leq \mathbf{N}$ is set up internally (this is the "general" default, as specified above). However, if no input vales of \mathbf{DGM} are specified, and if $\mathbf{NGM} = 0$ has not been specified (so that \mathbf{NGM} retains its built-in default value which is > 0), then "solar default" values of \mathbf{DGM}_i will be computed from \mathbf{DGMZ}_j , $1 \leq j \leq \mathbf{NGM}$. Here \mathbf{DGMZ} is a table appropriate for the quiet Sun, and is specified as a function of \mathbf{Z} , \mathbf{ZGM} . Values of \mathbf{DGM}_i corresponding to the input values of \mathbf{Z}_i are obtained by interpolation from the tables \mathbf{ZGM}_j and \mathbf{DGMZ}_j .

Note: $\mathbf{DGM}_i = 0$ is not acceptable.

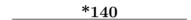
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The **CIMETHOD** and **CEMETHOD** statements each may contain an arbitrary number of nonnumeric codewords for specifying the set of methods for calculating automatic values of CI^j and/or $CE^{u,\ell}$. The **CIMETHOD** statement recognizes: CLARK, AR, VORONOV, JOHNSON, VS, SHAH, ONTHEFLY; while the **CEMETHOD** statement recognizes: SEATON, VREGE, SCHOLZ, PB, VS, JOHNSON, AGGRWL, ONTHEFLY. To enable a method, list its name in the pertinent statement; to turn off a method already enabled (say, because it is enabled by default) preface it with a minus sign (without intervening blank).

With these statements the user can specify method sets different from the default sets. It is necessary to turn off explicitly any unwanted methods that are already enabled! For example, to use only VS for all Hydrogen CI^j -values, use: "CIMETHOD (VS -SHAH -CLARK) ".

ONTHEFLY is a calculation mode, not a method.

See Section 19 for more details.



The **MATRIX** statement accepts control parameters for matrix manipulation. Their names are **DRPSW** (integer, default = 0), **EDJSW** (integer, default = 0), and **CRITJ** (floating point, default = 10^{-50}). When one or more of these names appear in a **MATRIX** statement, each name should be followed immediately by its desired input value. For example:

MATRIX (edjsw 1 critj 1.e-30)

When $\mathbf{DRPSW} = 1$: two lines of descriptive data will be written to the printout file for every matrix to be inverted.

When $\mathbf{EDJSW} = 1$ "junk" is edited out of every matrix prior to inversion or determinant calculation: find Y, the matrix element having the largest absolute value; compute $Z = \mathbf{CRITJ} \times |Y|$; and then set = 0 every matrix element whose absolute value is less than Z.

REFERENCE GUIDE

This is a listing of input parameters, in alphabetical order by description. Once a parameter's name has been identified by means of this list, its full specification can then be found in the main table at the start of this section.

KCOAA abbreviated form switch, Composite Line Analysis printout

KALHD Abort/Hi/Bye-system control parameter
 KALOR Abort/Hi/Bye-system control parameter
 LOGAS abscissa selector for location analysis graph

NABS absorber switch

AHM absorption coefficient for H-minus bound-free
BLIMG absorption/emission contributions graph limit
TLIMG absorption/emission contributions graph limit

JZOPT absorption/emission contributions graph Z-scale option

IPPOD absorption/emission dump, population ions

KONFORM absorption source function contributions detail print format switch

ABD abundance (see also Section 10)

RABD abundance ratio

IRPUN abundance ratio calculation output data switch

RABDL abundance ratio, logAEL added electrons

AL added recombination fractionACE added term for CE (default)ACI added term for CI (default)

CIJADD added term for CIJ
CKADD added term for CK

VX additional expansion velocity

NVX additional expansion velocity tables count
RKC additional photoionization parameter
TKR additional photoionization parameter
YKR additional photoionization parameter
WAVES additional wavelengths for opacity
WAVEMN additional wavelengths limit, automatic
WAVEMX additional wavelengths limit, automatic

PCE adjustment factor, FCE

INCH adjustment parameter (RHO weights)
SMP adjustment parameter (RHO weights)
WMN adjustment parameter (RHO weights)
WMX adjustment parameter (RHO weights)
WRMN adjustment parameter (RHO weights)
WRMX adjustment parameter (RHO weights)

CQM albedo multiplier
CQA albedo parameter
CQT albedo parameter
CLM albedo parameter
PNH albedo parameter
NAL ALN tables number

AOWXP alpha(old) weight exponent, Special-N1 (Diffusion)
IGMSW alternate GMMA for Hydrogen Lyman lines, PRD

BDAL Aluminum (neutral) departure coefficient
ALN Aluminum (neutral) level populations

ALK Aluminum-II (singly ionized) ground level population
LODCG ambipolar diffusion calculation graphs control code
NODCG ambipolar diffusion calculation graphs control code

CLEVELS ambipolar diffusion calculation parameter **IBETSW** ambipolar diffusion calculation parameter **IPDEE** ambipolar diffusion calculation parameter **FZION** ambipolar diffusion calculation parameter **IDFDI** ambipolar diffusion calculation parameter **IDFDM** ambipolar diffusion calculation parameter **IPDIJ** ambipolar diffusion calculation parameter ITN1R ambipolar diffusion calculation parameter KDIFD1 ambipoler diffusion calculation parameter MN1ambipolar diffusion calculation parameter MNG1 ambipolar diffusion calculation parameter NDSN1 ambipolar diffusion calculation parameter **NEFDF** ambipolar diffusion calculation parameter **ZXMIN** ambipolar diffusion calculation parameter **PALBET** ambipolar diffusion calculation term, Helium **PBETAL** ambipolar diffusion calculation term, Helium **PBETGM** ambipolar diffusion calculation term, Helium **PGMBET** ambipolar diffusion calculation term, Helium

AOWXP ambipolar diffusion, Special-N1, alpha(old) weight exponent NDSN1 ambipolar diffusion, Special-N1, calculation control switch SN1CC ambipolar diffusion, Special-N1, convergence criterion

N1NUP ambipolar diffusion, Special-N1, populations-of-the-run update switch ambipolar diffusion, Special-N1, simultaneous matrix print switch

WSN1D ambipolar diffusion, Special-N1, weight for N1 and NK

APDDIFC ambipolar diffusion velocity parameter
APDDTEXP ambipolar diffusion velocity parameter
APDXICA ambipolar diffusion velocity parameter
APDXICB ambipolar diffusion velocity parameter
APDXICC ambipolar diffusion velocity parameter
APDXICC ambipolar diffusion velocity parameter
ambipolar diffusion velocity parameter
ambipolar diffusion velocity parameter

SCTA amplitude, shock temperature SCVA amplitude, shock velocity

NANAL1 ANALYSIS depth selection parameter
 NANAL2 ANALYSIS depth selection parameter
 KANTNU analysis of TNU in radiative transitions

ADMAS angular diameter

IPERFA archive record, perfromance data, switch

ADS angular diameter ratio, Star/Sun

MFONT atmosphere data (Fontenla's format) output switch

JZATMO ATMOSPHERE zero-print mode switch

MODLAB atmospheric 'model name'NL atomic levels number

NSL atomic levels number, including supplementary levels

MASS atomic mass
NOION 'atom' switch

JZATOM ATOM zero-print mode switch

KXLYM augmentation switch for Lyman XK-table
 WAVEMN automatic additional wavelengths limit
 WAVEMX automatic additional wavelengths limit
 ESCTAU automatic use of escape probability

ZAUX auxiliary depths tableDDR auxiliary table for PRDXDR auxiliary table for PRD

IBNVIEW b calculation trace illustration, depth index for

NBS b smoothing level control index
 LSFFDB background for Line Source Function
 DOFDB background for Line Source Function

LEEDS background lines opacity debug printout switch (Helium-I)

 $\begin{array}{lll} \textbf{LHEDS} & \text{background lines opacity debug printout switch (Helium-II)} \\ \textbf{LYODS} & \text{background lines opacity debug printout switch (Hydrogen)} \\ \textbf{LOXDS} & \text{background lines opacity debug printout switch (Oxygen)} \\ \textbf{FNRMLA} & \text{background lines, Hydrogen Lyman } \alpha, \text{ normalizing factor} \\ \textbf{FNRMLB} & \text{background lines, Hydrogen Lyman } \beta, \text{ normalizing factor} \\ \end{array}$

BXI background lines standard frequencies

LSFBOC background opacity control

NLY background opacity, H Lyman lines limit

OML background opacity multiplier

NAB BANDL length

KARB 'banner' page character selector

VXS basic expansion velocity

IBNVIEW BD-calculation trace illustration, depth index for

BMWAC beam width parameter for eclipse continuum calculation

IBETSWbeta-equation selection switch, diffusion**IBETSW** β -equation selection switch, diffusion

TB blanketing temperature

DDL blended line components offsets
 DWN blended line components offsets
 CDL blended line components weights

SGRAF blended line emergent intensity graph switch

KBNDS boundary conditions switch for Special-N1 (diffusion)

AHM bound-free absorption coefficient for H-minus

EPCBR branching ratio

TX brightness temperature of illuminating source

BLCSW broadening components selector IBRDP broadening, ion, dump switch

V broadening velocity
VR broadening velocity

VNH broadening velocity, quiet Sun

MOPRNT built-in population-ion-model printout switch

DGM buoyancy factor (G-multiplier), HSE

DGMZ buoyancy factor (G-multiplier), HSE, standard table

KBX BXI length

KB1WA B1-weights depth indexKB1WB B1-weights depth index

KB1WS B1-weights type selection switch

BDCA Calcium (neutral) departure coefficient
CAN Calcium (neutral) level populations

CAK Calcium-II (singly ionized) ground level population

NCA CAN tables number

NCOSW Carbon Monoxide abundance computation switch

Carbon Monoxide lines = CO

NCOI Carbon Monoxide number density, input

MCON Carbon Monoxide number density output switch

BDC Carbon (neutral) departure coefficient
CN Carbon (neutral) level populations

CK Carbon-I (singly ionized) ground level population

FCE CE enhancement factors
CEMETHODCE method selection

INCEI CE-values comparion calculations depth index

ACE CE-values, default, addend

CEDMN CE-values default calculation parameter
CEDMX CE-values default calculation parameter
CEFEQ CE-values default calculation parameter
IXNCS CE-values default method switch (Hydrogen)

MCE CE-values, default, multiplier

JDMCE CE-values dump switch (Hydrogen)
IRFNC CE-values (Hydrogen) reference index

EXLYM change-over TAU for Lyman change-over TAU for Lyman

TSM change-over TAU for mean intensity and emergent intensity calculations

TMS change-over TAU for RT weight matrix method

TBAR change-over TAU for weight matrix KARB character selector for 'banner' page

NC charged particle density

IRFNC charged particle density reference value for CE and CI (Hydrogen)

LCEX charge exchange index

CCHX charge exchange, upper-level, parameter icxdp charge exchange, upper-level, parameter charge exchange, upper-level, parameter xrkh charge exchange, upper-level, term

XRLH charge exchange, upper-level, term

CIJADD CIJ added term IRATE CIJ printout

CIMETHOD CI method selection

INCEI CI-values comparion calculations depth index

ACI CI-values, default, addend

IXNCS CI-values default method switch (Hydrogen)

MCI CI-values, default, multiplier

JDMCI CI-values dump switch (Hydrogen)
IRFNC CI-values (Hydrogen) reference index

CKADD CK added term

WNJUNK 'cleanup' parameter for WN-matrix

NLC CN tables number

CO = Carbon Monoxide

CTCO CO abundance calculation temperature enhancement factor CTMX CO abundance calculation temperature enhancement limit

RCOMIN CO abundance, lower limitCOLINES CO isotope abundance ratio

ZRCO CO reference height

SHCOC CO scale height, chromospheric SHCOP CO scale height, photospheric

CTCO CO temperature enhancement factor
 CTMX CO temperature enhancement limit
 LCOD CO-lines absorption dump wavelength

LCOA CO-lines absorption limitLCOB CO-lines absorption limitCOLINES CO-lines control parameters

YCOL CO-lines method control parameter

COMU CO-lines mu value

SRCO CO-lines scattering ratio

NCOPT CO-lines statistics-keeping switch

MCOA CO-lines van der Waals damping multiplier

XCOL CO-lines wavelengths table

XCOMX CO-lines width limit

NCOI CO number density, input collisional excitation coefficient

CI collisional ionization coefficient

CKADD collisional ionization rate (CK), added term collisional transition rate (CIJ), added term

RFAC collision rates (all), reduction factor collision rates, forbidden transitions iCHDP collisions, Hydrogen, dump switch

LCH collisions, Hydrogen, codes ICHSW collisions, Hydrogen, switch

ZMASS column mass of gas

WFB component profiles weight, flow broadening

FMCDL components elimination criterion for Hydrogen Stark splitting
FRCDL components elimination criterion for Hydrogen Stark splitting

BLCSW components selector for line damping

KCOAA Composite Line opacity (Kurucz) abbreviated analysis printout

KODNTComposite Line opacity (Kurucz) data dump controlBANDEComposite Line opacity (Kurucz) eclipse switchALBKComposite Line opacity (Kurucz) parameterZALBKComposite Line opacity (Kurucz) parameter

BANDL Composite Line opacity (Kurucz) wavelength band
BANDU Composite Line opacity (Kurucz) wavelength band
LSFFDB constant background for Line Source Function
DOFDB constant background for Line Source Function

NDW constant Doppler width value index

NDWM constant Doppler width value index, for atmospheric model

CPRESS constant pressure

WPRESS constant pressure adjustment weight

KPC continuous opacity

MLC continuous opacity multiplier

SCOW Continuum Calculations output, selected wavelengths for

KAPDB continuum contributors control debug switch

BANDE continuum eclipse calculation switch

NECLIP continuum eclipse printout quantity selector

IFXDS continuum flux detail output control

YFLUX continuum flux weight matrix damping parameter

NUC continuum frequency interval, auxiliary

NUK continuum frequency interval

WNUC continuum frequency interval, auxiliary

WNUK continuum frequency interval

JSTCN 'continuum-only' run type switch

CSFCRIT Continuum Source Function convergence criterion

IDRCD Continuum Source Function debug printout disk ray index
 IMUCD Continuum Source Function debug printout MU index
 ISRCD Continuum Source Function debug printout shell ray index

TOPE 'Continuum Summary Graph' file

XK continuum transition standard frequencies
ICDIT continuum wavelengths selector for dI/dh
CORMAX CONTRIBUTORS printouts wavelength limit
CORMIN CONTRIBUTORS printouts wavelength limit
LSFBOC control parameter for line background opacity

MATRIX control parameter for matrix generation and inversion

PROGLI control parameter for profile graphs

BANDY control parameter for source function method YCONT control parameter for source function method YHMcontrol parameter for source function method YKR control parameter for source function method \mathbf{YL} control parameter for source function method YLINE control parameter for source function method YRATE control parameter for source function method **YWAVE** control parameter for source function method

NCOI CO number density, input

CSFCRIT convergence criterion for Continuum Source Function

EIDIF convergence criterion for NE-iterations **PRDCV** convergence criterion for PRD-iterations SN1CC convergence criterion, Special-N1 (diffusion) **IHSDD** convolved Hydrogen Stark profile dump switch **IHSDP** convolved Hydrogen Stark profile dump switch **HSBDMN** convolved Hydrogen Stark profile parameter **HSBDMX** convolved Hydrogen Stark profile parameter **HSBFEQ** convolved Hydrogen Stark profile parameter **HSBM** convolved Hydrogen Stark profile parameter **CSTARK** convolved Hydrogen Stark profile switch **IHSSW** convolved Hydrogen stark profile switch

KHFFS cooling rate components controlKOOLSUM cooling rate components control

BLIMG coordinate limit for graph of absorption contributors
 NGRL coordinate limit for graph of absorption contributors
 NGRR coordinate limit for graph of absorption contributors
 TLIMG coordinate limit for graph of absorption contributors

ICR coronal incident radiation
 COMU cosine of look-angle for CO
 MUF cosine of look-angle for flux
 MU cosine of look-angle for intensity

NCQ CQT length

criterion for automatic use of escape probability solution
 criterion for DEL in Line Source Function calculation
 criterion for rcheck (diffusion calculation, Special-N1)

RHOCR criterion for RHO calculation

SMATC criterion for selection for matrix samples output
CCHX cross-section multiplier, upper-level charge-exchange

LMZ cut-off for Lyman- α wing opacity

VOITC cut-off for Voigt profile function recomputation

TML cut-off TAU for intensity integralsBLCSW damping components selector

DPMULT damping multiplierY damping parameterYPRE damping parameter

YFLUX damping parameter for continuum flux KDAMP damping switch for Special-N1 (diffusion)

IDEDP d-coefficients (diffusion calculation) debug printout switch

IDFDI d-coefficients (diffusion calculation) dump index

IDFDMd-coefficients (diffusion calculation) method selection switchNEFDFd-coefficients (diffusion calculation) NE selection switch

IPDEE d-coefficients (diffusion calculation) print switch d-coefficients (diffusion calculation) smoothing

LDL DDL length

IPR01 debug printout limit index (Line Source Function)
 IPR02 debug printout limit index (Line Source Function)
 IPR03 debug printout limit index (Line Source Function)

IPR04 debug printout limit index (Line Source Function)

KAPDB debug printout switch for continuum contributors control

IDEDP debug printout switch for diffusion d-coefficients

LEEDS debug printout switch for Helium-I lines background opacity

LHEDS debug printout switch for Helium-II lines background opacity

JDMCE debug printout switch for Hydrogen CE-values
JDMCI debug printout switch for Hydrogen CI-values
ICHDP debug printout switch for Hydrogen collisions

LYODS debug printout switch for Hydrogen Lyman lines background opacity

ISMBD debug printout switch for intensity integration (SIMBA)
 IBRDP debug printout switch for ion broadening (Hydrogen)
 LOXDS debug printout switch for Oxygen lines background opacity

ISNUD debug printout switch for PRD SNU-shift

IXASM debug printout switch for smoothing-dump (IPEX=15) details

ISNDD debug printout switch for S(n) calculation
 ITRFI debug printout switch for TR-iteration
 CEDMN default CE-values calculation parameter
 CEDMX default CE-values calculation parameter
 CEFEQ default CE-values calculation parameter
 IXNCS default CE-values method selector (Hydrogen)

IXNCS default CE-values method selector (Hydrogen)
IXNCS default CI-values method selector (Hydrogen)

PMSK default Stark halfwidth multiplier

DELLIM DEL-criterion for DIRECT vs. FULL source function solution

DELWAVE deletion wavelengths

INFSM delimiter for Lyman RK-1 smoothing
 INLSM delimiter for Lyman RK-1 smoothing
 PROGLI delta-lambda limit for profile graphs

NWS DELWAVE length

DLSF denominator of line source function, limit for

VSMLL denominator = 0, replacement for

BD departure coefficient

BDAL departure coefficient, Aluminum
BDCA departure coefficient, Calcium
BDC departure coefficient, Carbon

WBDIR departure coefficient (direct) weight

DELTB departure coefficient editing parameter

BDFE departure coefficient, Iron **BDHE** departure coefficient, Helium BDHE2 departure coefficient, Helium-II **BDH** departure coefficient, Hydrogen **BDHM** departure coefficient, H-minus **BDMG** departure coefficient, Magnesium **BDO** departure coefficient, Oxygen BDO2departure coefficient, Oxygen-II departure coefficient, Oxygen-III BDO3 **BDSI** departure coefficient, Silicon BDSdeparture coefficient, Sulphur departure coefficient, Sodium **BDNA**

JBFSW departure coefficients method switch for supplementary levels

JBDNC departure coefficients ratio and Rho calculations bypass switch

NBS departure coefficients smoothing level index WBD departure coefficients updating weight

Z depth

ZAUX depth, auxiliary

IDRDP depth index for DRDMP

INCEI depth index for CI,CE comparison calculations

LHHSE depth index for H and M ins HSE

ICHDP depth index for Hydrogen collisions dump

JEDIT depth index for N-editing

IHEAB depth index for RHEAB calculation
 JSSV depth index for shock temperature
 ISSV depth index for shock velocity

ISOD depth index for Sobolev integration dump

IBNVIEW depth index for illustration of trace of BD- and ND-calculations

KLDIN depth interval for Lyman dump

IPRDD depth interval for partial redistribution printoutMN1 depth limit for N1 recalculation, ambipolar diffusion

IORICdepth-of-formation (line center) print switchNANAL1depth selection parameter for profile ANALYSISNANAL2depth selection parameter for profile ANALYSISRHEABdepth variation of total Helium abundance

KDIFD1 derivatives calculation method selection switch

LDFD1 derivatives smoothing control switch

LEVDES designation of atomic levelUSE designation of input file

IXFDS detail print control parameter for continuum flux
 IHDMP detail print control parameter for 'H' calculation
 JNEDP detail print control parameter for N-editing

LDINT detail print control parameter for transition terms
 LDTYP detail print control parameter for transition terms
 KONFORM detail print format switch for opacity and BHS

IDFSW detail print switch, dI/dh (line profiles)

IPPOD detail print switch, population ions absorption/emission

IXASM detail print switch, smoothing dump (IPEX=15) **LSTMP** detail print switch, STIM for GTN calculation

IWEIT detail print switch, weightingIRUNT development run switch

NGM DGMZ length

AW diagonal, integrated, of WN-matrix

ADS diameter, angular ADMAS diameter, angular

ICDIT dI/dh continuum wavelengths selector IDFSW dI/dh details print switch (line profiles)

IPDEE diffusion (ambipolar) d-coefficients print switch

LODCGdiffusion (ambipolar) graphs control codeNODCGdiffusion (ambipolar) graphs control code

CLEVELS diffusion (ambipolar) parameter diffusion (ambipolar) parameter **FZION IBETSW** diffusion (ambipolar) parameter **IDFDI** diffusion (ambipolar) parameter **IDFDM** diffusion (ambipolar) parameter **IPDEE** diffusion (ambipolar) parameter **IPDIJ** diffusion (ambipolar) parameter diffusion (ambipolar) parameter KDIFD1 MN1diffusion (ambipolar) parameter MNG1 diffusion (ambipolar) parameter **NEFDF** diffusion (ambipolar) parameter **ZXMIN** diffusion (ambipolar) parameter

IPDIJ diffusion analysis (DIJ) printout switch
 MXTAP diffusion calculation, KZAUG sum limit
 MXPPI diffusion calculation, KZAUG value limit

ITKZA diffusion calculation, Z-augmentation iteration limit

IDEDP diffusion d-coefficients debug printout switch

AOWXP diffusion (Special-N1) parameter CN1S diffusion (Special-N1) parameter I4DEQ diffusion (Special-N1) parameter I4DFM diffusion (Special-N1) parameter diffusion (Special-N1) parameter I4DIO **KBNDS** diffusion (Special-N1) parameter **KDAMP** diffusion (Special-N1) parameter **KDIAG** diffusion (Special-N1) parameter NDSN1 diffusion (Special-N1) parameter N₁MET diffusion (Special-N1) parameter N₁NUP diffusion (Special-N1) parameter

PALBETdiffusion term, HeliumPBETALdiffusion term, HeliumPBETGMdiffusion term, HeliumPGMBETdiffusion term, Helium

MDFG diffusion terms output switch

APDDIFC diffusion velocity (ambipolar) parameter diffusion velocity (ambipolar) parameter

MDFV diffusion velocity output switch IPDIJ DIJ printout switch, diffusion

DLU dilution factor

WBDIR 'direct' calculation of departure coefficient, weight
 DELLIM DIRECT calculation of Line Source Function
 LSFTYP DIRECT calculation of Line Source Function

OMIT disable program options

ISCRS disk file (temporary) control switch

R1N distance from illuminating source VSMLL divisor = 0, replacement for

IDNRT DNRT, DNRTC (Lyman) calculation switch

IDWIN Doppler width recomputation dump index increment

NDW Doppler width reference index

NDWM Doppler width reference index, for atmospheric model

ZNDW Doppler width reference index criterion

LMDL2 DR parameter, Hydrogen Lyman lines background opacity
LMDL3 DR parameter, Hydrogen Lyman lines background opacity
LMDR DR parameter, Hydrogen Lyman lines background opacity
LMXC DR parameter, Hydrogen Lyman lines background opacity
LMXP DR parameter, Hydrogen Lyman lines background opacity
LMXX DR parameter, Hydrogen Lyman lines background opacity

DDRDR parameter, PRD transitions DR parameter, PRD transitions DRLIM **TAUCL** DR parameter, PRD transitions \mathbf{XC} DR parameter, PRD transitions XCLDR parameter, PRD transitions XDRDR parameter, PRD transitions \mathbf{XP} DR parameter, PRD transitions \mathbf{XR} DR parameter, PRD transitions

IDRDP DRDMP depth indexKDRDP DRDMP frequency index

dump = debug printout

KLDIN dump, Lyman, depth intervalKLFIN dump, Lyman, frequency interval

JHBFD dump switch, H-bf background absorbers and emittersIPPOD dump switch, population ions absorption/emission

WORLDLY dump switch, storage management system

LCOD dump wavelength for CO-lines absorption calculation

ALBDUSTDust albedo (Type-1)ALBDTDust albedo (Type-2)

KDUST Dust constant

EPDUST Dust dilution factor

DFDUST Dust factor

ADT Dust opacity function

TDUST Dust temperature

TDST Dust temperature (Type-2)

DDT Dust temperature (Type-2) iteration criterion
 MDTR1 Dust temperature (Type-2) iteration criterion
 MDTR2 Dust temperature (Type-2) iteration criterion

LMDUST Dust wavelengths table

IDWIN DW recomputation dump index increment

BANDE eclipse calculation switch for Composite Line Opacity bands

BMWAC eclipse continuum calculation beam width parameter

ZECL eclipse continuum calculation Z values

ECLI eclipse line profiles switchNERM EDITH error messages limit

NED edit index for RHO

DELTB edit parameter for departure coefficients
 LME edit parameter for Lyman Epsilon-1
 LMF edit parameter for Lyman Epsilon-1
 LMT edit parameter for Lyman Epsilon-1

DRHO edit parameter for RHO
ISMVE edit switch, small values

A Einstein A

RZM electron-contributing metals multiplier NMT electron-contributing metals number

NE electron density

EIDIF electron density iterations convergence criterion

NEFDF electron density values for d-coefficients (diffusion)

ZMEelectron ratio, non-HAELelectrons, addedQNLelectrons, " $n\ell$ "ELEMENTelement data

NMT element data tables length

ELSYM element symbol of the ion of the run

FMCDL elimination criterion for Hydrogen Stark splitting components elimination criterion for Hydrogen Stark splitting components

IPPOD emission/absorption dump switch, population ions

DO enable program options

ELLED energy (particle) dissipation parameter

EMXED energy (particle) dissipation parameter NSPED energy (particle) dissipation parameter

FCE enhancement factors, CE RKMULT enhancement factors, RK

METEP Epsilon (Lyman) method parameter
QTAIL Epsilon (Lyman) Q-smoothing tail

EP1 Epsilon-1 (Lyman)

EPCBR Epsilon-1 (Lyman) branching ratio LMAEpsilon-1 (Lyman) edit parameter LMBEpsilon-1 (Lyman) edit parameter \mathbf{LME} Epsilon-1 (Lyman) edit parameter \mathbf{LMF} Epsilon-1 (Lyman) edit parameter LMREpsilon-1 (Lyman) edit parameter \mathbf{LMT} Epsilon-1 (Lyman) edit parameter WEP Epsilon-1 (Lyman) weighting parameter

EP2 Epsilon-2 (Lyman)

NERM error messages limit for EDITH

LSFTYP escape probability approximation for RHO **ESCTAU** escape probability criterion, for automatic use

SOBOLEV escape probability (Sobolev) parameter
SOBDMN escape probability (Sobolev) parameter
SOBDMX escape probability (Sobolev) parameter
SOBFEQ escape probability (Sobolev) parameter
vsb escape probability (Sobolev) parameter
escape probability (Sobolev) velocity
vsb every-line switch for ORIGIN printout
excitation coefficient, collsisional

TEX excitation temperature

IXSTA execution statistics printout control

VX expansion velocity, additional
 VXS expansion velocity, basic
 CVX expansion velocity parameter
 CVXS expansion velocity parameter

JSFEX explanation printing switch (line source function solution)

PW exponent in Stark broadening term
MTHEI exponential integral method selector
OPF extinction factor for incident radiation

IDEX extra standard-output (log file) information switch

IPEX extra printout switch (for debugging)

RFAC factor for all collision rates

DRIN factor for diffusion reduction (initial value)

CUTFE fast electrons calculation parameter **DQMAX** fast electrons calculation parameter **DQMIN** fast electrons calculation parameter NNDFE fast electrons calculation parameter **NVDFE** fast electrons calculation parameter NVFfast electrons calculation parameter NXFfast electrons calculation parameter fast electrons calculation parameter NZDFE RCCFE fast electrons calculation parameter **VMNFE** fast electrons calculation parameter **XJFE** fast electrons calculation parameter **XQMAX** fast electrons calculation parameter

PCEFCE adjustment factor NFEFEN tables number **BHORIZ** field strength, magnetic USE file designation for input **CVXF** flow broadening parameter \mathbf{CVXM} flow broadening parameter FBVMXflow broadening parameter FNHflow broadening parameter **HNDF** flow broadening parameter NFBflow broadening parameter NFH flow broadening parameter WFB flow broadening parameter

CHEFLOW flow constant, Helium, for RHEAB calculation

FNH flow velocity table, standard

VX fluid velocity
VXS fluid velocity

CDZ fluid velocity parameter
 CVSB fluid velocity parameter
 CVX fluid velocity parameter
 CVXS fluid velocity parameter

CVZ fluid velocity parameterFMVLIM fluid velocity parameter

LFLUX flux distribution (line) calculation control switch
DOFLUX flux distribution (line) calculation control switch

NFH FNH length

MFONT Fontenla atmosphere data output switch
 FROSCE forbidden transition, oscillator strength
 ISMSW format switch for iterative summaries

I4DEQ four-diagonal method control parameter, Special-N1 (diffusion)
 I4DFM four-diagonal method control parameter, Special-N1 (diffusion)
 I4DIO four-diagonal method control parameter, Special-N1 (diffusion)

LHM frequencies for H-minus

BXI frequencies, standard, for background linesXK frequencies, standard, for continuum transitions

XI frequencies, standard, for line transitions
XIBLU frequencies, standard, for line transitions
XIBLUT frequencies, standard, for line transitions
XIRED frequencies, standard, for line transitions
XIREDT frequencies, standard, for line transitions
XISYM frequencies, standard, for line transitions
XISYMT frequencies, standard, for line transitions

LSFFDB frequency-dependent background for Line Source Function **DOFDB** frequency-dependent background for Line Source Function

KDRDP frequency index for DRDMP

KLFIN frequency interval for Lyman dump

IPRDF frequency interval for partial redistribution printout

NU frequency intervalsWNU frequency intervals

MRR FRR length

IPIJG fudging of GNV in PIJ-calculation

DELLIMFULL calculation of Line Source Function**DGAMMA**gamma $(\gamma^{u\ell})$ parameter, PRD transitions**GAMMA**gamma $(\gamma^{u\ell})$ parameter, PRD transitions

ZMASS gas column mass

GK Gaunt factors for Level- \mathcal{N} -to-Continuum transfer calculation

Z geometrical depth

DGM G-multiplier, HSE

DGMZ G-multiplier, HSE, standard table

KDIFGA GNV-fudging depth indexKDIFGB GNV-fudging depth indexIPIJG GNV-fudging, PIJ-calculation

KDIFGS GNV-fudging switch

NGNV GNV suppression level limit

MNG1 GNV-1 replacement limit index (ambipolar diffusion)

XMU GR-weight-matrix MU table

LODCGgraph, diffusion calculations, control codeNODCGgraph, diffusion calculations, control codeLSFGCgraph, Line Source Function, control code

PROGLI graph, profiles, delta-lambda limit

NGRLgraph Z-scale limitNGRRgraph Z-scale limitIZOPTgraph Z-scale option

JZOPT graph Z-scale option for absorption/emission contributions

CLOGG gravity, surface, log of

CGR gravity ratio, with respect to Sun

LSTMP GTN calculation print switch for STIM details

LHHSE H (HSE) reference depth index

JHEAS HEABD (secret switch)

KARB 'header' page character selector

CHEFLOW Helium abundance calculation parameter
 HEABL Helium abundance calculation parameter
 Helium abundance calculation parameter
 RFHEAB Helium abundance calculation parameter
 RFHEAB Helium abundance coefficient reduction factor

RHEAB Helium abundance depth variationHEABL Helium abundance limit factor

PALBET Helium diffusion term
 PBETAL Helium diffusion term
 PBETGM Helium diffusion term
 PGMBET Helium diffusion term

LEEDS Helium lines background opacity debug printout switch

BDHE Helium (neutral) departure coefficient

HEN Helium (neutral) level populations

YH Helium-to-Hydrogen ratio

LHEDS Helium-II lines background opacity debug printout switch

BDHE2 Helium-II (singly ionized) departure coefficientHEK Helium-II (singly ionized) ground level population

HE2N Helium-II (singly ionized) level populations

HE304 Helium-II $\lambda 304$ line mean intensity

HE2K Helium-III (doubly ionized) ground level population

NLZ HEN tables number
NZ2 HE2N tables number
M304 HE304 reference index

KALHD Hi/Bye/Abort-system control parameter
 KALOR Hi/Bye/Abort-system control parameter
 AL higher levels recombination fraction

NLH HN tables number

HNAJL HND adjustment factor limit for HSE

NFH HNDF length
NVH HNDV length
CLNH HSE parameter
HNAJL HSE parameter
HTAU HSE parameter
LHHSE HSE parameter
PZERO HSE parameter

DGM HSE parameter (buoyancy factor, or G-multiplier)

DGMZ HSE parameter, standard table

HEL HSE weightHSEC HSE weight

JHBFD Hydrogen bound-free absorption and emission details printout

IXNCS Hydrogen CE-values method switch
 IXNCS Hydrogen CI-values method switch
 ICHDP Hydrogen collisions dump depth index

LCH Hydrogen collisions codesICHSW Hydrogen collisions switch

NH Hydrogen density

HNDF Hydrogen density table for FNHHNDV Hydrogen density table for VNH

CPRESS Hydrogen density recalculation parameterWPRESS Hydrogen density recalculation parameter

BDH Hydrogen departure coefficient

KHFFS Hydrogen free-free cooling rate controlIBRDP Hydrogen ion broadening dump switch

HN Hydrogen level populations

FNRMLA Hydrogen Lyman α simulated background profile normalizing factor **FNRMLB** Hydrogen Lyman β simulated background profile normalizing factor

IGMSW Hydrogen Lyman lines alternate GMMA, PRD

Hydrogen Lyman lines background opacity, DR parameter LMDL2LMDL3 Hydrogen Lyman lines background opacity, DR parameter Hydrogen Lyman lines background opacity, DR parameter LMDR LMXC Hydrogen Lyman lines background opacity, DR parameter \mathbf{LMXP} Hydrogen Lyman lines background opacity, DR parameter LMXX Hydrogen Lyman lines background opacity, DR parameter **JHLSK** Hydrogen Lyman lines background opacity parameter LLY Hydrogen Lyman lines background opacity parameter **LMCR** Hydrogen Lyman lines background opacity parameter LMDL2 Hydrogen Lyman lines background opacity parameter Hydrogen Lyman lines background opacity parameter

LMDL3
Hydrogen Lyman lines background opacity parameter
LMDR
Hydrogen Lyman lines background opacity parameter
LMH
Hydrogen Lyman lines background opacity parameter
LMXC
Hydrogen Lyman lines background opacity parameter
LMXP
Hydrogen Lyman lines background opacity parameter
LMXX
Hydrogen Lyman lines background opacity parameter
LMXX
Hydrogen Lyman lines background opacity parameter
NQLYM
Hydrogen Lyman lines background opacity parameter

IGMSW Hydrogen Lyman lines GMMA, PRD

NLY Hydrogen Lyman lines limit, background opacity

YK Hydrogen recombination parameter

KHFFS Hydrogen-run total cooling rate components control
KOOLSUM Hydrogen-run total cooling rate components control
HSBDMN Hydrogen Stark broadening calculation parameter
HSBDMX Hydrogen Stark broadening calculation parameter
HSBFEQ Hydrogen Stark broadening calculation parameter
HSBM Hydrogen Stark broadening calculation parameter
HYDROGEN STARK Broadening calculation table limits

IHSSM Hydrogen Stark broadening calculation table limits

IHSDD Hydrogen Stark broadening dump switchIHSDP Hydrogen Stark broadening dump switch

CSTARK Hydrogen Stark broadening switch **IHSSW** Hydrogen Stark broadening switch **CSDW** Hydrogen Stark splitting parameter **FMCDL** Hydrogen Stark splitting parameter FRCDL Hydrogen Stark splitting parameter **FSTKM** Hydrogen Stark splitting parameter **ISTARK** Hydrogen Stark splitting parameter **STARKI** Hydrogen Stark splitting parameter **IHSSP** Hydrogen Stark splitting switch

AHM H-minus bound-free absorption coefficient

YHM H-minus Continuum Source Function method control parameter

BDHM H-minus departure coefficient LHM H-minus wavelengths table

NHTWS H2 abundance computation switch
CEQMX H2 abundance control parameter
MH2N H2 number density output switch

TX illuminating source brightness temperature

IBNVIEW illustration of trace of BD- and ND-calculations, depth index for

R1N illuminating source distance

CEDMN impact-parameter CE-values calculation parameter
 CEDMX impact-parameter CE-values calculation parameter
 CEFEQ impact-parameter CE-values calculation parameter

TX incident radiation, brightness temperature of illuminating source

ICR incident radiation, coronal

DLU incident radiation dilution factor

OPF incident radiation extinction parameter
IRTIS incident radiation input interpolation switch

FINK incident radiation input parameter
XINK incident radiation input parameter

NBS index for b-smoothing KB1WA index for B1-weights KB1WB index for B1-weights

INCEI index for CE-values comparison calculations

ICXDP index for charge-exchange (upper-level) dump printout

INCEI index for CI-values comparison calculations
 IDFDI index for d-coefficients detailed printout
 PROGLI index for delta-lambda axis in profile graphs

KKPR index for detailed Lyman printout

IDRCD index for disk rays, Continuum Source Function debug printout

IDRDP index for DRDMP
 KDRDP index for DRDMP
 KDIFGA index for GNV-fudging
 KDIFGB index for GNV-fudging
 LHHSE index for HSE H and M

KOLEV index for Level- \mathcal{N} -to-Continuum transfer calculation

NMLR index for mass-loss-rateJEDIT index for N-editing

JH1 index for photoionization rates multiplierJH2 index for photoionization rates multiplier

NDW index for reference Doppler width

NDWM index for reference Doppler width, for atmospheric model M304 index for reference value of He-II λ 304 line mean intensity

IHEAB index for RHEAB calculationJSSV index for shock temperatureISSV index for shock velocity

ISRCD index for shell rays, Continuum Source Function debug printout

ISOD index for Sobolev integration dump

IBNVIEW index for illustration of trace of BD- and ND-calculations
 IMUCD index for XMU, Continuum Source Function debug printout

IDWIN index-increment for DW dump

ISCRS 'in memory' scratch I/O mode switch

NT INPAIR length
USE input file designation

INDRN input number densities, renormalization switch

REFLM input TAUK reference wavelength

INRHO input-RHO-only switch

AW integrated diagonal of WN-matrix

ISOD integration (Sobolev) dump depth index

YRATE integrations wavelengths damping parameter for rates calculations

WRATMN integrations wavelengths limit for rates calculationsWRATMX integrations wavelengths limit for rates calculations

TML intensity integral TAU cut-offTSM intensity integral TAU cut-off

ISMBD intensity integration (SIMBA) dump intervalIRTIS interpolation switch for incident radiation data

KLDIN interval, depth, for Lyman dump

IPRDDinterval, depth, for partial redistribution printoutISMBDinterval for intensity integration (SIMBA) dump

KLFIN interval, frequency, for Lyman dump

IPRDF interval, frequency, for partial redistribution printout

TRFLI interval limit for TR-effective calculation

MATRIX inversion control parameters

IBRDP ion broadening (Hydrogen) dump switch

ISCRS I/O (scratch) mode switch
CI ionization coefficient, collisional

CP ionization data, K-shell QIN ionization data, K-shell

IXNCS ionization potential lowering (Hydrogen)

IONSTAGE ionization stage of ion of run

MASS ion massNAME ion name

 ${\bf RUNTOPOP}$ ion-of-the-run level correspondences

NOION ion switch

BDFE Iron (neutral) departure coefficient
FEN Iron (neutral) level populations

FEK Iron-II (singly ionized) ground level population
NFB isotropic flow broadening velocities, number of
ITRFI iteration (effective TR) debug output control

HSLITER iteration limitIOMX iteration limitISUB iteration limitLYMITER iteration limit

ITN1R iteration limit (diffusion calculation)

ITPRD iteration limit, PRD

ISMSW iterative summaries format switch

WORLDLY IWORLD dump control switchJNUNC JNU input switch for PRDWNJUNK 'junk' criterion for WN-matrix

TE kinetic temperature

KMMAX KM limit

CP K-shell photoionization data
QIN K-shell photoionization data

Kurucz Composite Line Opacity control parameter
 KODNT
 Kurucz Composite Line Opacity data dump control
 BANDL
 Kurucz Composite Line Opacity wavelength band
 BANDU
 Kurucz Composite Line Opacity wavelength band

ALBK Kurucz opacity parameter
CQA Kurucz opacity parameter
CQM Kurucz opacity parameter
CQT Kurucz opacity parameter
ZALBK Kurucz opacity parameter

MKURU Kurucz spectrum calculations data output switchKUDNT Kurucz Statistical Line Opacity data dump control

KUR
 KURIN
 KURUZ Statistical Line Opacity parameter
 KURMA
 KURMI
 KURMI Kurucz Statistical Line Opacity parameter
 KURMI Kurucz Statistical Line Opacity parameter
 MXTAP
 KZAUG sum limit (diffusion calculation)
 MXPPI
 KZAUG value limit (diffusion calculation)

LDLMAX LDL maximumNDT LDT lengthLEVDES level designation

NBS level index for b-smoothing

NL levels number

NSL levels number, including supplementaries

MHM LHM length

HEABL limit factor for RHEAB calculationFMVLIM limit for fluid velocity multiplier

NLY limit for Hydrogen Lyman lines, background opacity

HNAJL limit for NH adjustment in HSE calculation
PARTLIM limit for partition function component

LN limit for saturation approximation in Lyman calculation

XCOMX limit for width of CO-lines

MNG1 limit index for GNV-1 replacement (ambipolar diffusion)
MN1 limit index for N1 recalculation (ambipolar diffusion)

IPR01 limit index for 'PERDMPn' debug printouts
 IPR02 limit index for 'PERDMPn' debug printouts
 IPR03 limit index for 'PERDMPn' debug printouts
 IPR04 limit index for 'PERDMPn' debug printouts

BLIMG limiting index for graph of absorption/emission contributors

TLIMG limiting index for graph of absorption/emission contributors

DLSF limiting value for denominator of line source function

KMMAX limiting value for XIFUL length

TLTR limiting multiplier for TDST recalculation
TRFLI limit interval for TR-effective calculation
NERM limit on some error messages from EDITH

CORMAX limit wavelength for ORIGINS and CONTRIBUTORS printouts
CORMIN limit wavelength for ORIGINS and CONTRIBUTORS printouts

DDL line, blended, component offset
 DWN line, blended, component offset
 CDL line, blended, component weight
 BLCSW line broadening components switch

IORIC line-center depths-of-formation print switch

LFLUX Line Flux Distribution (H) calculation control switch
DOFLUX Line Flux Distribution (H) calculation control switch

LSFBOC line opacity background control
OML line opacity background multiplier

OLL line opacity multiplier

LWNT 'Line Opacity' printout wavelengths interval

PROGLI line profiles graphs control parameter
PROGLI line profiles graphs delta-lambda axis limit

LOGAS line profiles graphs switchSGRAF line profiles graphs switch

DOPROF line profiles switchPROF line profiles switch

Line Source Function background

DOFDB Line Source Function background

ISCOMP Line Source Function comparisons printout details switch

IPR01 Line Source Function debug printout limit index
 IPR02 Line Source Function debug printout limit index
 IPR03 Line Source Function debug printout limit index
 IPR04 Line Source Function debug printout limit index
 DLSF Line Source Function denominator, limiting value for
 JSFEX Line Source Function explanation printing switch

LSFGC Line Source Function graph control code

ESCTAU Line Source Function method selection criterion

DOSFPRNT Line Source Function printout **LSFPRINT** Line Source Function printout LSFTYP Line Source Function type selector XIline transitions standard frequencies **XIBLU** line transitions standard frequencies **XIBLUT** line transitions standard frequencies **XIRED** line transitions standard frequencies **XIREDT** line transitions standard frequencies **XISYM** line transitions standard frequencies **XISYMT** line transitions standard frequencies **INPAIR** list of indices defining line transitions

LDU LMDUST lengthJM LMM lengthLLY LMXX length

LOGAS location analysis graph switch

CLOGG log(surface gravity)

MUF look-angle cosines for fluxMU look-angle cosines for intensity

IXNCS lowering of ionization potential (Hydrogen)

NS lower level of reference transition RCOMIN lower limit for CO abundance

LMZ Lyman- α wing background opacity cut-off

LN Lyman calculation parameter

EXLYM Lyman change-over TAU parameter
TGLYM Lyman change-over TAU parameter

XK Lyman continuum transitions standard frequencies

KKPR Lyman detail print frequency index

IDNRT Lyman DNRT, DNRTC calculation switch

KLDIN Lyman dump depth intervalKLFIN Lyman dump frequency intervalMETEP Lyman Epsilon method parameter

EP1 Lyman Epsilon-1

LMA
 Lyman Epsilon-1 edit parameter
 LMB
 Lyman Epsilon-1 edit parameter
 LME
 Lyman Epsilon-1 edit parameter
 LMF
 Lyman Epsilon-1 edit parameter
 LMR
 Lyman Epsilon-1 edit parameter
 LMT
 Lyman Epsilon-1 edit parameter
 LMT
 Lyman Epsilon-1 weighting parameter
 WEP

EP2 Lyman Epsilon-2
 GK Lyman Gaunt factor
 LYMITER Lyman iteration limit
 KOLEV Lyman level index

LYODS Lyman lines background opacity debug switch **JHLSK** Lyman lines background opacity parameter \mathbf{LLY} Lyman lines background opacity parameter LMCR Lyman lines background opacity parameter LMDL2 Lyman lines background opacity parameter LMDL3 Lyman lines background opacity parameter LMDRLyman lines background opacity parameter LMHLyman lines background opacity parameter LMXCLyman lines background opacity parameter \mathbf{LMXP} Lyman lines background opacity parameter $\mathbf{L}\mathbf{M}\mathbf{X}\mathbf{X}$ Lyman lines background opacity parameter **NQLYM** Lyman lines background opacity parameter

INFSM Lyman RK-1 smoothing delimiter
 INLSM Lyman RK-1 smoothing delimiter
 WSM Lyman RK-1 smoothing parameter
 LN Lyman saturation approximation limit
 XKLYM Lyman XK-table augmentation switch

LHHSE M (HSE) reference depth index

BDMG Magnesium (neutral) departure coefficient
MGN Magnesium (neutral) level populations

MGK Magnesium-II (singly ionized) ground level population

BHORIZ magnetic field strengthNMLR mass loss rate index

LPMLR mass loss rates printout switch

VM mass motion velocity

MASS mass of atom
ZMASS mass of gas column

RFMAS mass, reference

MAMAS matrix elements magnitude scan switch

MATRIX matrix inversion and generation control parameter

SMATC matrix sample output selection criterion FBVMX maximum value of flow broadening velocity

LDLMAX maximum value of LDL

KMMAX maximum value of XIFUL length

JBAR mean intensity

HE304 mean intensity of He-II λ 304 line

M304 mean intensity of He-II λ 304 line reference index

TSM mean intensity change-over TAU

NERMmessages limit for EDITHRZMmetal-electrons multiplierZMEmetal-electrons ratio

ELEMENT metals data

YCOL method control parameter YCONT method control parameter YCR method control parameter YHM method control parameter YKRmethod control parameter YLmethod control parameter YLDT method control parameter YLINE method control parameter **YLYM** method control parameter YRATE method control parameter **YWAVE** method control parameter

IDFDM method control parameter for d-coefficients (diffusion calculation)

IXNCSmethod control parameter for Hydrogen CI-valuesMETEPmethod control parameter for (Lyman) Epsilons

I4DEQ method control parameter for Special-N1 (diffusion)
I4DFM method control parameter for Special-N1 (diffusion)
I4DIO method control parameter for Special-N1 (diffusion)
KBNDS method control parameter for Special-N1 (diffusion)
KDAMP method control parameter for Special-N1 (diffusion)
KDIAG method control parameter for Special-N1 (diffusion)
N1MET method control parameter for Special-N1 (diffusion)

METSE method control parameter for statistical equilibrium equations
 METSEDG method control parameter for statistical equilibrium equations
 METSEDW method control parameter for statistical equilibrium equations

CEMETHOD method selection, CE calculation **CIMETHOD** method selection, CI calculation

NMG MGN tables number
 V microturbulence velocity
 VR microturbulence velocity

VNH microturbulence velocity, quiet Sun
IRATE 'minimal' RATES calculation printout

MODLAB 'model name,' atmospheric

ISCRS mode switch for scratch I/O

molecular Hydrogen = H2

NHTSW molecular Hydrogen abundance computation switch

LF MUF lengthCOMU MU for COMUF MU for flux

XMU MU for GR-weight matrix

MU MU for intensityL MU length

MLC multiplier for background opacity

MCE multiplier for CE (default)
MCI multiplier for CI (default)

MCOA multiplier for CO-lines van der Waals damping
 DGM multiplier for G (HSE); or buoyancy factor
 DGMZ multiplier for G (HSE), standard table

DPMULT multiplier for total damping

OML multiplier for line background opacity

OLL multiplier for line opacity

CQM multiplier for scattering albedoPMSK multiplier for Stark halfwidth

JH1 multiplier index for photoionization rateJH2 multiplier index for photoionization rate

FMVLIM multiplier limit for fluid velocity

MN1 N1 recalculation limit depth (ambipolar diffusion)

NAME name of ion

NNA NAN tables length

CTCO NCO calculation temperature enhancement factor CTMX NCO calculation temperature enhancement limit

ZRCO
 NCO calculation temperature enhancement reference height
 SHCOP
 NCO calculation temperature enhancement scale height
 SHCOC
 NCO calculation temperature enhancement scale height

IBNVIEW ND-calculation trace illustration, depth index for

ZNDW NDW-default criterion
JEDIT N-editing depth index

JNEDP N-editing details printout switch

JNEDP N-editing dump switch

ISTARK NE-index for Stark splitting of Hydrogen lines
STARKI NE-index for Stark splitting of Hydrogen lines

EIDIF NE-iterations convergence criterion

net radiative bracket = RHO

KRATE net-vs.-single rate switch for statistical equilibrium equations

NEFDF NE-values for d-coefficients (diffusion calculation)
 HNAJL NH adjustment factor limit for HSE calculation
 WSN1D NK weight, Special-N1 calculation (diffusion)

QNL " $n\ell$ " electrons NOION 'no ion' switch

ZME non-H electrons ratio

FNRMLA normalizing factor for simulated background Hydrogen Lyman α profile FNRMLB normalizing factor for simulated background Hydrogen Lyman β profile

ND number densities

ALN number densities, Aluminum
CAN number densities, Calcium
CN number densities, Carbon
HEN number densities, Helium

HE2N number densities, Helium-IIHN number densities, Hydrogen

INDRN number densities, input, renormalization switch

FEN number densities, Iron

MGN number densities, Magnesium onnumber densities, Oxygen O2Nnumber densities, Oxygen-II O3Nnumber densities, Oxygen-III SIN number densities, Silicon **NAN** number densities, Sodium SNnumber densities, Sulphur NKnumber density, protons

ALK number density, Aluminum-II (singly ionized) ground state
CAK number density, Calcium-II (singly ionized) ground state
CK number density, Carbon-II (singly ionized) ground state

NC number density, charged particlesMCON number density, CO, output switch

HEK number density, Helium-II (singly ionized) ground stateHE2K number density, Helium-III (singly ionized) ground state

MH2N number density, H2, output switch

FEK number density, Iron-II (singly ionized) ground state

MGK
 number density, Magnesium-II (singly ionized) ground state
 OK
 number density, Oxygen-II (singly ionized) ground state
 O2K
 number density, Oxygen-III (singly ionized) ground state
 O3K
 number density, Oxygen-IV (singly ionized) ground state
 SIK
 number density, Silicon-II (singly ionized) ground state
 NAK
 number density, Sodium-II (singly ionized) ground state
 SK
 number density, Sulphur-II (singly ionized) ground state

NL number of atomic levels

NFB number of isotropic flow broadening velocities

NSL number of supplementary atomic levels

TLARGE numerical control parameter for WN-matrix calculation
TSMALL numerical control parameter for WN-matrix calculation

WSN1D N1 weight, Special-N1 calculation (diffusion)

NLO ON tables number NO2 O2N tables number

NO3 O3N tables number

KONFORM opacity contributions details printout format switch

NABS opacity contributions switch

LSFBOC opacity control

ADT opacity function, dust
MLC opacity multiplier
OML opacity multiplier
OLL opacity multiplier

LMM opacity multiplier wavelengths

WAVES opacity, wavelengths for additional calculations

TS optical depth, standard

KTRANS optically-thin transitions descriptor

DO optionsOMIT options

KOELS ORIGINS printouts every-line switch limit
 CORMAX ORIGINS printouts wavelength limit
 CORMIN ORIGINS printouts wavelength limit

FROSCE oscillator strength for forbidden transitions

SCOW output, Continuum Calculations, selected wavelengths

IFXDS output control for continuum flux details
IRPUN output switch for abundance ratio calculation

MCON output switch for CO number density
 MDFG output switch for diffusion terms (GVL)
 MDFV output switch for diffusion velocity

MFONT output switch for Fontenla atmosphere data

MH2N output switch for H2 number density

MKURU output switch for Kurucz spectrum calculations data

MTREF output switch for TR-effective

IOMX overall iterations limit

LOXDS Oxygen lines background opacity debug printout switch

BDO Oxygen (neutral) departure coefficient
ON Oxygen (neutral) level populations

LX2DS Oxygen-II lines background opacity debug printout switch

BDO2 Oxygen-II (singly ionized) departure coefficient
OK Oxygen-II (singly ionized) ground level population

O2N Oxygen-II (singly ionized) level populations

BDO3 Oxygen-III (doubly-ionized) departure coefficientO2K Oxygen-III (doubly ionized) ground level population

O3N Oxygen-III (doubly ionized) level populations

LX3DS Oxygen-III lines background opacity debug printout switch

O3K Oxygen-IV (triply ionized) ground level population

ELLED particle energy dissipation parameter
 EMXED particle energy dissipation parameter
 NSPED particle energy dissipation parameter

PART Partition function

PARTLIM Partition function component limit

IWSMD Part-2 of WAVELENGTHS summary, switch

KTRANS passive transition descriptor

IPERFA performance data archive record switchIXSTA performance statistics printout control

NCOPT performance statistics switch for CO-lines opacity calculation

IPR01 PERSEUS 'PERDMPn' debug printout limit index
 IPR02 PERSEUS 'PERDMPn' debug printout limit index
 IPR03 PERSEUS 'PERDMPn' debug printout limit index
 IPR04 PERSEUS 'PERDMPn' debug printout limit index

TSM Phase-2 intensities change-over TAU
 RKC photoionization (additional) parameter
 TKR photoionization (additional) parameter
 YKR photoionization (additional) parameter

CP photoionization cross-section

RQCP photoionization cross-section ratios RRCP photoionization cross-section ratios

JATAW photoionization cross-section ratios, output switch

CP photoionization data, K-shellQIN photoionization data, K-shell

RK photoionization rate

JH1 photoionization rate multiplier index JH2 photoionization rate multiplier index

RL photorecombination rateZ photosphere depth

IPIJG PIJ-calculation, GNV fudging

IRATE PIJ printout

IPPOD population ion absorption/emission dump switch

RUNTOPOP population ion level correspondences

MOPRNT population-ion-model, built-in, printout switch

N1NUP populations-of-the-run update switch, Special-N1 (diffusion)

WPOP populations updating weightPOPUP population tables update switch

PRD = partial redistribution

DDRPRD DR parameter, transitions **DRLIM** PRD DR parameter, transitions **TAUCL** PRD DR parameter, transitions \mathbf{XC} PRD DR parameter, transitions \mathbf{XCL} PRD DR parameter, transitions XDRPRD DR parameter, transitions \mathbf{XP} PRD DR parameter, transitions \mathbf{XR} PRD DR parameter, transitions

IGMSW PRD GMMA for H Lyman alph and betaPRDCV PRD iterations convergence criterion

ITPRD PRD iterations limitJNUNC PRD JNU input switchSCH PRD on/off switch

IPRDD PRD printout depth intervalIPRDF PRD printout frequency interval

IGII PRD RII-function approximation selector

ISNUD PRD SNU-shift debug dump switch

NSPRD PRD switch (secret)

NLPAIR principal quantum number

KONFORM print format switch

JZATMO print mode switch (zeroes) for ATMOSPHERE

JZATOM print mode switch (zeroes) for ATOM

KCOAA print switch, abbreviated form of Composite Line Analysis

IPDEE print switch, diffusion d-coefficients

JSFEX print switch, Line Source Function explanation

MSSPR print switch, Special-N1 simultaneous solution matrix

IWEIT print switch, weighting details

IPEX printout, extra, switch (for debugging)

MOPRNT printout switch for built-in population-ion-model

NECLIP printout switch for continuum eclipse calculation

IPDIJ printout switch for DIJ (diffusion)

ISCOMP printout switch for Line Source Function comparisons details

LPMLR printout switch for mass loss rates
 JNEDP printout switch for N-editing details
 LPVEL printout switch for profile velocities

IRUNT production run switch

NANAL1 profile ANALYSIS depth selection parameterNANAL2 profile ANALYSIS depth selection parameter

VX profiles expansion velocity (additional)
PROGLI profiles graphs delta-lambda axis limit

SGRAF profiles graphs switch

FNRMLA profile simulation normalizing factor, background Hydrogen Lyman α FNRMLB profile simulation normalizing factor, background Hydrogen Lyman β

DOPROF profiles switchPROF profiles switch

LPVEL profile velocities printout switch

NP proton density

NLPAIR quantum number, principalNLPAIR quantum number, rotationalVNH quiet Sun broadening velocity

MQT QTAIL length

TRN radiation temperature

FINK radiation (incident) input parameter
XINK radiation (incident) input parameter

ICR radiation, incident coronal
 CRD radiative damping halfwidth
 KTRANS radiative transition descriptor
 INPAIR radiative transitions indices

FRR radius fraction

IRATE RATES calculation printout switchWRAT rates integrations wavelengths

WRATMN rates integrations wavelengths limit, (standard table)WRATMX rates integrations wavelengths limit, (standard table)

JATAW rates integrations wavelengths output switch

YRATS rates integrations wavelengths, standard, damping parameter

ADS ratio of angular diameters, Sun/Star

KPCR ratio of input opacities

RRCP ratio of photoionization cross-sections

JATAW ratio of photoionization cross-sections, output switch

NTAN ray-selection parameter for WN-matrix, spherical coordinates

MSKIP ray-selection parameter for WN-matrix, spherical coordinates

CN1S rcheck criterion (diffusion calculation, Special-N1)

AL recombination fraction, added

APARAD recombination parameter (Aldovrandi and Pequignot)

APCDP recombination parameter

APCI recombination parameter (Romanik)
APEI recombination parameter (Romanik)

APETA recombination parameter (Aldovrandi and Pequignot)
APWRA recombination parameter (Aldovrandi and Pequignot)
APWRB recombination parameter (Aldovrandi and Pequignot)

NAPKNT recombination parameter (Romanik)

NAPWRA recombination parameter (Aldovrandi and Pequignot)NAPWRB recombination parameter (Aldovrandi and Pequignot)

YK recombination parameter (Hydrogen)
RFAC reduction factor, all collision rates

FSTKM reduction factor, for Hydrogen Stark splitting
RFHEAB reduction factor, for RHEAB calculation
LHHSE reference depth index for H and M, HSE

ZRCO reference height, NCO calculation temperature enhencement

ZNDW reference index criterion for Doppler width

NDW reference index for Doppler width

NDWM reference index for Doppler width (for atmospheric model)

M304 reference index for He-II λ 304 line mean intensity IRFNC reference index for Hydrogen CE and CI calculation

IHEAB reference index for RHEAB calculation

RFMAS reference mass

NS reference transition lower level index
 MS reference transition upper level index
 REFLM reference wavelength for input TAUK
 INDRN renormalization of input number densities

CRS resonance broadening halfwidth

RHEAB = depth dependence of total Helium abundance

CHEFLOW RHEAB calculation parameter
 HEABL RHEAB calculation parameter
 IHEAB RHEAB calculation parameter
 RFHEAB RHEAB calculation parameter

JHEAS RHEAB (secret switch)

JBDNC RHO and departure coefficients ratio calculations bypass switch

RHOCR
 NED
 RHO editing index
 DRHO
 RHO editing parameter
 INRHO
 RHO, input-only, selector
 CWJ
 RHOJ calculation parameter
 CHI
 RHO-like line transfer quantity

CHLIM
CHOP
RHO selection parameter
RHOPT
RHO selection parameter
RHOPT
RHO selection parameter
RHOPT
RHO smoothing parameters

WR RHO-weighting factor

RHOWT RHO weightsRHWT RHO weights

INCH RHO weights adjustment parameter SMPRHO weights adjustment parameter WMNRHO weights adjustment parameter $\mathbf{W}\mathbf{M}\mathbf{X}$ RHO weights adjustment parameter **WRMN** RHO weights adjustment parameter WRMX RHO weights adjustment parameter IGII RII-function approximation selector, PRD **IRKCOMP** RK-components initial calculation switch

RKMULT RK enhancement factors

RKW RK-weights RKWT RK-weights

IRLCOMP RL-components initial calculation switch

NLPAIR rotational quantum number

MR RRNU length
IRUNT run type switch

LN saturation approximation limit in Lyman calculation

SHCOC scale height, chromospheric, NCO temperature enhancement sHCOP scale height, photospheric, NCO temperature enhancement

SCTS scale height, shock temperature **SCVS** scale height, shock velocity CQMscattering albedo multiplier \mathbf{CQA} scattering albedo parameter \mathbf{CQT} scattering albedo parameter CLMscattering albedo parameter **PNH** scattering albedo parameter **SRCO** scattering ratio for CO lines

NSW SCOW length

ISCRS scratch I/O mode switch

NSPRD secret PRD switch

SCOW selected wavelengths for Continuum Calculation output

SMATC selection criterion for matrix sample output

IBETSW selection parameter for beta-equation, diffusion

KB1WS selection parameter for b-1 weights

IDFDM selection parameter for d-coefficients (diffusion calculation)

NEFDF selection parameter for d-coefficients NE-values (diffusion calculation)

MSKIP selection parameter for WN-matrix rays, spherical coordinates

NTAN selection parameter for WN-matrix rays, spherical coordinates

BLCSWselectors for line broadening **BLCSW** selectors for line damping **ASMCR** sequential smoothing parameter **NIASM** sequential smoothing parameter **JSSV** shock temperature parameter SCTA shock temperature parameter **SCTS** shock temperature parameter **ISSV** shock velocity parameter **SCVA** shock velocity parameter **SCVB** shock velocity parameter **SCVS** shock velocity parameter

BDSI Silicon (neutral) departure coefficient

SIN Silicon (neutral) level populations

SIK Silicon-II (singly ionized) ground level population

ISMBD SIMBA (intensity integration) dump interval

FNRMLA simulated background profile normalizing factor, Hydrogen Lyman α FNRMLB simulated background profile normalizing factor, Hydrogen Lyman β

MSSPR simultaneous solution matrix print switch, Special-N1

KRATE single-vs.-net rate switch for statistical equilibrium equations

NDSN1 skip Special-N1 (ambipolar diffusion)

TMS small TAU change-over for RT

VSMLL small value to replace denominators = 0

ISMVE small values editing switch

IXASM smoothing debug printout (IPEX=15) details control index

IDFDS smoothing of d-coefficients (diffusion calculation)

NBS smoothing of departure coefficients, level control index

LDFD1 smoothing of derivatives (numerical)

SMOOTH smoothing of RHO

WSM smoothing parameter for Lyman RK-1

SMOOTHsmoothing parameters for RHOASMCRsmoothing ('sequential') parameterNIASMsmoothing ('sequential') parameterQTAILsmoothing tail for Lyman EP1 Q values

ISNDD S(n) calculation dump switch
 VXS source function expansion velocity
 SOBOLEV Sobolev calculation parameter
 SOBDMN Sobolev calculation parameter
 SOBDMX Sobolev calculation parameter
 SOBFEQ Sobolev calculation parameter

ISOD Sobolev integration dump depth index

VSB Sobolev velocity

CVSB Sobolev velocity parameter

BDNA Sodium (neutral) departure coefficient NAN Sodium (neutral) level populations

NAK Sodium-II (singly ionized) ground level population

LSFFDBsource function (line) background typeDOFDBsource function (line) background typeISNDDsource function (line) dump switch

BANDY source function method control parameter
YCONT source function method control parameter
YHM source function method control parameter
YL source function method control parameter
YLINE source function method control parameter
YRATE source function method control parameter
YWAVE source function method control parameter

DOSFPRNT source function printout **LSFPRINT** source function printout

LSFTYP source function solution type selector

TX source temperature

AOWXP Special-N1 (diffusion), alpha(old) weight exponent

SN1CC Special-N1 (diffusion), convergence criterion

ITN1R Special-N1 (diffusion), iterations limitMSSPR Special-N1 (diffusion), matrix print switch

I4DEQSpecial-N1 (diffusion), method control parameterI4DFMSpecial-N1 (diffusion), method control parameterI4DIOSpecial-N1 (diffusion), method control parameterKBNDSSpecial-N1 (diffusion), method control parameterKDAMPSpecial-N1 (diffusion), method control parameterKDIAGSpecial-N1 (diffusion), method control parameterN1METSpecial-N1 (diffusion), method control parameter

N1NUP Special-N1 (diffusion), populations-of-the-run update switch

WSN1D Special-N1 (diffusion), weight for N1 and NK

MSKIPspherical coordinates WN-matrix ray selection parameterNTANspherical coordinates WN-matrix ray selection parameter

IONSTAGE stage of ionization of ion of run

standard frequencies for background linesxkstandard frequencies for continuum transitions

XI standard frequencies for line transitions
XIBLU standard frequencies for line transitions
XIBLUT standard frequencies for line transitions
XIRED standard frequencies for line transitions
XIREDT standard frequencies for line transitions
XISYM standard frequencies for line transitions
XISYMT standard frequencies for line transitions

IDEX standard-output (log file) extra data switch

FNH standard table of flow velocity

TS standard TAU table

YRATS standard wavelengths for rates integrations, damping parameter

WRATMN standard wavelengths for rates integrations, limit WRATMX standard wavelengths for rates integrations, limit

IHSDD Stark broadening, convolution, dump switch (Hydrogen) **IHSDP** Stark broadening, convolution, dump switch (Hydrogen) **HSBDMN** Stark broadening, convolution, parameter (Hydrogen) **HSBDMX** Stark broadening, convolution, parameter (Hydrogen) Stark broadening, convolution, parameter (Hydrogen) **HSBFEQ HSBM** Stark broadening, convolution, parameter (Hydrogen) **CSTARK** Stark broadening, convolution, switch (Hydrogen) **IHSSW** Stark broadening, convolution, switch (Hydrogen) **IHSKM** Stark broadening, convolution, table limit (Hydrogen) **IHSSM** Stark broadening, convolution, table limit (Hydrogen)

CSK Stark broadening halfwidth

PW Stark broadening halfwidth exponent

JHLSK Stark broadening switch, H Lyman lines background opacity

PMSKStark broadening halfwidth multiplier **CSDW** Stark splitting parameter (Hydrogen) **FMCDL** Stark splitting parameter (Hydrogen) **FRCDL** Stark splitting parameter (Hydrogen) **FSTKM** Stark splitting parameter (Hydrogen) **ISTARK** Stark splitting parameter (Hydrogen) **STARKI** Stark splitting parameter (Hydrogen) **IHSSP** Stark splitting switch (Hydrogen) ADSStar/Sun angular diameter ratio

WEIGHT statistical equilibrium equation parameter

METSEstatistical equilibrium equation method control parameterMETSEDGstatistical equilibrium equation method control parameterMETSEDWstatistical equilibrium equation method control parameterKRATEstatistical equilibrium equation net-vs.-single rate switchKUDNTStatistical Line Opacity (Kurucz) data dump control

FKUR Statistical Line Opacity (Kurucz) multiplier

ALBK Statistical Line Opacity (Kurucz) parameter

KURIN Statistical Line Opacity (Kurucz) parameter
 KURMA Statistical Line Opacity (Kurucz) parameter
 KURMI Statistical Line Opacity (Kurucz) parameter
 ZALBK Statistical Line Opacity (Kurucz) parameter

P statistical weight

LSTMP STIM for GTN calculation details print switch
WORLDLY storage management system dump control switch

ISUB sub-iterations limit

DELWAVE 'subtractional' wavelengths

BDS Sulphur (neutral) departure coefficient
SN Sulphur (neutral) level populations

SK Sulphur-II (singly ionized) ground level population

ISMSW summaries, iterative, format switch

NSL supplementary atomic levels

JBFSW supplementary levels b calculation methods switch NGNV suppression level limit for GNV (diffusion calculation)

CLOGG surface gravity (log)

IBETSW switch for beta-equation, diffusion

KB1WS switch for b-1 weights

NABS switch for controlling absorbers

POPUP switch for controlling updating of population tables

MCON switch for CO number density output

IDFDM switch for d-coefficients method (diffusion calculation)IDEDP switch for diffusion d-coefficients debug printout

MDFG switch for diffusion terms (GVL) output

MDFV switch for diffusion velocity output

KDIFGS switch for GNV fudging

MH2N switch for H2 number density output

IRTIS switch for incident radiation input data interpolation

JNUNC switch for input JNU data

INDRN switch for input number densities renormalization

INRHO switch for input-RHO-only

IBRDPswitch for ion broadening (Hydrogen) debug printoutMKURUswitch for Kurucz spectrum calculations data output

switch for Lyman DNRT, DNRTC calculationMAMASswitch for matrix elements magnitude scan

JNEDP switch for N-editing details printout
JNEDP switch for N-editing dump printout
KOELS switch for ORIGIN printout (every-line)
ISNUD switch for PRD SNU-shift debug printout

ISCRS switch for scratch I/O mode ISNDD switch for S(n) calculation dump

KRATE switch for statistical equilibrium equation (net-vs.-single rate)

WORLDLY switch for storage management system dump

ELSYM symbol, element, of ion of run

QTAIL tail for smoothing Lyman EP1 Q values
EXLYM TAU change-over parameter, Lyman
TGLYM TAU change-over parameter, Lyman

ESCTAU TAU criterion for automatic use of escape probability solution

TML TAU cut-off for intensity integrals

TAUKIN TAUK input values

REFLM TAUK input values reference wavelength

TS TAU, standard

TLTR TDST recalculation limiting multiplier

WTD TDST recalculation weight TB temperature, blanketing

TX temperature, brightness, of illuminating source

TDST temperature, Dust (Type-2)

TE temperature, electron

CTCO tempearture enhancement factor, NCO calculation
CTMX tempearture enhancement limit, NCO calculation

TEX temperature, excitation
 TE temperature, kinetic
 TRN temperature, radiation

SCTA temperature, shock, amplitude

JSSV temperature, shock, depth index

SCTS temperature, shock, scale height

TER temperature table for CE and CI

ISCRS temporary scratch disk file switch

NTE TER length

ACE term to be added to CE (default)
ACI term to be added to CI (default)

CIJADD term to be added to CIJ CKADD term to be added to CK

MCEterm to multiply CE (default)MCIterm to multiply CI (default)KTRANSthick transition descriptorKTRANSthin transition descriptor

LR TKR lengthKANTNU TNU analysis

KOOLSUM total cooling rates components control

CHEFLOW total Helium abundance calculation parameter
 HEABL total Helium abundance calculation parameter
 IHEAB total Helium abundance calculation parameter
 RFHEAB total Helium abundance calculation parameter
 RHEAB total Helium abundance, depth variation

KHFFS total Hydrogen cooling control

NH total Hydrogen density

KALHD traceback (Hi/Bye/Abort-system) control parameter
 IBNVIEW trace of BD- and ND-calculations, depth index for
 KALOR traceback (Hi/Bye/Abort-system) control parameter

KTRANS transition descriptorINPAIR transition indicesNT transitions number

LDINT transition terms detail print control parameter
LDTYP transition terms detail print control parameter

KTRANS transparent transition descriptor

ITRFI TR-effective calculation debug output control

TRFLI TR-effective calculation limit interval

MTREF TR-effective output switch (file .msc)

M TS length

VT turbulent pressure velocity
KTRANS two-photon transition descriptor

CCHX upper-level charge-exchange parameter
ICXDP upper-level charge-exchange parameter
RCHX upper-level charge-exchange parameter
XRKH upper-level charge-exchange term
XRLH upper-level charge-exchange term

MSupper level of reference transition

INRHO use input-RHO only

 \mathbf{CVW} van der Waals broadening halfwidth

MCOA van der Waals damping multiplier for CO-lines **MDFV** velocity, ambipolar diffusion, output switch **APDDIFC** velocity, ambipolar diffusion, parameter **APDDTFC** velocity, ambipolar diffusion, parameter **APDTEXP** velocity, ambipolar diffusion, parameter **APDXICA** velocity, ambipolar diffusion, parameter velocity, ambipolar diffusion, parameter APDXICB **APDXICC** velocity, ambipolar diffusion, parameter

velocity, ambipolar diffusion, parameter

velocity, broadening VRvelocity, broadening

APDXICD

WFB

VNHvelocity, broadening, quiet Sun VXvelocity, expansion, for profiles

 \mathbf{VXS} velocity, expansion, for source functions

CVXvelocity, expansion, parameter \mathbf{CVXS} velocity, expansion, parameter \mathbf{CVXF} velocity, flow broadening, parameter CVXMvelocity, flow broadening, parameter FBVMXvelocity, flow broadening, parameter NFBvelocity, flow broadening, parameter

velocity, flow broadening, parameter VMvelocity, mass motion \mathbf{V} velocity, microturbulence VR

VNHvelocity, microturbulence, quiet Sun

velocity, microturbulence

FMVLIM velocity multiplier limit CDZvelocity parameter \mathbf{CVZ} velocity parameter

SCVA velocity, shock, amplitude **ISSV** velocity, shock, depth index **SCVB** velocity, shock, parameter **SCVS** velocity, shock, scale height

VSBvelocity, Sobolev

CVSB velocity, Sobolev, parameterVT velocity, turbulent pressure

VOITC Voigt profile subroutine recomputation cut-off criterion

NVOIT Voigt profile subroutine execution statistics printout switch

IVOIT Voigt profile subroutine selection switch

NVX VX tables number

BANDL wavelength band limit for Composite Line opacity

BANDU wavelength band limit for Composite Line opacity

LWNT wavelength interval for 'Line Opacities' printouts

WAVEMN wavelength limit for automatic additional wavelengths

WAVEMX wavelength limit for automatic additional wavelengths

WAVEMX wavelength limit for H Lyman lines background opacity

CORMAX wavelength limit for ORIGINS and CONTRIBUTORS printouts **CORMIN** wavelength limit for ORIGINS and CONTRIBUTORS printouts

REFLM wavelength of input TAUK values

TKR wavelengths for additional photoionization

LDT wavelengths for Dust opacity calculation (Type-2)

XCOL wavelengths for each CO-line

LCR wavelengths for incident coronal radiation

LMM wavelengths for opacity multiplierWRAT wavelengths for rates integrations

JATAW wavelengths for rates integrations, output switch LWNT wavelengths interval for 'Line Opacity' printouts

SCOW wavelengths, selected, for Continuum Calculations output

ICDIT wavelengths selector, continuum, for dI/dhIWSMD WAVELENGTHS summary Part-2 switch

DELWAVE wavelengths to be deleted

NWV WAVES length

AOWXP weight exponent for alpha(old), Special-N1 (diffusion)

WPRESS weight for adjusting NH to constant pressure
 WBD weight for departure coefficient updating
 WBDIR weight for 'direct' departure coefficient

WFB weight for flow-broadened component profilesNQLYM weight for H Lyman lines background opacity

HEL weight for HSE calculation**HSEC** weight for HSE calculation

WEP weight for Lyman EP1, EP2WPOP weight for populations updating

WSN1D weight for Special-N1 and -NK (diffusion)

WTD weight for TDST recalculation
 WZM weight for Z-from-mass calculation
 WZ weight for Z-from-TAUKIN calculation

TBAR weight matrix change-over TAU

XMU weight matrix MU table

MSKIP weight matrix (spherical) ray selection parameter NTAN weight matrix (spherical) ray selection parameter

IWEIT weighting details print switch
 RHOWT weights for RHO calculation
 RHWT weights for RHO calculation
 RKW weights for RK-1 calculation
 RKWT weights for RK-1 calculation

WEIGHT weights for statistical equilibrium equations

XCOMX width limit for CO-lines

TLARGE WN-matrix calculation numerical control parameter
TSMALL WN-matrix calculation numerical control parameter

WNJUNK WN-matrix 'cleanup' parameter AW WN-matrix integrated diagonal

MATRIX WN-matrix inversion and generation control parameter

WNJUNK WN-matrix 'junk' parameter

MSKIP WN-matrix (spherical) ray selection parameter NTAN WN-matrix (spherical) ray selection parameter

WORLDLY WORLD dump control switch

NCL XCOL length
NDR XDR length
K XI length
KB XIBLU length
KBT XIBLUT length
KBTMAX XIBLUT length limit

KR XIRED lengthKRT XIREDT lengthKRTMAX XIREDT length limit

KS XISYM length

KST XISYMT lengthKSTMAX XISYMT length limitKMMAX XIFUL length limit

INK XINK lengthKK XK length

KXLYM XK-table, Lyman, augmentation switch

LG XMU length

TAUCL XXC parameter (partial redistribution)XCL XXC parameter (partial redistribution)

N Z length

NKA ZALBK length

ITKZA Z-augmentation (diffusion calculation) iteration limit

MAUXZAUX indexLZAZAUX lengthNZEZECL length

JZATMO zero-print mode switch for ATMOSPHERE

JZATOMzero-print mode switch for ATOMCPRESSZ-from-mass calculation parameterWPRESSZ-from-mass calculation parameterWZMZ-from-mass calculation weightWZZ-from-TAUKIN calculation weightFZIONZION multiplier (ambipolar diffusion)ZXMINZION parameter (ambipolar diffusion)

NGRL Z-scale limit for graphsNGRR Z-scale limit for graphs

JZOPT Z-scale option for absorption/emission contributions graphs

IZOPT Z-scale option for graphsZGM Z-table for DGMZ (HSE)

ZECL Z-table for eclipse continuum calculation

(Section 5 – last revised: 2007 Apr 13)

Section 6: **Program Options**

Many features of PANDORA may be enabled or disabled, as desired. Some of these optional features are controlled by assigning particular values to certain input parameters; all others are controlled through the following two input statements:

```
"DO ( OPTION_1 OPTION_2 OPTION_3 ... OPTION_n ) ", i.e. DO ( ADDCOPR EPSW ) , and "OMIT ( OPTION_1 OPTION_2 OPTION_3 ... OPTION_n ) ", i.e. OMIT ( FELE SCOPRNT QSFEDIT ) ,
```

where $OPTION_i$ is the alphanumeric code name, to be described below, of a particular processing or output feature of PANDORA. Options appearing in **DO** statements will be enabled, those appearing in **OMIT** statements will be disabled. Only the OPTIONs appearing in the following table are valid. There may be any number of **DO** and/or **OMIT** statements, and a particular OPTION may appear several times – however, only the status resulting from its last appearance will prevail. Every OPTION not mentioned in **DO** and/or **OMIT** statements will retain its default setting.

All OPTIONS are listed and defined on the following table. This list is in alphabetical order by option name; the default settings are given in parentheses. After this table of definitions there follows an alphabetized listing of keywords and descriptive phrases for each OPTION – this last list should be consulted when an OPTION's significance or function are only vaguely known, and its name is sought. After the OPTION name has been located in the keywords list, the complete definition can then be found in the first part of this section.

See next page for important information about automatic options adjustments.

Note:

After all **DO** and/or **OMIT** statements have been read, and before the printout OPTIONS is produced, some options are reset automatically as follows, in the sequence shown:

- If PHASE2 is off: LIGHT, ECLIPSE and EMERINT are turned off;
- If FINITE is off: REFLECT is turned off;
- If FINITE and INCRFRNT are both off: INCIDNT is turned off;
- If SPHERE is on: SPHOUT, GDS, ENHANCE, HSE, INCIDNT and INCIFRNT are turned off;
- If USETRIN is off: CSWITCH is turned off;
- If ORT is on: GDS is turned off;
- If SPECSAV is on: CONSAV and PROSAV are turned on.
- \bullet If SPHERE and PRODMP are both on: ECLIDMP and LINTDMP are turned on.

ACSFPRNT (off):

print abbreviated results of continuum source function calculation (used only if CSFPRNT is on).

ADDCOPR (off):

print continuum data for additional wavelengths.

ADN1DMP (off):

print details of "sepcial N1" calculation (used only when ADN1PRNT is on).

ADN1PRNT (on):

print "special N1" calculation results (used only if AMBPRNT is on).

AEDIT (off):

replace negative final A-values (frequency integration weights) with zero.

AHSEPRNT (off):

print abbreviated results of HSE calculation.

AINDPRNT (off):

print abbreviated version of INPUT listing (used only when INDAPRNT is on).

AINTPRNT (off):

print abbreviated frequency integrations data.

ALL (off):

provide complete printout for all overall iterations, not just the last one.

ALLY (off):

provide complete Lyman and HSE printouts for every iteration, not just the last one.

ALSFPRNT (off):

print abbreviated results of Line Source Function calculation.

ALUPRNT (off):

print Aluminum populations and departure coefficients.

ALYMPRNT (off):

print abbreviated results of Level- \mathcal{N} -to-Continuum transfer calculation.

AMBPRNT (on):

print data from ambipolar diffusion calculations, (used only when AMDIFF is on).

AMDDMP (off):

print details of ambipolar diffusion calculations, (used only when AMBPRNT is on).

AMDIFF (off):

include ambipolar diffusion (only in Hydrogen or Helium runs).

AMDN1 (on):

use "special N1" calculation for ambipolar diffsuion, (used only when AMDIFF is on). Caution: AMDN1 should **not** be turned off (this switch is provided for testing only).

ANALYSIS (off):

print details of line absorption profile calculations (note input parameters NANAL1, NANAL2).

AOPTPRNT (off):

print abbreviated version of OPTIONS listing (used only when OPTPRNT is on).

APHICOPR (on):

print continuum data for additional photoionization wavelengths.

APHIPRNT (off):

print results and details of generalized additional photoionization calculation.

APOPPRNT (off):

print abbreviated populations of the ion-of-the-run.

APRFPRNT (off):

print abbreviated line profile calculation results.

ARHODMP (off):

print detailed sets of 'transition terms' (uses input parameter LDINT).

ATMOPRNT (on):

print ATMOSPHERE input data listing.

ATOMPRNT (on):

print ATOM input data listing.

ATOMSAV (off):

save computed default atomic model parameters in output file.

AVCON (off):

calculate the average of the continuum intensity.

AVELOP (off):

use Averaged Line opacities.

AVOPRNT (on):

print Averaged Line opacities data table as used in this run (also uses the value of LWNT).

BDCALC (off):

departure coefficients calculated from all level equations, rather than from the continuum equation.

BDGRAF (on):

print graphs of departure coefficients.

BDMP (off):

print details of departure coefficients calculation.

BDPRNT (off):

print complete sets of BDR, BDJ, BDS, and S* from 'RHO + RBD' calculation (only if RHBPRNT is on).

BEDIT (off):

edit departure coefficients.

BLENDMP (off):

print Voigt function details for each blended line component, (used only when ANALYSIS is on).

BRATDMP (off):

print details of b-ratios calculation (uses input parameter LDINT).

BSMOOTH (off):

do "alternate" sequential smoothing for departure coefficients (note input parameter ASMCR).

CALCOOL (off):

calculate net cooling rates.

CALHEAT (off):

calculate net heating rates.

CALPRNT (off):

print Calcium populations and departure coefficients.

CARPRNT (off):

print Carbon populations and departure coefficients.

CEFACTS (off):

update CE-enhancement factors where possible and needed.

CHEXLO (off):

use lower-level charge exchange.

CHEXLOL (off):

use LTE hydrogen number density for lower-level charge exchange.

CHEXUP (off):

use upper-level charge exchange.

CHKGRAF (on):

print graphs of CHECKs for all iterations.

CHKPRNT (on):

print Consistency CHECKs from 'RHO + RBD' calculation.

CHXDMP (off):

print details of upper-level charge-exchange calculation.

CHXPRNT (on):

print results of upper-level charge-exchange calculation (used only when CHX-CNG is on).

CIJPRNT (off):

print the bound-bound collision rates CIJ (for 'minimal' printout, see input parameter IRATE).

CLNORM (on):

compute H Lyman lines normalization factors.

CNFLXDMP (off):

print debug dump output from continuum flux calculation.

COCLIPSE (off):

calculate emergent continuum eclipse intensities for CO lines wavelengths.

COCOPR (off):

print continuum data for CO-lines opacity wavelengths.

COCRID (off):

print details of CO-lines cooling rate wavelength integration.

CODMP (off):

print details of CO-lines absorption calculation.

COLHPRNT (on):

print calculated rates for collisions with Hydrogen atoms.

COLTEMP (off):

calculate color temperatures.

COMCRID (off):

print details of Composite Lines cooling rates wavelength integration.

COMOPAN (off):

Composite Line Opacity analysis.

COMPCOPR (off):

print continuum data for Composite Line Opacity wavelengths.

COMPRK (off):

print comparison RKs.

CONFLUX (off):

calculate continuum flux.

CONSAV (off):

write continuum spectrum data in Special Spectrum Save File, (this option will be turned on automatically when SPECSAV is on).

COOLCO (off):

calculate CO-lines cooling rate, (used only when CALCOOL is on).

COOLCOM (on):

calculate Composite Lines cooling rate, (used only when CALCOOL is on).

COOLINT (off):

calculate integrated net heating and cooling rates, (used only when CALCOOL is on).

COOLXRAY (on):

calculate X-rays cooling rate, (used only when CALCOOL is on).

COOLSAV (off):

write cooling and heating rates in a save file.

CPSW (on):

adjust total Hydrogen density to give constant pressure, (used only when HSE is off).

CSF (on):

use calculated background continuum source function when calculating line source function.

CSFB (off):

set BC in line source function calculation = min(CSF, B), instead of = CSF, (used only when CSF is on).

CSFDMP (off):

print debug dump output for background continuum source function calculation.

CSFPRNT (on):

print results from background continuum source function calculation.

CSFGRAF (off):

print graphs of background continuum opacity and background continuum source function.

CSWITCH (off):

use TR (level 1), instead of TE, in the stimulated emission factor (BETA) for BC in the line source function calculation, (this option will be turned off automatically when USETRIN is off).

DELABORT (on):

try to read all the input before stopping because of error(s).

DIDHC (off):

print dI/dh for emergent continuum intensities (see also input parameter ICDIT).

DIDHL (on):

print and save dI/dh for emergent line intensity profiles.

DIFFANA (on):

analyze results of diffusion calculations (used only if AMDIFF is on and/or VELGRAD is on) for radiative CRD transitions.

DOION (on):

do all the normal calculations pertaining to the ion-of-the-run.

DPDWPRNT (off):

print results of Doppler Width and Damping Paramater calculations.

DRDMP (off):

print debug details of PRD DR calculation for transition (MS/NS) at depth IDRDP and frequency KDRDP.

DSMOOTH (off):

smooth the calculated diffusion terms with the sequential smoothing procedure.

DUSTCOPR (on):

print continuum data for Dust opacity wavelengths, (used only when DUSTEMP is on).

DUSTDMP (off):

print debug dump output from Type-2 Dust temperature recalculation.

DUSTEMP (on):

calculate new values of TDST, (used only when DUSTYPE is on).

DUSTYPE (off):

use Type-2 version of Dust background continuum opacity.

ECLIDMP (off):

print debug dump output from Eclipse calculation.

ECLIGRAF (on):

print graphs of results of Line Eclipse calculation.

ECLIPSE (off):

calculate emergent continuum Eclipse intensities, (pertains to WAVES $_i < 0$ only).

ECLISAV (off):

write Eclipse emission data to an output file.

ELECPRNT (off):

print and plot results of electron density calculations.

EMERBACK (off):

calculate intensity and flux emerging from back face (far face) of finite atmosphere.

EMERINT (on):

calculate emergent continuum intensities for all wavelengths for which background continuum calculations were done.

EMIGRAF (off):

print graph of emitters.

EMINDMP (off):

print debug dump output from emergent continuum intensity calculations.

EMIPRNT (off):

print detailed analysis of the contributions to the background continuum emission.

EMISUM (off):

print an 'Emitters Summary'.

ENHANCE (off):

use R^2 source function enhancement factor in emergent intensity calculations, (used only when SPHERE is off).

ENL (off):

edit negative values out of tables of EP1 (Lyman Epsilon-1) by interpolating from neighboring positive values.

ENL2 (off):

edit negative values out of tables of EP1 (Lyman Epsilon-1) by shifting the entire EP1 and EP2 tables.

EPCOMP (off):

print comparison of the results obtained from the various methods for the Lyman EP1, EP2 calculations.

EPDMP (on):

print intermediate details of the Lyman EP1, EP2 calculations, (also uses the value of LDINT).

EPSNEDC (off):

eliminate negative values of EP1 (Lyman Epsilon-1) when using the CHAIN method.

\mathbf{EPSW} (off):

replace any line-source-function-epsilons < -0.9999 by -0.9999.

EVERY (off):

print complete printout for all sub-iterations, not just the last one.

EXPAND (off):

the atmosphere is expanding.

FDBCOPR (off):

print continuum data for FDB (frequency-dependent line source function background) wavelengths.

FDBDMP (off):

print frequency-dependent background terms for FDB transitions.

FELE (off):

use results from fast electrons calculation.

FELEC (off):

calculate fast electrons.

FELEDMP (off):

print debug dump output from fast electrons calculation.

FELEPRNT (on):

print results of fast electrons calculations.

FEPRNT (off):

print Iron populations and departure coefficients.

FINITE (off):

the atmosphere is finite, instead of semi-infinite.

FLUXDMP (off):

print details of emergent continuum flux calculation at each wavelength, (also uses the value of IFXDS).

FLUXSAV (off):

write integrated flux quantities to an output file.

FLWBPRNT (off):

print component profiles of flow broadening.

FLWBROAD (off):

compute flow-broadened profiles, (used only when EXPAND is off).

GDMP (on):

print debug dump consisting of all 'geometric dilution matrices', (used only when GDS is on).

GDS (off):

calculate geometric dilution.

GDSDMP (off):

print geometric dilution terms, (used only when GDS is on).

GNVCALC (off):

compute the diffusion term GNV1 from the non-local N1 calculation, (used only when AMDIFF is on).

GTNSMTH (on):

smooth STIM when calculating GTN(u,l).

GTNSTIM (off):

use departure coefficients, instead of number densities, in STIM for GTN(u,l).

HBROAD (on):

in a Hydrogen run, use ion collision broadening for transitions above level 5.

HEABD (off):

calculate depth dependence of Helium abundance (used only when AMDIFF is on).

HELPRNT (off):

print Helium populations and departure coefficients.

HEL2PRNT (off):

print Helium-II populations and departure coefficients.

HENORM (on):

renormalize Helium number densities in the diffusion calculations.

HFFCOOLD (off):

print details of H free-free and H-minus free-free net cooling rates integrations.

\mathbf{HMS} (off):

calculate H-minus departure coefficient.

HMSCOPR (off):

print continuum data for H-minus departure coefficient calculation wavelengths.

HMSJPRNT (off):

print values of mean intensity used in H-minus departure coefficient calculation.

HMSONLY (off):

use only continuum data pertaining to 'H-minus wavelengths' in the H-minus departure coefficient calculation.

HNPRNT (on):

print Hydrogen populations and departure coefficients.

HSE (off):

recalculate NE and NH via the hydrostatic equilibrium equation.

HSEDMP (off):

print debug dump output from the hydrostatic equlibrium calculation, (used only when HSE is on).

HSEV (on):

include mass motion velocity in the hydrostatic equilibrium calculations, (used only when HSE is on).

HSTSUMM (on):

print summary of calculation of Stark splitting of Hydrogen lines.

ILR (on):

calculate incident line radiation terms, (used only when INCIDNT is on).

INBED (off):

edit negative values out of tables of BDIJ values calculated from unfudged input RHO values.

INCIDNT (off):

there is external radiation shining upon the atmosphere, and it is shining on the back face (far face).

INCIFRNT (off):

the external incident radiation is shining upon the front face of the atmosphere, (used only when INCIDNT is on).

INDAPRNT (on):

print miscellaneous INPUT data listing.

INDPRNT (off):

print the input values of number density and departure coefficient of the ion of the run.

INDXDMP (off):

print debug dumps of the contents of the random-access scratch file indices.

INPEX (on):

extrapolate input tables to added depths, instead of just extending the end values.

INNBPRNT (on):

print input values of NK, ND and BD.

INPEXW (on):

print input table extrapolation warning messages.

INSCARD (on):

write the current iterates to the restart files for every iteration, not just for the last iteration only. (Note: the results for iteration i+1 will overwrite the results for iteration i.)

INTAPRNT (on):

print frequency integrations data for all radiative transitions.

INTEDIT (off):

use edited TE values instead of input.

INTGRAF (on):

print graphs of the results of emergent line profile calculations, and graphs of S and B vs. Z with the emergent line profile calculation.

INTRPRNT (on)

print input values of RHO, JBAR, CHI and AW.

IRHWED (on):

edit input values of RHOWT.

IRUNT (off):

print the most detailed execution performance and version description data.

ISCRS (on):

use 'in-memory' scratch I/O to the extent possible.

ITDMP (off):

print debug dump of 'Iterative Summary File' contents summary.

ITERB (on):

print Iterative Summary of values of departure coefficients.

ITERCHI (off):

print Iterative Summary of CHI.

ITERCHK (on):

print Iterative Summary of values of consistency checks.

ITERN (on):

print Iterative Summary of values of number densities.

ITERNE (on):

print Iterative Summary of values of electron density.

ITERNH (on):

print Iterative Summary of values of total Hydrogen density.

ITERRHO (on):

print Iterative Summary of values of net radiative bracket.

ITERRK (on):

print Iterative Summary of values of Lyman RK-1.

ITERRWT (off):

print Iterative Summary of values of RHO-weights.

ITERS (on):

print Iterative Summary of values of line source functions.

ITERTAU (off):

print Iterative Summary of values of line core optical depths.

ITERTD (on):

print Iterative Summary of values of TDST (Type-2 Dust temperature).

ITERZ (on):

print Iterative Summary of values of Z.

IVALICK (on):

check 'validity' of emergent intensity integrations.

IXSTA (on):

print performance statistics.

JBDNC (off):

bypass the calculation of unused Rhos and b-ratios.

JLYSAV (off):

save Lyman-continuum JNU (=JB).

JNTRPOL (off):

interpolate input values of PRD JNU to new Z-scale (instead of simply assigning values to the new Z-scale), in runs for which TAUKIN is specified.

JNUPRNT (off):

print values of mean intensity for PRD transitions, for each iteration.

JSTIN (off):

just read and check all the input, then stop.

KOMPRNT (off):

print Composite Line Opacity (Kurucz) data table, as used in this run (also uses the value of LWNT).

KROSSID (off):

print details of Rosseland mean opacity wavelength integration.

KSHLCOPR (off):

print continuum data for K-shell wavelengths.

KURPRNT (off):

print Statistical Line Opacity (Kurucz) data table, as used in this run (also uses the value of LWNT).

LBDPRNT (on):

print summary of line center background.

LFDPRNT (off):

print full arrays of values of Line Flux Distribution.

LIGHT (on):

calculate emergent line intensity and flux profiles.

LINECDMP (off):

print details of scattering albedo analysis (used only when LINECOMP is on).

LINECOMP (off):

compare results from Line Source Function and Composite Line calculations.

LINECOPR (off):

print continuum data for line core wavelengths.

LINTDMP (off):

print debug dump output from emergent line intensity calculation.

LNUMDMP (off):

print dump of number density calculations.

LONGNBM (off):

use the long, detailed version of the error message that is printed when a calculated value of $\mathrm{BDIJ} < 0$.

LSCALE (off):

print graph of logs of TAU scales.

LSFFULL (on):

print full set of standard line source function calculation results (used only if the basic set of results is printed).

LSFGRAF (on):

print Line Source Function graphs for all transitions, not just for those with LSFPRINT = 1.

LSFPRNT (on):

print results of Line Source Function calculations for all transitions, not just for those with LSFPRINT = 1.

LTE (off):

calculate LTE versions of emergent line intensity and flux profiles.

LTEDATA (on):

print LTE values of S and FR, (used only when LTE is on).

LYMAN (off):

calculate Level- \mathcal{N} -to-Continuum transfer in detail (the 'Lyman' calculation).

LYMCOPR (off):

print continuum data for Level- \mathcal{N} -to-Continuum transfer calculation wavelengths, (used only when LYMAN is on).

LYMDMP (off):

print debug dump output from Level- \mathcal{N} -to-Continuum transfer calculation, (used only when LYMAN is on).

MAGPRNT (off):

print Magnesium populations and departure coefficients.

MAKIX (on):

insert place-markers in printout file, and generate the corresponding index file.

MCINPUT (on):

accept lower- and MiXed-case input statements, instead of UPPER-case only.

METPRNT (off):

print details of automatic Statistical Equilibrium Equation Method selection, (used only when METSW is on).

METSW (off):

try the other Statistical Equlibrium Equation methods whenever a value of line-source-function-epsilon < -0.9999.

MITPRNT (off):

provide only a bare minimum printout for each iteration, (used only when ALL is off or EVERY is off).

MONOTAU (off):

force all sets of calculated optical depths to increase monotonically.

NBPRNT (off):

print final, weighted values of number density and departure coefficient.

NEDIT (off):

edit number densities to insure positive line source functions.

NESWICH (on):

recalculate NE in detail, instead of setting NE = NP.

NHADJ (on):

adjust the calculated values of NH so that TAU5000 = 1 where Z = 0, (used only when HSE is on; will be turned off automatically when HSE is off).

NRSMOOTH (on):

smooth the $n\ell/n1$ ratios in the diffusion calculations.

NVOIT (on):

print Voigt function calculations execution statistics.

OPAGRAF (off):

print graph of absorbers.

OPANEG (on):

edit negative Line Opacity only to keep Total Opacity positive.

OPAPRNT (off):

print detailed analysis of the contributions to the background opacity.

OPASUM (off):

print an 'Absorber Summary'.

OPTHINL (off):

use the optically-thin-limit approximation.

OPTPRNT (on):

print OPTIONS listing.

ORIGIN (off):

provide 'long version' of analyses of regions of formation of values of emergent intensity.

ORSHORT (off):

provide 'short version' of analyses of regions of formation of values of emergent intensity, (used only when ORIGIN is on).

ORT (off):

radiation flows in the 'outward' direction only, instead of isotropically.

OXYPRNT (off):

print Oxygen populations and departure coefficients.

OXY2PRNT (off):

print Oxygen-II populations and departure coefficients.

OXY3PRNT (off):

print Oxygen-III populations and departure coefficients.

PARTPRNT (off):

print the tables of Ionization Potentials, Partition Functions and/or Partition Function ratios.

PARTVAR (on):

use depth-varying values of Partition Functions (instead of constant values).

PASSPRNT (on):

print results and details of line source function calculations for passive transitions.

PDCHECK (off):

print debug checksums.

PDETPRNT (on):

print details of BD and ND calculations, illustrated at depth # IBNVIEW (used only when POPPRNT is on).

PED (off):

print results and details of particle energy dissipation calculation.

PEDDMP (off):

print debug dump output from particle energy dissipation calculation.

PEGTNALL (on):

print GTN-editing messages for every iteration, not just the last one.

PERDMP0 (off):

print debug dump output from PERSEUS for transition (MS/NS): contents of data blocks, (see Note 59, Section 5).

PERDMP1 (off):

print debug dump output from PERSEUS for transition (MS/NS): but without details of frequency/angle summations, (see Note 59, Section 5).

PERDMP2 (off):

print debug dump output from PERSEUS for transition (MS/NS): details of frequency/angle summations, (see Note 59, Section 5).

PERDMP3 (off):

print debug dump output from PERSEUS for transition (MS/NS): PRD data arrays, (see Note 59, Section 5).

PESRJALL (off):

print S, RHO and JBAR editing messages in every iteration, not just the last one.

PHASE2 (on):

calculate emergent spectrum, and provide summary analyses.

PIJPRNT (off):

print the bound-free collision rates PIJ (for 'minimal' printout, see input parameter IRATE).

POPBSW (off):

set the departure coefficients for higher levels equal to those for the highest calculated level (instead of their LTE values), for 'population update ions' only.

POPGRAF (on):

print graph of number densities.

POPPRNT (on):

print results and details of the number densities calculations.

PRDCOPR (off):

print continuum data for PRD (partial redistribution profile points) wavelengths (see also input parameter **IPRDF**).

PRDITER (off):

print results of all PRD-iterations, not just the last one.

PRDMETH (on):

Use the Hubery-Lites, instead of the Kneer-Heasley, formulation for PRD.

PRDPRNT (off):

print results and details of PRD calculations.

PROCPRNT (on):

print line profile-specific emergent continuum intensities.

PRODMP (off):

print debug dump output from emergent intensity calculations.

PROSAV (off):

write emergent line profile data in the Special Spectrum Save File, (this option will be turned on automatically when SPECSAV is on).

PTN (on):

edit negative values out of tables of TAU integrands.

QSFEDIT (on):

edit negative values out of tables of QSF (PRD modified source function).

RABDAT (on):

save data needed for separate RABD calculation.

RATEALL (off):

print complete details of rates integrations.

RATECOPR (off):

print continuum data for rates integrations wavelengths.

RATEFULL (on):

print details of the rates integrations.

RATEGRAF (on):

print graphs of the TR sets and JNU sets used in rates calculations.

RATEPRNT (off):

print results and details of the 'SETTUP' calculation, *i.e.*, rates calculation (for 'minimal' printout, see input parameter IRATE).

RATESUMM (off):

print rate integration summary for every level.

RCOMPRNT (on):

print details of recombination calculation.

REFLECT (off):

the plane-parallel atmosphere is symmetric about the lowest depth value.

RHBPRDT (on):

print details of 'RHO + RBD' calculation for each radiative transition (only if RHBPRNT is on).

RHBPRNT (on):

print Explanation, and Results (optional), of the 'RHO + RBD' calculations (see also options BDPRNT, RHBPRDT, RHBPRSM).

RHBPRSM (off):

print final sets of Rho and b-ratios from 'RHO + RBD' calculation (only if RHBPRNT is on).

RHEDIT (off):

edit the calculated values of RHO (net radiative bracket).

RHOFUDGE (off):

'fudge' RHO's as necessary for calculation of BDIJ, (to assure positive values of BDIJ).

RHOWOPT (on):

use the same 'artificial' set of TAU values for all transitions when computing RHO/W, instead of the line-core TAUs of each transition.

RIJPRNT (on):

print ratio of collision rates RIJ.

RKINCR (off):

artificial RK enhancement.

RSMOOTH (off):

smooth the calculated RHO sets using the sequential smoothing procedure.

RSQUARE (off):

use depth-varying (instead of constant) dilution factor, (used only when IN-CIDNT is on).

SCALE (off):

print collated TAU scales.

SDIRECT (off):

replace negative Line Source Function values in "Direct" calculations by interpolated positive ones.

SEBUG (off):

print intermediate details of the statistical equlibrium calculations for transition (MS/NS), (also uses the value of LDINT).

SECOMP (off):

print comparative analysis of the results from the different Statistical Equlibrium methods.

SEDIT (on):

edit negative values out of calculated sets of Line Source Functions obtained by the "Full" solution.

SEDITIF (off):

edit negative values out of frequency-dependent Line Source Functions used for intensity and flux profiles.

SEPRNT (off):

print results and details of Statistical Equilibrium calculations.

SETIME (off):

print timings for the different Statistical Equilibrium methods, (used only when SECOMP is on).

SILPRNT (off):

print Silicon populations and departure coefficients.

SLFGRAF (off):

print graph of SLF for transition (MS/NS).

SLFPRNT (off):

print SLF for transition (MS/NS).

SLFSAV (off):

save SLF in the Special Spectrum Save File.

SLYR (on):

smooth the calculated Lyman RK- $\mathcal N$ set.

SNUSHFT (off):

apply frequency-shift to PRD SNU in emergent profile calculations.

SOBDMP (off):

print debug dump output from Sobolev escape probability calculation.

SOBINT (off):

print Sobolev integration details, (used only when SOBDMP is on).

$\mathbf{SODPRNT} \ (\mathrm{off}) :$

print Sodium populations and departure coefficients.

SPECSAV (off):

save all spectrum data in the Special Spectrum Save File, (this is equivalent to turning on both CONSAV and PROSAV).

SPECSUM (off):

provide a 'Spectrum Summary'.

SPHEGEOM (off):

print complete sets of all Z-dependent geometrical quantities, (used only when SPHERE is on).

SPHERE (off):

the atmosphere is spherically symmetric, instead of being plane-parallel and semi-infinite.

SPHETAU (off):

calculate optical depths along rays by quadratic integration, instead of by trapezoidal rule, (used only when SPHERE is on).

SPHOUT (off):

use spherically-symmetric geometry in computing emergent line and continuum flux, (used only in cases where the line source functions were calculated with plane-parallel coordinates).

SQSMDMP (off):

print details of sequential smoothing, (used only when SQSMPRNT is on).

SQSMPRNT (off):

print brief messages for all occurrences of sequential smoothing.

SSMOOTH (off):

do "alternate" sequential smoothing for S-from-number densities.

STANDARD (on):

print various basic numerical data.

STANCOPR (off):

print results of continuum calculations for standard background wavelengths.

STANPRNT (off):

print provisional depth-dependent input tables, before interpolation to the standard Z table of this run.

STAUREDM (on):

print short version of TAU-reduction error message from the WN-matrix calculation.

STIMPRNT (off):

print values of stimulated emission factors.

STKWATT (on):

attenuate Hydrogen line Stark splitting components outside the Doppler core at each depth.

SULPRNT (off):

print Sulphur populations and departure coefficients.

SUMGRAF (on):

print 'iterative summaries' in graphical, rather than in tabular, form, (used only when SUMMARY is on.

SUMMARY (on):

print 'iterative summaries,' and a fudging summary.

SUMTREND (on):

print Iteration Trends summary.

TANG (on):

include the ray tangent to the first depth (*i.e.* shell) in the angle integrations for spherical geometry, (used only when NTAN = 1, and only when SPHERE is on).

TAUDMP (off):

print debug dump output from all optical depth integrations (TAU calculations).

TAUPLOT (on):

print TAU scales for all transitions beneath the departure coefficient graphs.

TAUPRNT (off):

print results and details of the line-core optical depth calculations.

TAUSUM (off):

print a 'TAU Summary'.

TEGRAF (on):

print graph of temperature vs. optical depth.

TOPE (off):

save data for separate 'Continuum Plots' program.

TRANSAV (off):

save transitions data in special file (.tsf).

TRPRNT (off):

print computed effective radiation temperatures.

TRUECONT (off):

compute "true continuum" as needed for residual line profiles.

TRUECOPR (off):

print results of "true continuum" calculations needed for residual line profiles.

ULNORM (on):

use H Lyman lines normalization factors.

USENCJ (on):

calculate background continuum JNU directly, instead of from the source function.

USETRIN (off):

calculate values of the rates RK and RL with the 'old' method, which requires input values of TR.

USETSM (off):

eliminate TAU values smaller than TSM in emergent intensity and continuum mean intensity calculations.

USEWTAB (on):

use standard rates integrations wavelengths.

VELGDMP (off):

print details of velocity gradient terms calculation, (used only when VLGPRNT is on).

VELGRAD (off):

include velocity gradient terms in statistical equilibrium equations (only in Hydrogen or Helium runs).

VELS (off):

use calculated diffusion velocity in source function calculations.

VESCAPE (off):

use Voigt expression for the escape probability.

VLGPRNT (on):

print data from velocity terms calculation (used only when VELGRAD is on).

VSWITCH (off):

use two broadening velocity sets, instead of just one.

VTV (on):

set VT = V.

WATESTE (on):

use logarithmic style of weighting for Lyman EP1, EP2.

WATESTR (on):

use logarithmic style of weighting for all RHO sets.

WAVENUMB (off):

print results in wavenumber instead of wavelength units.

WAVEPRNT (on):

print Continuum Wavelengths summary table (also uses the value of LWNT).

WISFILE (off):

write an 'iterative studies' save file for transition (MS/NS).

WNDMP (off):

print debug dump output for all WN-matrix calculations.

WTABPRNT (off):

print standard rates integrations wavelengths.

XRAYCRID (off):

print details of X-ray cooling rates wavelength integration.

ZCOMP (off):

when mass is prescribed, adjust Z to match the input mass scale.

ZPRNT (off):

reprint input values of Z and TE to nine significant figures.

REFERENCE GUIDE

This is a listing of OPTION names, in alphabetical order by description. Once an OPTION's name has been identified by means of this list, its full specification can then be found in the main table at the start of this section.

ACSFPRNT abbreviated continuum source function calculation printout

AHSEPRNT abbreviated HSE calculation printout

AINDPRNT abbreviated INPUT printout

APRFPRNT abbreviated line profile calculation results

ALSFPRNT abbreviated Line Source Function calculation printout

ALYMPRNT abbreviated LYMAN calculation printout **APOPPRNT** abbreviated number densities printout

AOPTPRNT abbreviated OPTIONS listing

APOPPRNT abbreviated POPULATIONS printout **DELABORT** abort, delayed, during input reading

OPASUM absorber summary printout

OPAGRAF absorbers (background continuum opacity contributors) graph
OPAPRNT absorbers (background continuum opacity contributors) printout

ANALYSIS absorption profiles, line, details printout
HEABD abundance, Helium, depth dependence
RABDAT abundance ratio calculation data

APHICOPR additional photoionization background continuum data printout

APHIPRNT additional photoionization details printout

ADDCOPR additional wavelengths continuum data printout
NHADJ adjustment of NH (Hydrostatic Equilibrium)
CPSW adjustment of NH (not Hydrostatic Equilibrium)

LINECOMP albedo, scattering, analysis LINECOMP albedo, scattering, analysis

RATEALL all integration data should be printed for Rates Integrations

BSMOOTH 'alternate' sequential smoothing procedure for departure coefficients 'alternate' sequential smoothing procedure for S-from-number density

ALUPRNT Aluminum populations printout

DIFFANA ambipolar diffusion, analysis of results

NRSMOOTH ambipolar diffusion, smoothing of number density ratios

AMDIFF ambipolar diffusion terms

AMDN1 ambipolar diffusion terms alternative

GNVCALC ambipolar diffusion terms alternative

AMDDMP ambipolar diffusion terms detail printout

AMBPRNT ambipolar diffusion terms printout

COMOPAN analysis of Composite Lines (Kurucz) opacity contribution

RHOWOPT artificial TAU in RHO/W calculation

ATMOPRNT ATMOSPHERE data printout

EXPAND atmosphere stationary or expanding

ATOMPRNT ATOM data printout

ATOMSAV atomic model parameters in output file

AINTPRNT attenuate Hydrogen lines Stark splitting components
AINTPRNT A-values (frequency integration weights) printout
A-values (frequency integration weights) printout
AEDIT A-values (frequency integration weights) editing

AVCON averaged continuum intensity

AVELOP Averaged Lines opacity

AVOPRNT Averaged Lines opacity details printout

INTRPRNT AW input values printing

CSWITCH b-for-PERSEUS temperature selector

BDCALC b from all level equations
BDCALC b from continuum equation

JBDNC b-ratios and RHO calculation bypass
BRATDMP b-ratios calculation debug details
LONGNBM b-ratios calculation error message
BDPRNT b-ratios printout (complete)

EMERBACK backface emergent spectrum backface incident radiation

LBDPRNTbackground data (summary at line core wavelengths) printoutUSEWTABbackground wavelengths (standard), for rates calculationWTABPRNTbackground wavelengths (standard), for rates calculation

STANDARD basic numerical data printouts

CSF BC (Line Source Function calculation option)
CSFB BC (Line Source Function calculation option)

BDMP BD calculations details

PDETPRNT BD calculations trace, using IBNVIEW

BDGRAF BD graph printout

INNBPRNT BD input values printing

ITERB BD iterative summary printing
LONGNBM BDIJ calculation error message

BDGRAF BDIJ graph printout

RHBPRDT BDIJ printoutRHBPRNT BDIJ printoutRHBPRSM BDIJ printout

BDPRNT BDIJ printout (complete)
BLENDMP blended lines components dump

CIJPRNT bound-bound collision rates CIJ printout
PIJPRNT bound-free collision rates PIJ printout

HBROAD broadening, ion (Hydrogen)

broadening velocity = microturbulence velocity

VSWITCH broadening velocities switch

JBDNC bypass b-ratios and RHO calculation JBDNC bypass RHO and b-ratios calculation

CALPRNT Calcium populations printout
CARPRNT Carbon populations printout

CEFACTS CE-enhancement factors, using and updating

CHXDMP charge-exchange calculation dump
CHXPRNT charge-exchange calculation printout

CHEXLO charge-exchange, lower-level

CHEXLOL charge-exchange, lower-level, Hydrogen populations

CHEXUP charge-exchange, upper-level

IVALICK check validity of emergent intensity integrations

CHKGRAF CHECKs graphs, for all iterations

PDCHECK checksums printing

INTRPRNT CHI input values printingITERCHI CHI iterative summary printing

CIJPRNT CIJ printout control

CODMP CO-lines absorption calculation details printout

COCLIPSE CO-lines continuum eclipse calculation

COOLCO CO-lines cooling rate calculation

COCRID CO-lines cooling rate calculation details printout
COCOPR CO-lines wavelengths continuum data printout

SCALE collated TAU scales printout

CIJPRNTcollision rates, electrons, CIJ printoutPIJPRNTcollision rates, electrons, PIJ printoutRIJPRNTcollision rates, electrons, ratio RIJ printoutCOLHPRNTcollision rates, Hydrogen atoms, printout

COLTEMP color temperatures

LINECOMP comparison of Line Source Function and Composite Line calculations comparison of Line Source Function and Composite Line calculations

EPCOMP comparison of Lyman Epsilons methods

SECOMP comparison of Statistical Equilibrium methods

SETIME comparison of Statistical Equilibrium methods timing

COMPRK comparison RKs

FLWBPRNT component profiles (flow-broadened) printout COOLCOM Composite Lines cooling rate calculation

COMCRID Composite Lines cooling rate calculation detail printout

COMOPAN Composite Lines opacity analysis

KOMPRNT Composite Lines opacity details printout

COMPCOPR Composite Lines opacity wavelengths continuum calculations printout

LINECDMP Composite Lines scattering albedo analysis
 LINECOMP Composite Lines scattering albedo analysis
 ITERCHK Consistency Checks iterative summary

CNKPRNT Consistency Checks printout
CPSW constant pressure NH adjustment
STANDARD constants (physical) printout

OPAGRAF continuum absorbers (continuum opeacity contributors) graph
OPAPRNT continuum absorbers (continuum opeacity contributors) printout

TRUECONT continuum calculation, "true"

APHICOPR continuum data (additional photoionization) printout ADDCOPR continuum data (additional wavelengths) printout

COCOPR continuum data (CO-lines)

COMPCOPR continuum data (Composite Lines opacity wavelengths) printout

DUSTCOPR continuum data (dust) printout

FDBCOPR continuum data (FDB wavelengths) printout

HMSCOPR continuum data (H-minus departure coefficient wavelengths) printout

KSHLCOPR continuum data (K-shell wavelengths) printout
LINECOPR continuum data (Line Core wavelengths) printout

LYMCOPR continuum data (Lyman calculation wavelengths) printout

PRDCOPR continuum data (PRD wavelengths) printout

RATECOPR continuum data (rates calculations wavelengths) printout
STANCOPR continuum data (standard background wavelengths) printout
LBDPRNT continuum data (summary at line core wavelengths) printout

TRUECOPR continuum data ("true continuum") printout

CONSAV continuum emission special output

EMIGRAF continuum emitters (Continuum Source Function) graph
EMIPRNT continuum emitters (Continuum Source Function) printout

CONFLUX continuum flux

CNFLXDMP continuum flux debug printout **FLUXDMP** continuum flux detail printout

SPHOUT continuum flux using spherical coordinates

EMERINT continuum intensity

AVCON continuum intensity, averaged EMINDMP continuum intensity debug printout

DIDHC continuum intensity, dI/dh

PROCPRNT continuum intensity, line profile-specific
CONIPRNT continuum intensity, "true," printout
USENCJ continuum JNU method selection
LYMAN continuum (Lyman) transfer calculation

OPAGRAF continuum opacity contributors (absorbers) graph
OPAPRNT continuum opacity contributors (absorbers) printout

TOPE 'Continuum Plots' data

CSFGRAF Continuum Source Function and opacity graph
ACSFPRNT Continuum Source Function calculation printout
CSFPRNT Continuum Source Function calculation printout

EMIGRAF Continuum Source Function contributors (emitters) graph
EMIPRNT Continuum Source Function contributors (emitters) printout

WAVEPRNT Continuum Wavelengths summary printout STANDARD control parameters (numerical) printout

COOLCO cooling rate, CO-lines

COOLCOM cooling rate, Composite Lines

COOLXRAY cooling rate, X-rays

COOLSAV cooling rates calculation special output for plotting

COCRID cooling rates debug printout, CO-lines

COMCRID cooling rates debug printout, Composite Lines

HFFCOOLD cooling rates debug printout, H and H-minus free-free

XRAYCRID cooling rates debug printout, X-rays

CALCOOL cooling rates (net radiative)CSFDMP CSF calculation debug printout

CSFPRNT CSF calculation printout
DPDWPRNT damping parameter printout

PDCHECK debug checksums

AMDDMP debug printout, ambipolar diffusion

BLENDMP debug printout, blended lines components

BRATDMP debug printout, b-ratios calculation

CHXDMP debug printout, charge-exchange calculation
COCRID debug printout, CO-lines cooling rate integration

COMCRID debug printout, Composite Lines cooling rate integration

CNFLXDMP debug printout, continuum flux calculation

CSFDMP debug printout, CSF calculation
ECLIDMP debug printout, eclipse calculation

EMINDMP debug printout, emergent continuous intensity

FDBDMP debug printout, FDB terms

GDMP debug printout, geometrical dilution

HFFCOOLD debug printout, H and H-minus free-free net cooling ratesHSEDMP debug printout, hydrostatic equilibrium calculation

LINTDMP debug printout, line intensity calculation
PRODMP debug printout, line intensity calculation

PERDMP0 debug printout, Line Source Function calculation PERDMP1 debug printout, Line Source Function calculation PERDMP2 debug printout, Line Source Function calculation PERDMP3 debug printout, Line Source Function calculation **LYMDMP** debug printout, Lyman continuum calculation **EPDMP** debug printout, Lyman Epsilons calculation **TAUDMP** debug printout, optical depth integrations **PEDDMP** debug printout, particle energy dissipation

PERDMP0 debug printout, PERSEUS
PERDMP1 debug printout, PERSEUS

PERDMP3 debug printout, PERSEUS debug printout, PERSEUS

DRDMP debug printout, PRD DR calculation
INDXDMP debug printout, random access files indices

KROSSID debug printout, Rosseland-mean opacity integration

SQSMDMP debug printout, sequential smoothing

SOBDMP debug printout, Sobolev escape probability calculation
SOBINT debug printout, Sobolev escape probability calculation
SEBUG debug printout, statistical equilibrium calculation

VELGDMP debug printout, velocity gradient terms
WNDMP debug printout, weight matrix calculations
XRAYCRID debug printout, X-rays cooling rates integration
ATOMSAV default atomic model parameters in output file

DELABORT delayed abort during input reading
BDMP departure coefficients calculation details

BEDIT departure coefficients editing

BDCALC departure coefficients from all level equations
BDCALC departure coefficients from continuum equation

BDGRAF departure coefficients graph
TAUPLOT departure coefficients graph
HMS departure coefficients, H-minus

GTNSTIM departure coefficients, instead of Ns, in STIM for GTN(u,l)

ITERB departure coefficients iterative summary POPBSW departure coefficients, populations ions

RHOFUDGE departure coefficients ratios calculation RHO fudging

BSMOOTH departure coefficients smoothing

NBPRNT departure coefficients supplementary printout

HEABD depth-dependent abundance, Helium

ITERZ depth scale recalculation iterative summary printing

RSQUARE depth variation of dilution factor

AMDDMP detail printout for ambipolar diffusion terms
CHXDMP detail printout for charge-exchange calculation

FLUXDMP detail printout for emergent continuous flux calculation
CODMP detail printout for CO-lines absorption calculation

LINECDMP detail printout for LINECOMP options

EPDMP detail printout for Lyman Epsilons calculation

LNUMDMP detail printout for number density calculation
 RCOMPRNT detail printout for recombination calculation
 LINECDMP detail printout for scattering albedo analysis
 ADN1DMP detail printout for "special N1" calculation

SEBUG detail printout for statistical equilibrium calculation
VELGDMP detail printout for velocity gradient terms calculation

DIDHC dI/dh, emergent continuum
DIDHL dI/dh, emergent line profiles

AMDIFF diffusion, ambipolar

AMDN1 diffusion, ambipolar, alternative

DIFFANA diffusion, ambipolar, analysis of results
 AMDDMP diffusion, ambipolar, detail printout
 GNVCALC diffusion, ambipolar, GNV1 method
 HENORM diffusion, ambipolar, He renormalization

AMBPRNT diffusion, ambipolar, printout diffusion, ambipolar, smoothing

NRSMOOTH diffusion, ambipolar, smoothing of number density ratios

DIFFANA diffusion analysis

VELS diffusion velocity in Line Source Function

RSQUARE dilution factor depth variation

SDIRECT 'direct' Line Source Function editing option

DPDWPRNT Doppler width printout **DRDMP** DR (PRD) debug printout

DUSTDMP dust calculation: print numerical details of temperature recalculation

DUSTEMP dust calculation: recompute temperature

DUSTYPE dust calculation: Type-2

ITERTD dust temperature recalculation iterative summary printoutDUSTCOPR dust temperature recalculation continuum data printout

ECLIDMP eclipse calculation debug printout
ECLISAV eclipse emission special output
ECLIPSE eclipse intensity calculations

COCLIPSE eclipse intensity calculations, for CO lines

ECLIGRAF eclipse intensity graphs, for Lines

BEDIT edit departure coefficients

OPANEG edit GTN

INBED edit input values of b-ratios

INTEDIT edit input values of TE

OPANEG edit Line Opacity

SDIRECT edit Line Source Function
SEDIT edit Line Source Function

EPSW edit Line-Source-Function-epsilons

ENL edit Lyman Epsilon-1
ENL2 edit Lyman Epsilons
EPSNEDC edit Lyman Epsilons

OPANEG edit negative Line Opacity

NEDIT edit number densities to insure positive line source functions

QSFEDIT edit QSF (PRD modified source function)

RHEDIT edit RHO

IRHWED edit RHOWT input values

SEDITIF edit SLF

PTN edit TAU integrands

PEGTNALL editing messages from GTN calculation

PESRJALL editing messages form S, RHO and JBAR calculation

TRPRNT effective radiation temperature printout
ELECPRNT electron density calculation details printout

NESWICH electron density calculation switch

ITERNE electron density iterative summary printing

EMERINT emergent continuous intensity

EMINDMP emergent continuous intensity debug printout

DIDHC emergent continuous intensity, dI/dh

PROCPRNT emergent continuous intensity, line profile-specific

SPECSAV emergent intensity special output
CONSAV emergent intensity special output
STIMPRNT emission factors, stimulated, printout

EMISUM emitter summary printout

EMIGRAF emitters (Continuum Source Function contributions) graph
EMIPRNT emitters (Continuum Source Function contributions) printout

CEFACTS enhancement factors for CE, using and updating

RKINCR enhancement factors for RK, artificial

ENHANCE enhancement (R-squared) for emergent intensities

ENL Epsilon-1 (Lyman) editing

EPSW Epsilons (Line Source Function) editing

METSW Epsilons (Line Source Function) for Statistical Equlibrium calculations

EPDMP Epsilons (Lyman) debug printout

ENL2 Epsilons (Lyman) editing EPSNEDC Epsilons (Lyman) editing

EPCOMP Epsilons (Lyman) methods comparison
LONGNBM error message from BDIJ calculation

STAUREDM error message from WN-matrix calculation
SOBDMP escape probability (Sobolev) calculation dump
VESCAPE escape probability (Sobolev) Voigt expression

IRUNT execution statisticsIXSTA execution statistics

NVOIT execution statistics for Voigt function calculations

EXPAND expanding atmosphere

HSEV expansion velocity in hydrostatic equilibrium calculation

STANDARD exponentials and exponential integrals control parameter printout

INPEX extrapolate input tables

INPEXW extrapolate input tables, warning messages

FELE... fast electrons calculation options

FDBCOPR FDB wavelengths continuum printout

ZPRNT figures, significant, printed **REFLECT** finite atmosphere, reflective

FLWBPRNT flow broadeningFLWBROAD flow broadeningPHASE2 flux calculations

SPHOUT flux calculations using spherical coordinates

CONFLUX flux, continuum

CNFLXDMP flux, continuum, debug printout
 FLUXDMP flux, continuum, detail printout
 FLUXSAV flux, integrated, to be saved

LIGHT flux, Line

SEDITIF flux, Line, edit SLF for

LTE flux, Line, LTE

ORIGINformation regions of computed emergent intensitiesORSHORTformation regions of computed emergent intensitiesFDBDMPfrequency-dependent background terms printout

FDBCOPR frequency-dependent background wavelengths continuum printout

frequency-dependent line source function = SLF

AINTPRNTfrequency integrations data printoutINTAPRNTfrequency integrations data printoutAEDITfrequency integrations weights editing

SNUSHFT frequency shift for PRD SNU in emergent profile calculation

INCIFRNT frontface incident radiation

RHOFUDGE fudge RHOs
SUMMARY fudging summary
BDPRNT full b-ratios printout
GDS geometrical dilution

GDSDMP geometrical dilution canonical printout
GDMP geometrical dilution debug printout

SPHEGEOM geometrical Z-dependent quantities printout (spherical geometry) **STANDARD** geometrical Z-dependent quantities printout (spherical geometry)

VELGRAD gradient, velocity

VELGDMP gradient, velocity, dump printout

OPAGRAF graph of absorbers (background continuum opacity contributors)

CHKGRAF graph of CHECK, for all iterations
 BDGRAF graph of departure coefficients
 TAUPLOT graph of departure coefficients

CSFGRAF graph of Continuum Source Function and opacity

EMIGRAF graph of emitters (Absorption Source Function contributors)

ECLIGRAF graph of Line eclipse results

LSFGRAF graph of Line Source Function calculation results

LSCALE graph of logs of TAU scales
POPGRAF graph of number density

CSFGRAF graph of opacity and Continuum Source Function

TEGRAF graph of temperature vs. optical depth

RATEGRAF graph of TR and JNU, from rates calculation
 GTNSTIM GTN calculation, formulation of STIM for
 GTNSMTH GTN calculation, smoothing of STIM for

OPANEG GTN editing

PEGTNALL GTN-editing messages

HFFCOOLD H and H-minus free-free net cooling rate debug printout

CALHEAT heating rates (net radiative)

HFFCOOLD H-minus and H free-free net cooling rate debug printout

HMS H-minus departure coefficient

HMSCOPR H-minus departure coefficient continuum data printoutHMSONLY H-minus integration continuum wavelengths selection

HMSJPRNT H-minus JNU printout

HEABD Helium abundance, depth dependent

HENORM Helium populations renormalization (diffusion calculation)

HELPRNT Helium-I populations printoutHEL2PRNT Helium-II populations printout

AHSEPRNT HSE printout option

ALLY HSL iterations general printout frequency control

PRDMETH Hubeny-Lites PRD formulation

COLHPRNT Hydrogen atoms collision rates printout ITERNH Hydrogen density iteration summary

NHADJ Hydrogen density recalculation adjustment (HSE)

CPSW Hydrogen density recalculation adjustment (not HSE)

HBROAD Hydrogen, ion broadening

HSTSUMM Hydrogen lines Stark splitting summary

CLNORM Hydrogen Lyman lines (background) normalization factors
 ULNORM Hydrogen Lyman lines (background) normalization factors
 CHEXLOL Hydrogen populations for lower-level charge exchange

HNPRNT Hydrogen populations printout

STKWATT Hydrogen Stark splitting components attenuation

HSE hydrostatic equilibrium

HSEDMP hydrostatic equilibrium calculation debug printout

HSEV hydrostatic equilibrium (expansion velocity)HSEV hydrostatic equilibrium (mass motion velocity)

NHADJ hydrostatic equilibrium NH adjustment

AHSEPRNT hydrostatic equilibrium printout

PDETPRNT IBNVIEW-illustrated trace of BD and ND calculations

ILR incident Line radiation term
 INCIDNT incident radiation, backface
 INCIFRNT incident radiation, frontface
 MAKIX index file for printout file

INDXDMP index (random access file) dumps

ISCRS 'in-memory' scratch I/O

INBED input BDIJ (from unfudged RHOs) editing

AINDPRNT INPUT data printout INDAPRNT INPUT data printout

JSTIN 'input only'

MCINPUT input reading: accept mixed case statements

DELABORT input reading: delayed abort **INPEX** input tables extrapolation

INPEXW input tables extrapolation warning

INTEDIT input TE values editing

ZCOMP input values of mass, to be matched by adjusted Z values

INDPRNT input values of ND (number density)INNBPRNT input values of NK, ND and BD

INTRPRNT input values of RHO, JBAR, CHI and AW

MAKIX insertion of printout place-markers

INSCARD insurance restart data file PTN integrands (TAU) editing

FLUXSAV integrated flux quantities to be saved

INTRPRNT integrated mean intensity (JBAR) input values printing

COOLINT integrated net radiative cooling and heating rates

IVALICK integration (intensity) validity checking
 AINTPRNT integration, frequency, data printout
 INTAPRNT integration, frequency, data printout
 AEDIT integration, frequency, weights editing
 TAUDMP integrations debug printout for TAUs
 SOBINT integration (Sobolev) dump index

PHASE2 intensity calculations
EMERINT intensity, continuum

PROCPRNT intensity, continuum, line profile-specific CONIPRNT intensity, continuum, "true," printout

SPECSAV intensity data save file

LIGHT intensity, line

LINTDMPintensity, line, debug printoutPRODMPintensity, line, debug printoutSEDITIFintensity, line, edit SLF for

INTGRAF intensity, line, graphs, and S & B vs. Z graphsIVALICK intensity, line, integration validity checking

LTE intensity, line, LTE

SPECSAV intensity, line, special output
 PROSAV intensity, line, special output
 ORIGIN intensity, regions of formation
 ORSHORT intensity, regions of formation

CONIPRNT intensity, "true" continuum, printout

JNTRPOL interpolation of input JNU HBROAD ion broadening (Hydrogen)

INNBPRNT ionized number density input values printing

DOION ion-of-the-runISCRS I/O, scratch

FEPRNT Iron populations printout
MITPRNT iterations minimum printout

WISFILE iterative studies file
PHASE2 iterative summaries
SUMMARY iterative summaries

SUMGRAF iterative summaries in graph form

ITDMP iterative summary file contents index printout

ITERCHI iterative summary of CHI

ITERCHK iterative summary of consistency checks
 ITERB iterative summary of departure coefficient
 ITERNE iterative summary of electron density

ITERNH iterative summary of HND

ITERNH iterative summary of Hydrogen densityITERS iterative summary of Line Source Functions

ITERN iterative summary of NDITERNE iterative summary of NE

ITERN iterative summary of number densitiesITERTAU iterative summary of optical depth

ITERRHO iterative summary of RHO
 ITERRWT iterative summary of RHOWT
 ITERRK iterative summary of RK (Lyman)

ITERSiterative summary of SITERTAUiterative summary of TAUITERTDiterative summary of TDST

ITERNH iterative summary of total Hydrogen density

ITERZ iterative summary of Z

SUMTREND iterative trends summary

JLYSAV JB (Lyman continuum) save switch

PESRJALL JBAR editing message
INTRPRNT JBAR input values printing

USENCJ JNU (continuum) method selection

HMSJPRNT JNU (H-minus) printing

JNTRPOL JNU input (PRD) interpolation

RATEGRAF JNU(level), TR summary and JNU summary graphs

JLYSAV JNU (Lyman continuum) save switch

JNUPRNT JNU (PRD) printing

RATEGRAF JNU (rates calculation) graphsPRDMETH Kneer-Heasley PRD formulation

KSHLCOPR K-shell calculation background continuum calculation printout

KOMPRNT Kurucz Composite Line opacity details printout **KURPRNT** Kurucz Statistical Line opacity details printout

Level- \mathcal{N} -to-Continuum transfer = Lyman

ANALYSIS Line absorption profiles details printout

LBDPRNT Line center, background (continuum) data summary printout

ECLIGRAF Line eclipse calculation graphs

LIGHT Line flux calculation

SPHOUT Line flux profiles using spherical coordinates

PROSAV Line flux special output

LTE Line flux, LTE

KURPRNT Line haze opacity (statistical line opacity) details printout

LIGHT Line intensity and flux calculation

PROCPRNT Line intensity and flux, emergent continuum for

LINTDMP Line intensity debug printout
PRODMP Line intensity debug printout

DIDHL Line intensity, dI/dh APRFPRNT Line intensity printout

PROSAV Line intensity special output

LTE Line intensity, LTE OPANEG Line opacity editing

CSF Line Source Function calculation BC option
 CSFB Line Source Function calculation BC option
 PERDMP0 Line Source Function calculation debug printout

PERDMP1 Line Source Function calculation debug printout
PERDMP2 Line Source Function calculation debug printout
PERDMP3 Line Source Function calculation debug printout

LISEBRAF Line Source Function calculation graph
ALSEBRAT Line Source Function calculation printout
LISEBRAF Line Source Function calculation printout
LISEBRAF Line Source Function calculation printout

VELS Line Source Function calculation velocity (diffusion)

SDIRECT Line Source Function editing
SEDIT Line Source Function editing

PESRJALL Line Source Function editing message

Line Source Function, frequency-dependent = SLF

ITERS Line Source Function iterative summary

NEDIT Line Source Function, positive values, editing number densities LINECOPR line wavelengths background continuum calculations printout

LSCALE logs-of-TAU-scales graph

LONGNBM long error message from b-ratios calculation

MCINPUT lower-case input statements

CHEXLO lower-level charge-exchange calculation

CHEXLOL lower-level charge-exchange calculation, Hydrogen populations

LTEDATA LTE calculations printout

CHEXLOL LTE Hydrogen populations for lower-level charge exchange

LTE Line intensity and flux

Lyman = Level- \mathcal{N} -to-Continuum transfer

LYMCOPR Lyman continuum background continuum calculations printout

LYMDMP Lyman continuum calculation debug printout
JLYSAV Lyman continuum JNU (=JB) save switch
LYMAN Lyman continuum transfer calculation

EPDMP Lyman Epsilons debug printout

ENL2 Lyman Epsilons editing
EPSNEDC Lyman Epsilons editing

EPCOMP Lyman Epsilons methods comparisonsWATESTE Lyman Epsilons weighting method

ENL Lyman Epsilon-1 editing

CLNORM Lyman lines (Hydrogen) (background) normalization factors
ULNORM Lyman lines (Hydrogen) (background) normalization factors

ALYMPRNT Lyman printout

ITERRK Lyman RK iterative summary printing

SLYR Lyman RK smoothing

MAGPRNT Magnesium populations printout

ZCOMP mass, input values, to be matched by adjusted Z values

HSEV mass motion velocity in hydrostatic equilibrium calculation

STANDARD matrix calculations control parameters printout
INTRPRNT mean intensity, integrated, (JBAR), printing
EPCOMP methods comparison (Lyman Epsilons)

SECOMP methods comparison (Statistical Equilibrium calculation)

USENCJ methods switch for background continuum JNU microtrubulence velocity = broadening velocity

MITPRNT minimum printout for each iteration

MCINPUT mixed-case input statements

MONOTAUmonotonic TAUEXPANDmoving atmosphere

STANDARD MU integration weights printout

ZPRNT 9 significant figures

AMDN1 N1 calculation, diffusion calculation

ADN1DMP N1 calculation, diffusion calculation, details printout

ADN1PRNT N1 calculation, diffusion calculation, printout

LNUMDMP ND calculations details

PDETPRNT ND calculations trace, using IBNVIEW

POPGRAF ND graph

INNBPRNT ND input values printingITERN ND iterative summary printing

POPPRNT ND printing

NESWICH NE calculation switch
OPANEG negative GTN editing

OPANEG negative Line Opacity editing
ITERNE NE iterative summary printing

INTRPRNT net radiative bracket (RHO) input values printing

CALCOOL net radiative cooling rates
CALHEAT net radiative heating rates

NHADJ NH adjustment (Hydrostatic Equilibrium calculation)

CPSW NH adjustment (without Hydrostatic Equilibrium calculation)

ITERNH NH iterative summaryINNBPRNT NK input values printing

DOION 'no ion'

CLNORM normalization factors for background Hydrogen Lyman lines
ULNORM normalization factors for background Hydrogen Lyman lines

LNUMDMP number densities dump

NEDIT number densities editing for positive line source functions

POPGRAF number densities graph

INDPRNT number densities input values printingINNBPRNT number densities input values printing

GTNSTIM number densities, instead of BDs, in STIM for GTN(u,l)

ITERN number densities iterative summary

APOPPRNT number densities printout **POPPRNT** number densities printout

NRSMOOTH number densities ratios smoothing, diffusion calculations

NBPRNT number densities supplementary printout

STANDARD numerical data printout

CSFGRAF opacity and background continuum source function graph

AVOPRNT opacity (Averaged Lines) details printout
KOMPRNT opacity (Composite) details printout
KURPRNT opacity (Statistical) details printout

SPHETAU optical depth along ray by quadratic integration

TAUPRNT optical depth calculation printout

TAUDMP optical depth integrations debug printout

ITERTAU optical depth iterative summary
 MONOTAU optical depth monotonicity
 TAUSUM optical depth summary printout
 OPTHINL optically-thin-limit approximation

AOPTPRNT OPTIONS printout
OPTPRNT OPTIONS printout

ORIGIN origin regions of computed intensities
ORSHORT origin regions of computed intensities

ORT outward-only radiation

ALL overall iterations general printouts frequency control

OXYPRNT Oxygen populations printout
OXY2PRNT Oxygen-II populations printout

OXY3PRNT Oxygen-III populations printout
PED particle energy dissipation calculation

PEDDMP particle energy dissipation calculation details dump

PARTVAR partition function, mode PARTPRNT partition function, printout

PASSPRNT 'passive transitions' source function printout

IRUNT performance statisticsIXSTA performance statisticsNVOIT performance statistics

PERDMP0 PERSEUS calculation debug printout
PERDMP1 PERSEUS calculation debug printout
PERDMP2 PERSEUS calculation debug printout
PERDMP3 PERSEUS calculation debug printout

CSWITCH PERSEUS calculation selector of temperature for b

APHICOPR photoionization (additional), background continuum data printout

APHIPRNT photoionization (additional), details printout

STANDARD physical constants printout

PIJPRNT PIJ printout control

MAKIX place-markers in printout file

POPBSW populations ions departure coefficients

PHASE2 post-processing

PRDCOPR PRD background continuum data printout

DRDMP PRD DR debug printout

PRDITER
PRD iterations printout control
PRD JNU input interpolation
PRD JNU printout control
PRD JNU printout control

PRDMETH PRD method selector

QSFEDIT PRD modified source function (QSF) editing

PRDITERPRD printoutPRDPRNTPRD printout

SNUSHFT PRD SNU frequency shift for profile calculation **STANDARD** precalculated integration weights printout

MAKIX printout file place markers

ALLY printout frequency control for HSL iterations
ALL printout frequency control for overall iterations
EVERY printout frequency control for sub-iterations

MITPRNT printout: minimum per iteration

SNUSHFT profile calculation PRD SNU frequency shift

APRFPRNT profile calculation printout
PROSAV profile emission special output

FLWBPRNT profiles, flow-broadened profiles, flow-broadened profiles, line, details printout profiles, line, edit SLF for

PROCPRNT profile-specific emergent continuum intensity and flux

IRUNT program version descriptionSTANPRNT provisional input tables printout

QSFEDIT QSF editing

RABDAT RABD calculation data

USETRIN radiation temperatures used for rates calculation

ILR radiation, incident
 INCIDNT radiation, incident
 INCIFRNT radiation, incident
 ORT radiation, outward only

TRPRNT radiation temperature, effective, printout

CALCOOL radiative cooling ratesCALHEAT radiative heating rates

INDXDMP random access file indices dumps

RATECOPR rates calculation background continuum data printout

USETRIN rates calculation, from TR
RATEPRNT rates calculation printout

RATEGRAF rates calculation TR and JNU graphs
RATEALL rates integrations details printout
RATEFULL rates integrations details printout
RATESUMM rates integrations summary printout
USEWTAB rates integrations wavelengths, standard
WTABPRNT rates integrations wavelengths, standard

CALCOOL rates (net radiative cooling)CALHEAT rates (net radiative heating)

RIJPRNT ratios of collision rates RIJ printout
BDGRAF ratios of departure coefficients graph

RHOFUDGE ratios of departure coefficients RHO fudging

SPHETAU ray-optical-depth by quadratic integration

DELABORT reading input: delayed abort

RCOMPRNT recombination calculation details printout

REFLECT reflective finite slab

ORIGIN regions of formation of computed intensities
ORSHORT regions of formation of computed intensities

HENORM renormalization of Helium populations (diffusion calculation)

INSCARD restart file insurance

JBDNC RHO and b-ratios calculation bypass

RHOWOPT RHO calculation
RHEDIT RHO editing

PESRJALL RHO editing message

RHOFUDGE RHO fudging for calculating ratios of departure coefficients

INTRPRNT RHO input values printing

ITERRHO RHO iterative summary printing

RHBPRDT RHO printout
RHBPRNT RHO printout
RHBPRSM RHO printout

RSMOOTH RHO smoothing (sequential)
WATESTR RHO weighting method

ITERRWT RHO weights iterative summary

RHOWOPT RHO/W calculation
IRHWED RHOWT input editing
RIJPRNT RIJ printout control
RKINCR RK enhancement factors
COMPRK RK, Lyman, comparisons

ITERRK RK, Lyman, iterative summary

SLYR RK, Lyman, smoothing

KROSSID Rosseland mean opacity integration details printout

RSQUARE R-squared depth variation of dilution factor
ENHANCE R-squared enhancement for emergent intensities

PESRJALL S editing message

SSMOOTH S-from-number density smoothing

ITERS S iterative summary

INTGRAF S & B vs. Z graphs, and intensity graphs (Phase 2)

ATOMSAV save computed atomic model parameters

TOPE save 'Continuum Plots' data

COOLSAV save cooling rates data for plotting FLUXSAV save integrated flux quantities save Lyman-continuum JNU (=JB)

RABDAT save RABD calculation data

TRANSAV save transitions data in special file

ISCRS scratch I/O

LINECOMP scattering albedo analysis
LINECOMP scattering albedo analysis

SQSMDMP sequential smoothing details printout

SQSMPRNT sequential smoothing messages

BSMOOTH sequential smoothing of departure coefficients

DSMOOTH sequential smoothing of diffusion terms **RSMOOTH** sequential smoothing of RHO values

SSMOOTH sequential smoothing of S-from-number density values

RATEPRNT SETTUP printout

RATEFULL SETTUP, rates integrations details printout **STAUREDM** short error message from WN-matrix calculation

ZPRNT significant figures printed, more SILPRNT Silicon populations printout

SLF = frequency-dependent line source function

SEDITIF SLF editing

SLFGRAF SLF graph printing

SLFPRNT SLF printing

SLFSAV SLF saving in Special Spectrum Save File

BSMOOTH smoothing of departure coefficients

DSMOOTH smoothing of diffusion terms
SLYR smoothing of Lyman RK values

NRSMOOTH smoothing of number densities ratios, diffusion calculations

RSMOOTH smoothing of RHO

SSMOOTHsmoothing of S-from-number densityGTNSMTHsmoothing of STIM for GTN(u,l)SQSMDMPsmoothing, sequential, details printout

SQSMPRNT smoothing, sequential, messages

SOBDMP Sobolev escape probability solution details printout

SOBINT Sobolev integration dump index

SODPRNT Sodium populations printout

source function: see also Line Source Function

SPHERE source function calculations using spherical coordinates

ENHANCE source function enhancement (R-squared) for emergent intensities

EPSW source-function-epsilons printing

PASSPRNT source function printout, passive transitions

AMDN1 "special N1" calculation

ADN1DMP "special N1" calculation, details printout

ADN1PRNT "special N1" calculation, printout **SPECSAV** special output, calculated spectra

CONSAV special output, continuum intensity calculation

ECLISAV special output, eclipse intensities

PROSAV special output, profiles
PHASE2 spectrum calculations

SPECSAV spectrum calculations save file

SPECSUM spectrum summary

SPHOUT spherical coordinates for line and continuum fluxes **SPHERE** spherical coordinates for source function calculations

TANG spherical coordinates, use of tangent ray

SPHEGEOM spherical coordinates, Z-dependent quantities printout **STANDARD** spherical coordinates, Z-dependent quantities printout

USEWTAB standard background wavelengthsWTABPRNT standard background wavelengths

STANCOPR standard background wavelengths continuum data printout

STKWATT Stark splitting, Hydrogen, components attenuation

HSTSUMM Stark splitting, Hydrogen, summary

EXPAND stationary atmosphere

SEBUGstatistical equilibrium debug printoutSECOMPstatistical equilibrium methods comparisonMETSWstatistical equilibrium methods selection

METPRNT statistical equilibrium methods selection printout

SEPRNTstatistical equilibrium printoutSETIMEstatistical equilibrium timing dataKURPRNTStatistical Line opacity detailsGTNSTIMSTIM for GTN(u,l), formulation ofGTNSMTHSTIM for GTN(u,l), smoothing of

STIMPRNT stimulated emission factors printout
EVERY sub-iterations printout frequency control

SULPRNT Sulphur populations printout

PHASE2 summaries

SUMMARY summary and fudging printout
OPASUM summary printout, absorbers

WAVEPRNT summary printout, continuum wavelengths

EMISUM summary printout, emitters

SUMGRAF summary printout, graphical form

HSTSUMM summary printout, Hydrogen lines Stark splitting
ITDMP summary printout, iterative summary records index

LBDPRNT summary printout, line center background (continuum) data

RATESUMM summary printout, rates integrations

SPECSUM summary printout, spectrum TAUSUM summary printout, TAU

WAVEPRNT summary printout, wavelengths (Continuum)

NBPRNT supplementary number densities and departure coefficients printout

TANG tangent ray in spherical coordinates

SPHETAU TAU along ray by quadratic integration

PTN TAU integrands editing

TAUDMP TAU integrations debug printout

ITERTAU TAU iterative summary

LSCALETAU (logs) graphMONOTAUTAU monotonicityTAUPRNTTAU printout

STAUREDM TAU-reduction (WN-matrix calculation) error message

TAU scales printout
TAUPLOT
TAUSUM
TAUSUM
TAUSUM
TAUSTEMP
TOST iterative summary
TDST recalculation

DUSTDMP TDST recalculation numerical details printout

INTEDIT TE (input) editing ZPRNT TE printout, extra

TEGRAF temperature vs. optical depth graph
CSWITCH temperature selector for b (for PERSEUS)

SETIME timing comparison of statistical equilibrium methods

ITERNH total Hydrogen density iterative printout

PDETPRNT trace of BD and ND calculations at depth # IBNVIEW

RIJPRNT transition rates printout control
TRANSAV transitions data, save in special file

RATEGRAF TR graph
TRPRNT TR printout

TRUECONT "true continuum" calculation

TRUECOPR "true continuum" calculation printout
CONIPRNT "true continuum" intensity printout

USETRIN TR used for rates calculation

USETSM TSM use control

VTV turbulent pressure velocity default

DUSTYPE Type-2 dust opacity calculation

MCINPUT upper-case input statements

CHEXUP upper-level charge-exchange calculation

CHXDMP upper-level charge-exchange calculation dump
CHXPRNT upper-level charge-exchange calculation printout

USETSM use TSM

IVALICK validity checking of intensity integrations

velocity, broadening = velocity, microturbulent

VSWITCH velocity, broadening, switch

VELS velocity, diffusion, in Line Source Function

VELGRAD velocity gradient terms

DIFFANA velocity gradient terms, analysis

VELGDMP velocity gradient terms, details printout

VLGPRNT velocity gradient terms, printout

velocity, microturbulent = velocity, broadening

VTV velocity, microturbulent pressure, defaults

IRUNT version description

VESCAPE Voigt expression for escape probability

NVOIT Voigt function calculations execution statistics

VTV VT default

WAVEPRNT wavelengths (Continuum) summary printout
WAVENUMB wavelengths printed in spectrum output
WAVENUMB wavenumbers printed in spectrum output

WNDMP weight matrix calculations debug printouts

NWRHO weight (RHO) adjustment procedureWATESTE weighting method for Lyman Epsilons

WATESTR weighting method for RHO
COOLXRAY X-rays cooling rate calculation

XRAYCRID X-rays cooling rate integration details printout ZCOMP Z adjustment to match input mass values

ITERZ Z iterative summary printing

ZPRNT Z printout, extra

(Section 6 – last revised: 2007 Jan 29)

Section 7: Program Execution

PANDORA is written in Fortran; work on it began in 1966. It has run on various computers and operating systems, both at CfA and other places; currently at CfA it runs under Solaris (a flavor of Unix) on a SUN workstation.

PANDORA uses a large program address space, supplemented by a scratch disk file which can grow large (several Gbytes) depending on the run.

Internally, PANDORA refers to I/O files by Fortran unit numbers "nn." Externally, under Unix these files bear the generic names "fort.nn." I use a script called schema which supervises a pandora run and links variously-named I/O files to the proper Fortran units. While users are free to set up pandora runs and I/O file names as they wish, they are also free to use schema. In the listing overleaf, I give both the Fortran unit numbers and the specific file names or schema's file "extension codes" by which I refer to these files.

I recommend that users make their own copies of pandora, of schema (if used), and of the commonly available data files (such as atomic model files, Line Opacity data files, etc). This insulates users from the changes I routinely make to these files without prior warning. Users can then choose to make fresh copies whenever convenient.

Section 99 is a tutorial introduction to PANDORA and how to set up the input files.

The **Input Files** are connected to the following units:

- 3 general run-specific input (—.dat);
- 4 atmosphere model (—.mod);
- 7 atomic model (—.atm);
- 8 run-specific restart data (—.res);
- 9 JNU restart values for a PRD run (—.jnu);
- 10 required for Statistical Line opacity (statistical, see Section 9);
- 11 required for Composite Line opacity (composite, see Section 9);
- 12 required for Averaged Lines opacity (average, see Section 9).

Intermixed reading from files 3, 4, 7 and 8 is controlled by the **USE** statement. Part A of the input statements (see Section 3) must be in file 3 (—.dat); the very first occurrence of **USE** must also be in file 3 (—.dat).

The **Output Files** are connected to the following units:

- 15 general printout (—.aaa, see Section 11);
- 16 error messages and 'debug' data (—.aer, see Section 11);
- 19 restart data, PANDORA input format (—.rst);
- 20 restart data, mostly PANDORA input format (—.msc);
- 21 restart data, PANDORA input format (—.pop);
- 22 PRD JNU values, PANDORA input format (—.jnr);
- 23 results from the emergent spectrum calculations (—.spc);
- 24 calculated cooling rates (—.coo);
- 25 continuum data, for use by separate programs (—.csp);
- 26 sample matrices, for use by separate programs (—.mat);
- 27 Source-Function-related data (transitions data) (—.tsf);
- 28 run_archive (see below);
- 29 journal file: copies of the input data statements as read (—.jrl);
- 30 iterative studies data, for use by separate programs (—.itr);
- 31 printout index (—.aix, see Section 11);
- 32 checksums, for use by separate programs (—.cks).

The **Scratch File** is connected to unit 1 (—.tmp); it is a temporary file, used in direct access mode (see Section 5, Note 20).

The run_archive file is used to collect a 'performance data record' from each PANDORA run. This is a permanent file, opened for 'append access' as needed.

(Making a 'performance data record' depends on input parameter ${\bf IPERFA}.)$

(Section 7 – last revised: 2003 Jul 30)

Section 8: Output Files

Besides the printout files (described in Sections 7 and 11), PANDORA provides output in several additional files. Some of these contain data that can be used to restart the run (and may also contain data that is neither needed nor permissible for restarting – such files must be edited appropriately). Other files provide collections of data and results that are useful for various special purposes. See also Section 7.

Each of the four basic restart data files begins with the set of four "Run ID" lines (in the form of PANDORA comments), containing the run **HEADING**, program version number, two time stamps (one expressed in Smithsonian Days), and a summary of basic run data. Copies of the **HEADING** line also appear at various places in several files.

File fort.19 contains general restart data, as follows:

- \bullet Always —
- Run ID
- ullet Always —

for all radiative transitions u, ℓ : $\mathbf{METSE}^{u,\ell}$ (if METSW is on), $\mathbf{RHO}_i^{u,\ell}$, $\mathbf{RHWT}_i^{u,\ell}$, $\mathbf{JBAR}_i^{u,\ell}$, $\mathbf{CHI}_i^{u,\ell}$, $\mathbf{AW}_i^{u,\ell}$

- If option LYMAN is on for level j = KOLEV: IRKCOMP^j = 0, RK^j, RKWT $_i$, IRLCOMP^j = 0, RL^j, EP1 $_i$, EP2 $_i$
- Always —

 $\mathbf{N}\mathbf{K}_i,\,\mathbf{N}\mathbf{D}_i^j$ for all levels $j;\,\mathbf{B}\mathbf{D}_i^j$ for all levels j

 $\bullet \ Always --$

"USE (INPUT) "

File fort.20 contains miscellaneous restart and other data, as follows:

• Always —

Run ID

• Always —

 N, Z_i, TE_i

• If **POPUP** is on but \neq HYDROGEN — \mathbf{NE}_i , \mathbf{ZME}_i , \mathbf{NC}_i

• If option HSE is on —

 $\mathbf{MASS}_i,\,\mathbf{PGS}_i,\,\mathbf{PTO}_i,\,\mathbf{TE}_i,\,\mathbf{VT}_i,\,\mathbf{VM}_i,\,\mathbf{GD}_i,\,\mathbf{T5000}_i$

• If option ATOMSAV is on and default values of atomic parameters were computed —

atomic model parameter values

- ullet If options DUSTEMP and DUSTYPE are both on ${f TDST}_i$
- If MH2N = 1 —

 $H2N_i$

• If MCON = 1 — CON_i

• If POPUP = HYDROGEN and MFONT = 1 — atmosphere model data tables for Juan Fontenla

ullet $If\ \mathbf{NAME} = \mathtt{HELIUM2} - \mathbf{N},\ \mathbf{Z}_i,\ \mathbf{HE304}_i$

• If this is a K-shell run —

 N, Z_i, QIN_i

• If IRPUN = 1 —

two sets of data for a separate program (CENSUS) which calculates abundance ratios of ions of the same element

(these data include **Z**, and FLVSL and FIONL, as they appear in the 'POPULATIONS' printout; if AMDIFF is on and this is a Helium run, then a second set of these data will appear)

• If option JLYSAV is on —

Level- $\mathcal N$ -to-Continuum (Lyman) J-bar values

ullet If option USETRIN is off and f MTREF=1 — Effective Radiation Temperature values

• If MDFV = 1 and AMDIFF is on —

 $\mathbf{N}, \mathbf{Z}_i, \mathbf{TE}_i, \mathbf{VM}_i, \mathbf{VAMB}_i, \mathbf{VBMB}_i, \mathbf{VCMB}_i, \mathbf{VDMB}_i, \mathbf{VH}_i, \mathbf{VP}_i, \mathbf{VE}_i, \mathbf{V1}_i, \mathbf{V2}_i, \mathbf{V3}_i$

- If $\mathbf{MDFG} = 1$ and \mathbf{AMDIFF} is on \mathbf{GVL}_{i}^{j} , $1 \leq j \leq \mathbf{NL}$
- If RHEAB was recomputed N, Z_i, RHEAB_i
- If NAME = HELIUM or HELIUM2 and AMDIFF is on —
 N, Z_i, and either: PALBET_i, PBETAL_i if HELIUM; or PGMBET_i,
 PBETGM_i if HELIUM2
- If option CHEXUP is on and this is one of the 10 "charge exchange" ions $\mathbf{N}, \mathbf{Z}_i, \mathbf{XRKH}_i^j, \mathbf{XRLH}_i^j, 4 \leq j \leq \mathrm{NPQMX}$
- If MKURU = 1 —

then data for Kurucz's spectrum programs

(these data comprise the computed departure coefficients of the ion-of-the-run plus, if this is a Hydrogen run, some atmosphere data tables)

• If option CALCOOL is on —

data for separate program to calculate new TE values

(these data include **NE**, **NH**, **TE**, SUM [which is called 'Total Rate' in the 'NET RADIATIVE COOLING RATES' printout], and, in a Hydrogen run, SUMSM [i.e., smoothed values of SUM])

• If option FLUXSAV is on —

data for separate programs to calculate new TE values

(these data include **Z** and **TE**, and 'Integrated Flux', 'Integrated Derivatives' and 'Effective Temperature', as they appear in the 'CONTINUUM FLUX INTEGRALS' printout)

• If option ECLISAV is on —

results of eclipse emergent profile calculations

(these data include **R1N**, **Z** and **FRR**, and 'DL', 'ID' and 'IS', as they appear in the 'ECLIPSE INTENSITY AND FLUX' printout)

• If option CLNORM is on and this run calculates H Lyman α and/or β — FNRMLA and FNRMLB

(used by PANDORA to adjust the simulated H Lyman α and β lines in the background)

File fort.21 contains populations restart data as follows:

• Always —

Run ID

- If option HSE is on, and **POPUP** is set, and **NAME** = HYDROGEN NE_i , ZME_i , NC_i
- If option HMS is on **BDHM**_i
- If option AMDIFF or option VELGRAD is on, and VBMB $\neq 0$ $VBMB_i$
- If option HSE is on, or if option HSE is off and option CPSW is on \mathbf{NH}_i
- ullet If $\mathbf{POPUP} = \mathtt{HYDROGEN}$ —

for all levels j such that $1 \leq j \leq 15$: \mathbf{NP}_i , \mathbf{HN}_i^j , \mathbf{BDH}_i^j , plus all those 'population ions' populations tables (in the order shown just below) for which there was at least some input

• If POPUP = CARBON —

for all levels j such that $1 \le j \le 8$: \mathbf{CK}_i , \mathbf{CN}_i^j , \mathbf{BDC}_i^j

• If POPUP = SILICON —

for all levels j such that $1 \le j \le 8$: \mathbf{SIK}_i , \mathbf{SIN}_i^j , \mathbf{BDSI}_i^j

• If POPUP = HELIUM —

for all levels j such that $1 \le j \le 13$: \mathbf{HEK}_i , \mathbf{HEN}_i^j , \mathbf{BDHE}_i^j

• If POPUP = HELIUM2 —

for all levels j such that $1 \le j \le 8$: $\mathbf{HE2K}_i, \, \mathbf{HE2N}_i^j, \, \mathbf{BDHE2}_i^j$

• If POPUP = ALUMINUM —

for all levels j such that $1 \le j \le 8$: \mathbf{ALK}_i , \mathbf{ALN}_i^j , \mathbf{BDAL}_i^j

• If POPUP = MAGNESIUM —

for all levels j such that $1 \leq j \leq 8$: \mathbf{MGK}_i , \mathbf{MGN}_i^j , \mathbf{BDMG}_i^j

• If POPUP = IRON —

for all levels j such that $1 \le j \le 8$: \mathbf{FEK}_i , \mathbf{FEN}_i^j , \mathbf{BDFE}_i^j

- If POPUP = SODIUM —
- for all levels j such that $1 \le j \le 8$: \mathbf{NAK}_i , \mathbf{NAN}_i^j , \mathbf{BDNA}_i^j
- If POPUP = CALCIUM —

for all levels j such that $1 \leq j \leq 8$: \mathbf{CAK}_i , \mathbf{CAN}_i^j , \mathbf{BDCA}_i^j

• If POPUP = OXYGEN —

for all levels j such that $1 \le j \le 14$: \mathbf{OK}_i , \mathbf{ON}_i^j , \mathbf{BDO}_i^j

• If POPUP = OXYGEN2 —

for all levels j such that $1 \le j \le 8$: $\mathbf{O2K}_i, \, \mathbf{O2N}_i^j, \, \mathbf{BDO2}_i^j$

• If POPUP = OXYGEN3 —

for all levels j such that $1 \leq j \leq 8$: $\mathbf{O3K}_i,\,\mathbf{O3N}_i^j,\,\mathbf{BDO3}_i^j$

• If POPUP = SULPHUR —

for all levels j such that $1 \le j \le 8$: \mathbf{SK}_i , \mathbf{SN}_i^j , \mathbf{BDS}_i^j

File fort.22 contains special restart data as follows:

- Always Run ID
- $\mathbf{JNU}_{i,k}^{u,\ell}$ for all PRD transitions

<u>File fort.23 contains</u> data from all emergent spectrum calculations, to make them available to various auxiliary programs; this file is written only if options SPECSAV, PROSAV and/or CONSAV are on.

(These data include much of the input for the continuous intensity and flux calculations, and for the line intensity and flux calculations – mostly labelled in the file. The various quatities in the file can be identified by comparing them with the detailed normal printout. Note that, for Continuum Flux, the value printed is $4\pi H$, while the value saved is H. Both continuous intensity and line intensity are given for each value of μ , as is obvious. Extra data are saved when there is incident radiation – again, this should be clear. *Note*: flow-broadened profiles are indicated by setting the value of the velocity table index $\mathbf{NVY} = 0$. *Note* the effect of options WAVENUMB and INCIFRNT)

<u>File fort.24 contains</u> results of the cooling and heating rates calculations, for separate plotting programs; this file is written only when options CALCOOL and COOLSAV are both on.

(These data include almost all the quantities that appear in the two COOLING RATES and the two HEATING RATES printouts)

<u>File fort.25 contains</u> data for separate programs to produce 'continuum data' plots; this file is written only when the option TOPE is on.

(These data include, for each wavelength, the complete 'Continuum Data Blocks' (which contain all the information that appears in complete 'CONTIN-UUM DATA' printouts), followed by, again for each wavelength, the computed continuous emergent intensities and intermediate results from those computations. Since these data are not normally accessible, they are provided in this special file.

<u>File fort.26 contains</u> contains data for separate programs to analyze the performance of PANDORA's matrix inversion algorithms; this file is written only when the switch $\mathbf{SMATC} > 0$ and qualifying matrices were encountered; (this file is only of use to me, as the program developer)

<u>File fort.27 contains</u> final values of data from the line source function calculations for all radiative transitions, as they appear in the printout file; this file has them in a format intended to be more convenient for user-written analysis and plotting programs. This file is written when the option TRANSAV is on.

(These data include **Z** and **TE**, and then 'TAU', 'S', 'RHO', 'JBAR' and ST, the total source function as plotted)

<u>File fort.30 contains</u> 'iterative studies' data for a separate program to analyze the performance of PANDORA's iterative procedures, and provides various graphical displays of the data.

(These data include **Z** and **TE**, and 'EPSILON', 'S', 'TAU' and 'JBAR', as they appear in the 'LINE SOURCE FUNCTION' printout, for transition (**MS/NS**) *only*, for every iteration)

<u>File fort.32 contains</u> debug checksums, for separate program RELAX that compares checksum data files from different runs.

(This is not intended for routine use; it is a debugging aid for ongoing program development)

(Section 8 – last revised: 2007 Feb 05)

Section 9: Background Line Opacities

PANDORA's calculation of line source functions requires knowledge of the background opacity; this opacity is referred to casually as the "background continuum." Opacity from other lines may contribute to this background continuum for any given line. When such other lines are lines of the ion-of-the-run, then PANDORA's "blended line" mechanism is available to handle it. Some background lines due to H, He-II, and CO can be included explicitly (see the table printed by PANDORA as part of the ATMOSPHERE printout). In addition, general background line opacity can be included in three other ways: Statistical Line opacity, Composite Line opacity, and/or Averaged Line opacity; these are all added into the total background continuum.

This section describes the *control*, the *input* and the *data* requirements of these background absorbers. Note that the necessary input files are also mentioned in Section 7.

These three Background Line opacities are mutually exclusive: only one of them can be used at any given wavelength. Averaged Line opacity has highest priority: if it is used, then neither of the other two is used. Composite Line opacity has the next highest priority: if it is used, then Statistical Line opacity is not used; thus the latter is used only if neither of the others is used.

A) Scattering albedo

Each of these Background Line opacities is apportioned between an absorption part and a scattering part by means of an albedo table that is a function of depth.
This table is obtained by interpolation from the input tables \mathbf{ZALBK}_{ℓ} and \mathbf{ALBK}_{ℓ} , $1 \leq \mathbf{NKA}$.

When **NKA** = 0, then the scattering albedo = $1/(1 + Q_i)$, where Q_i is a function of depth and wavelength

$$Q_i = X_i \left(1 + \mathbf{CLM} \frac{10^4}{LM} \right) + PNH \left(\frac{\mathbf{NH}_i}{\mathbf{NH}_N} \right),$$

and X_i is either

$$X_i = \frac{\mathbf{XNE}_i}{1.07 \times 10^{14}} \left(\frac{LM}{5000}\right)^3 \frac{1}{\mathbf{CQM}}, \quad \mathbf{CQM} > 0,$$

or

$$X_i = \frac{\mathbf{XNE}_i}{1.07 \times 10^{14}} \left(\frac{LM}{5000}\right)^3 \frac{1}{\mathbf{CQA}(\mathbf{TE}_i)}, \quad \mathbf{CQM} \le 0.$$

Here LM is wavelength in Angstroms, and \mathbf{CQM} and \mathbf{CQA} (a tabulated function of \mathbf{CQT}_k , $1 \le k \le \mathbf{NCQ}$) are input parameters (see Section 5, Note *117). The default values of this tabulated parameter are:

\mathbf{CQT}	\mathbf{CQA}
4000	0.0001
5000	0.001
6000	0.01
7000	0.1
8000	1.0

B) Statistical Line opacities

PANDORA can use opacity distribution functions computed by Kurucz, as described in VAL II. Ten component opacity distributions, identified by k=1 through k=10, are given for 11×9 grids of temperature and electron density, at each of 53 wavelength grid points in the range 1269.80-8352.95 Å.

Temperature grid: log(TE) =

3.60 3.64 3.68 3.72 3.76 3.80 3.84 3.88 3.92 3.96 4.00 Density grid: $\log(NE) =$

 $9.0 \quad 10.0 \quad 11.0 \quad 12.0 \quad 13.0 \quad 14.0 \quad 15.0 \quad 16.0 \quad 17.0$

The necessary tabulated numerical data from Kurucz are in a special data file, "statistical," which must be connected to logical unit 10 (see Section 7). Using the actual input tables of \mathbf{TE}_i and \mathbf{NE}_i , $1 \leq i \leq \mathbf{N}$, at the start of a run PANDORA constructs an array of $53 \times \mathbf{N}$ values of Statistical opacity, using the specified component distribution function. For ultimate control over the computed values of this array, a table of *ad hoc* multipliers, \mathbf{FKUR}_{ℓ} , $1 \leq \ell \leq 53$, (i.e. one for each of the given wavelength values), can be specified in the input; normally all values of $\mathbf{FKUR} = 1$.

The input parameter **KURIN** is used to specify which component distribution should be used: k = KURIN. (When the value of **KURIN** = 0, then no Statistical opacities are computed, and the data file need not be provided.) A subset of the available wavelength range can be selected by specifying a lower limit, **KURMI** (printed as LLMIN), and an upper limit, **KURMA** (printed as LL-MAX).

When option KURPRNT is on then a printout and a graph appear. Values of Statistical opacity are printed for all \mathbf{N} depths, at wavelength points # 1 and every \mathbf{LWNT} 'th wavelength point thereafter. Values of Statistical opacity are plotted for all 53 wavelengths, at five depths whose indices are:

KINMAX + KININT, KINMAX, KINMAX - $1 \times$ KININT, KINMAX - $2 \times$ KININT, and KINMAX - $3 \times$ KININT.

A dump of raw data (as read from statistical), at wavelength points # 1 and every **KUDNT**'th wavelength point thereafter, appears if **KUDNT** > 0.

C) Composite Line opacities

Kurucz has calculated the composite opacity due to all known atomic and molecular lines (circa mid-1989) as a function of temperature, pressure, velocity and wavelength, assuming local thermodynamic equilibrium. His opacities are given for 56 values of temperature, 21 values of pressure, 5 values of velocity, and 35093 wavelength grid points in the range 8.97666-9998.56236 nm.

Temperature grid: log(TE) =

Pressure grid: log(P) =

Velocity grid: V (km/s) =

$$0.0 \quad 1.0 \quad 2.0 \quad 4.0 \quad 8.0$$

These $35,093 \times (56 \times 21 \times 5) = 35,093 \times 5,880 = 206,346,840$ opacity values have been written to six binary files, as follows:

File name	# points	Range (nm)
BSAMHE	4659	8.97666-22.78209
BSAMLY	6936	22.78377 - 91.16094
BSAMBA	6934	91.17535 - 364.62911
BSAMVI	6163	364.70183 - 1249.82029
BSAMIR1	6934	1250.0 - 4999.28118
BSAMIR2	3467	5000.0 - 9998.56236

PANDORA works with a reduced set of $1,750 \times 5,880 = 10,290,000$ opacity values at 1,750 wavelength grid points covering almost the same range, at the same temperatures, pressures and velocities. This reduction is done by PROCURE, a separate program; its output file, "composite," must be connected to logical unit

11 (see Section 7). (CONCUR, a second separate program, selects a specified, unreduced subset of Kurucz's data; its output file has the same format as that produced by PROCURE.) PANDORA cannot read Kurucz's original files—it only reads files produced by PROCURE (or CONCUR).

Reduction Procedure

- 1) The original set of 35,093 wavelengths is cut into 350 blocks of 100 consecutive "original" wavelengths each (the last 93 original wavelengths are ignored).
- 2) Such a block pertains to "original" wavelengths $W_j, 1 \leq j \leq 100$, and contains $100 \times 5,880$ opacity values.
- 3) "Nominal" wavelength values, $N_i, 1 \leq i \leq 5$, are computed such that $N_i = W_1 + (2 \times i 1) \times (W_{100} W_1)/10$.
- 4) In each original block the opacity values pertaining to a given (TE,P,V)-triple are treated as a separate table of opacity vs. W_i .
- 5) Such a table of 100 opacity values is sorted into increasing order. The 10^{th} , 30^{th} , 50^{th} , 70^{th} and 90^{th} entries of this ordered opacity table, together with their associated (original) values of W_j , are pulled out. These opacity values constitute the "reduced" opacity table.
- 6) The 5 selected opacity values are then ordered so that their associated (original) wavelengths W_i are in increasing order.
- 7) The 5 "nominal" wavelengths N_i are then assigned to these 5 (ordered) opacity values of the "reduced" table.
- 8) This is done for all 5,880 (TE,P,V)-triples, so that 5,880 "reduced" tables of 5 entries each are obtained.
- 9) In this manner, each original block of data pertaining to 100 "original" wavelengths is replaced by a reduced block of data pertaining to 5 "nominal" wavelengths, for all values of temperature, pressure and velocity.

A typical PANDORA run need not use all 1750 wavelengths of the reduced data set, since it uses only those that fall within the wavelength bands specified in the input. There are **NAB** such band(s), and Composite Line opacity will be computed at all those wavelengths W (in Å), arising in the context of a given PANDORA run, such that **BANDL** $_{\ell} \leq W \leq BANDU_{\ell}$, $1 \leq \ell \leq NAB$. (When **NAB** = 0, then no Composite Line opacities will be computed, and the data file need not be provided.) Using the input tables of **TE**_i and **V**_i, and a computed

table of P_i , $1 \le i \le N$, PANDORA constructs an array of KOMP \times N values of Composite opacity at the start of a run; here KOMP is the count of all the wavelength points of the input 'reduced' data set that are contained within the specified band(s).

PANDORA automatically computes 'continuum data' for these KOMP wavelength points. Values of the 'method control parameters' for the relevant Continuum Source Function calculations can be specified, for each band, using the input values of **BANDY**. Printout from these continuum calculations is controlled by option COMPCOPR.

When option KOMPRNT is on then a printout and a graph appear. Values of Composite opacity are printed for all **N** depths, at wavelength points # 1 and every **LWNT**'th wavelength point thereafter. Values of Composite opacity are plotted for all KOMP wavelengths, at five depths selected by **KINMAX** and **KININT** as with Statistical opacity, above.

A dump of raw data (as read from composite), at wavelength points # 1 and every **KODNT**'th wavelength point thereafter, appears if **KODNT** > 0.

Note: Kurucz's original data files (BSAMHE, etc) no longer exist; thus the reduction and extraction procedures described here are of historical interest only. We have used our "standard" reduced file composite for many years; it is the only data input file now available.

D) Averaged Line opacities

PANDORA can use arbitrary opacity distributions specified as functions of arbitrary grids of depth (in km, like the \mathbf{Z} table) and of wavelength (in Å). These opacity sets are interpolated to the values of depth and wavelength that are needed for the calculation. If option AVELOP is on, then PANDORA expects a special data file, connected to logical unit 12 (see Section 7). If there is data in this file (*i.e.*, if a wavelength grid is specified), then Averaged Line opacity will be used at all wavelengths within the range of the wavelength grid.

This special data file is a binary file that PANDORA attempts to read as in the following quasi-Fortran code fragment:

```
integer KWA, NT, NP, NZ
real*8 WAVES(KWA), ZGRID(NZ), AVOP(NZ)
----
read (12) KWA, NT, NP, NZ
----
if (KWA .gt. 0) then
    read (12) (WAVES(I), I = 1,KWA)
    read (12) (ZGRID(I), I = 1,NZ)
----
do 999 J = 1,KWA
    read (12) (AVOP(I), I = 1,NZ)
----
999 continue
end if
----
```

(The parameters NT and NP provide for possible future program additions; currently they should both be set = 0.)

As each set of NZ opacity values pertaining to a given value of the wavelength grid is read, the data are interpolated to the \mathbf{Z} table of the run; this process produces a final data array of size KWA \times \mathbf{N} .

When option AVOPRNT is on then a printout and a graph appear. Values of Averaged opacity are printed for all \mathbf{N} depths, at wavelength points # 1 and every \mathbf{LWNT} 'th wavelength point thereafter. Values of Averaged opacity are plotted

for all KWA wavelengths, at five depths selected by \mathbf{KINMAX} and \mathbf{KININT} as with Statistical opacity, above.

(Section 9 – last revised: 2006 Nov 02)

Section 10: Element Data

Numerical data pertaining to electron-contributing elements are required for the electron density (**NE**) calculations. These data comprise an 'element table,' of **NMT** rows and 9 columns, that is set up for the run. Each row of the table pertains to a different ion; the default value of **NMT** = 38. The columns are for: element symbol (M), atomic number (atno), abundance realtive to Hydrogen (AB), ionization potential (CHI), partition function U-I and U-II (UI and UII), logarithmic abundance on a scale such that Hydrogen = 12.0 (LAB), default value of logarithmic abundance (DEF), and an integer (k) identifying the source of the abundance value. The default element table is given at the end of this section. *Note* option MCINPUT.

Data other than the default values (listed below) can be input with **NEWELE** and **ELEMENT** statements, as follows:

NEWELE (j M atno AB CHI UI UII LAB DEF k)

where j (an integer quantity) is the index of a group of entries (*i.e.* a row) in the element table; M (an alphanumeric quantity) must be a valid chemical element symbol; and n and k (integer quantities) and AB, CHI, UI, UII, LAB and DEF (floating point quantities) will constitute the j^{th} row of the element table. These fields must be given in the order shown. A **NEWELE** statement provides all the data for element M, which will override the entire current contents of the j^{th} row.

ELEMENT ($M I_1 I_2 \dots I_n$)

where M must be a valid chemical element symbol, and I_i is one or more phrases,

each consisting of a pair of input fields: $A\ V$. The field A must be alphanumeric and is an identifier; it can take on the values: AB (= abundance), LAB (= logarithmic abundance), UI (= partition function), UII (= partition function), CHI (= ionization potential), or ATNO (= atomic number). The field V is numeric, and must be integer for A = ATNO, but floating point otherwise. Upon reading the phrase $I = A\ V$, PANDORA will set the value of A for element M equal to V. Examples:

- 1) ELEMENT (FE AB 3.5E-5 CHI 7.87 UI 24.) specifies Iron, and sets the abundance, ionization potential and the partition function UI equal to 0.000035, 7.87 and 24.0, respectively.
- 2) ELEMENT (FE CHI 7.87)
 ELEMENT (fe ui 24. ab 3.5e-5)

is one of many configurations equivalent to example (1).

Note that an **ELEMENT** statement is normally used to override single existing entries in the current element table. The **NEWELE** statement is provided to allow emergency wholesale changes in the built-in default element data; (the preferred way to make bulk permanent changes in this table is to modify the PAN-DORA source code). In general the **NEWELE** statement should be avoided since, during input reading, **ELEMENT** statements are checked much more carefully for correctness and consistency than **NEWELE** statements.

PANDORA sets the value of **NMT** to its default before Part B of the input is read, and sets up the default values for **NMT** rows of the element table before Part D of the input is read (see Section 3). This makes a number of things possible; for instance:

- If "NMT (5)" occurs, then the element table of the run will contain only 5 rows, whose default data will be set equal to those contained in the first five rows of the default element table (see below).
- If "NMT (39)" occurs, then the element table of the run will contain 39 rows; the default data for the first 38 rows will be equal to those contained in the default element table (see below), while the default entries of the 39^{th} row will all be blanks or zero, respectively. Note that the input value of **NMT** may not exceed 50.
- Any of the numeric entries in the element table may be changed from their default values by mentioning them explicitly in **ELEMENT** statements. For example, if only AB(Na) (*i.e.* the abundance of Sodium) needs to be changed, to 0.00001, then there need not be an **NMT** statement, and only "Element (NA AB 1.E-5)" would be needed in Part D of the input.
- If **NMT** is explicitly input as greater than 38, then additional ions, with their associated data, can be input with **ELEMENT** statements. When an **ELE-MENT** statement is processed, its element symbol (M), is compared with those currently present in the element table. If there is no match, and if there is at least one empty row, then the new element symbol and its associated data will be accepted. Conversely, if an attempt is made to introduce more than **NMT** entries, then the run will be stopped. When a **NEWELE** statement is processed, it will override the contents of the j^{th} row, regardless.

Notes

Default Element Table

\underline{M}	\underline{atno}	\underline{AB}	<u>CHI</u>	<u>UI</u>	<u>UII</u>	\underline{LAB}	\underline{DEF}	\underline{k}
Н	1	0	13.595	2.00	1.00	0	12.00	
HE	2	0	24.58	1.00	2.00	0	11.00	
HE2	2	0	54.403	2.00	1.00	0	11.00	
LI	3	0	5.39	2.09	1.00	0	1.05	3
BE	4	0	9.32	1.02	2.00	0	1.38	3
В	5	0	8.296	6.03	1.00	0	2.70	1
\mathbf{C}	6	0	11.256	9.28	5.94	0	8.39	4
N	7	0	14.529	4.07	8.91	0	7.85	5
O	8	0	13.614	8.70	3.98	0	8.66	2
F	9	0	17.418	5.62	8.32	0	4.56	1
NE	10	0	21.558	1.00	5.37	0	7.84	3
NA	11	0	5.138	2.02	1.00	0	6.17	3
MG	12	0	7.644	1.01	2.01	0	7.53	3
AL	13	0	5.984	5.83	1.03	0	6.37	3
SI	14	0	8.149	9.26	5.82	0	7.51	3
P	15	0	10.474	4.46	8.12	0	5.36	3
\mathbf{S}	16	0	10.357	8.12	4.16	0	7.14	3
CL	17	0	13.014	5.25	7.76	0	5.50	1
AR	18	0	15.755	1.00	4.89	0	6.18	3
K	19	0	4.339	2.18	1.00	0	5.08	3
CA	20	0	6.111	1.03	2.29	0	6.31	3
SC	21	0	6.538	12.0	22.9	0	3.05	3
TI	22	0	6.818	30.2	56.2	0	4.90	3
V	23	0	6.738	41.7	43.7	0	4.00	1
CR	24	0	6.763	10.3	7.24	0	5.64	3
MN	25	0	7.432	6.45	7.76	0	5.39	1
FE	26	0	7.896	24.5	39.2	0	7.45	3
CO	27	0	7.863	31.6	27.5	0	4.92	1
NI	28	0	7.633	28.8	10.0	0	6.23	3
CU	29	0	7.724	2.29	1.02	0	4.21	1
ZN	30	0	9.391	1.00	2.00	0	4.60	1
GA	31	0	5.997	5.37	1.00	0	2.88	1
GE	32	0	7.899	8.13	4.37	0	3.58	3

RB	37	0	4.177	2.29	1.00	0	2.60	1
SR	38	0	5.693	1.26	2.19	0	2.92	3
Y	39	0	6.377	12.0	15.1	0	2.21	3
ZR	40	0	6.835	33.9	45.7	0	2.59	3
BA	56	0	5.210	2.29	4.17	0	2.17	3

(The source citations identified by the value of the integer k appear in the PAN-DORA printout; these are built into the source code, and cannot be changed by **ELEMENT** or **NEWELE** statements.)

When input reading is finished, the 'element table' exists only in *provisional* form. It is converted into *final* form by the following sequence of steps:

- 1) Look at every row. If any AB > 0, then compute the corresponding LAB from it; if AB \leq 0, then set LAB = DEF.
- 2) Look at every row. If any AB = 0, then compute it from the corresponding LAB; if $AB \le 0$, then set AB = 0 and LAB = 0. (AB < 0 is legitimate in **ELE-MENT** and **NEWELE** statements.)
- 3) If $\mathbf{FABD} \neq 0$, then look at every row *except* those of Hydrogen or Helium. Set the final value of $AB = \mathbf{FABD} \times AB$. If this final AB > 0, then compute LAB from it.
- 4) Squeeze out (eliminate) from the table every row whose AB = 0, and adjust the value of **NMT** accordingly.
- 5) If the Hamburg data (used to calculate depth-dependent partition functions when option PARTVAR is on) has usable CHI values for any of the ions in the final table, then such Hamburg values will replace the corresponding default or input values of CHI (regardless of the status of option PARTVAR).

(Section 10 – last revised: 2007 Feb 05)

Section 11: **Printout**

Initial PANDORA development occurred in a batch-oriented environment using a remote central computing system. Output was written to a file that was printed sometime after completion of the run. The printers were expected to use $11\times14\frac{7}{8}$ fan-fold paper providing about 60 lines per page and 132-136 character positions per line. The resulting hardcopy was called "output" or "printout." Things have changed. Now PANDORA runs on desktop workstations. (But it is not an interactive program—things have not changed that much.) The user still deals with output files and normally waits for a run to finish before doing so. Complete output files are no longer routinely printed but are stored on disk to be displayed and examined on CRT screens. Nevertheless, in this writeup we retain the old terms "output" and "printout" to refer to PANDORA's output files and their contents.

PANDORA has been revised to limit the lengths of lines in the output files to no more than 128 characters.

This Section consists of two parts. Part A has general information about output files and their use while Part B has detailed information about how to control their contents.

A) Printout Files

The 'general printout' file is connected to unit 15, and the 'error printout' file may be connected to unit 16; see Section 7.

The 'general printout' file is the main output file of the run. Its normal contents, while to some extend fixed, can generally be controlled by various switches and options (see Part B, below). In addition, PANDORA also prints various 'debug' data and/or error messages, and these are written to the 'error printout' file. Normally the general printout file and the error printout file are both connected to unit 15, so that normal and error printouts appear in one file, in a single, merged sequence. (A merged arrangement preserves the context of error messages.)

However, the **OUTPUT** statement can be used to make PANDORA connect the error printout file to unit 16. Thus the two types of output can be split. This makes for cleaner normal output, which may be especially desirable in those situations where various error messages are considered inconsequential. (But note that a 'split' arrangement tends to obscure the context of error messages.)

The general printout file can be very large—this can make it difficult to scan it interactively with an editor. Option MAKIX has been provided to help with this. When MAKIX is on, then a 'printout index' file (connected to unit 31; see Section 7) will be generated, as follows:

Every 'major' printout section in the general printout file will be preceded by a unique 'identifier line'. These indentifier lines, and these lines only, will also appear in the 'printout index' file. Having in hand a copy of this index, the user can decide which printout sections to examine, and can use the unique identifier string as an unambiguous target for a string-search.

LOOKAT

A separate program LOOKAT helps to display the 'general printout' file on a screen, and to select portions to be printed. It works best when the associated 'printout index' file is also available (see above). LOOKAT is intended to be self-contained,

self-explanatory, and easy to use.

B) Printout control

Most sections of PANDORA's output can be enabled or suppressed at will. The various program 'options' (*i.e.* those mentioned in **DO** and **OMIT** statements) provide most of the control facilities for this purpose, but some other input parameters (especially those that control various 'debug dumps' and 'details dumps') also can affect the amount of printout.

There follows a list of every 'section' of PANDORA's printout, with descriptions of the conditions that determine whether or not that section appears. Many of these descriptions mention 'subsections' of major 'parent' sections. Such subsections are *not printed* if conditions are such that the parent section does not appear. Many parent sections contain stuff in addition to the subsections mentioned; some do not.

Besides the printout sections listed below, there are some debugging aid printouts that are under 'option' control; these options are listed in the TEST/DEBUG part of the printout section OPTIONS. The option MITPRNT controls whether or not even a minimum of information appears for all but the last iteration. Also, some error printouts appear invariably whenever certain problems are detected.

Printed Graphs. PANDORA produces many graphs of selected tables. The resolution is crude: character positions. Nevertheless, in many cases these convenient graphs provide adequate pictures of what is poing on. Before any graph image is actually printed, however, PANDORA determines whether it is "interesting" (i.e., whether a 'sufficient' number of data points fall within, rather than on, the graph borders)—boring graphs are not printed. In such cases only a single print line, consisting of the graph title and the word "BORING," will appear.

The following **Notes** are referred to in the remainder of this Section:

Note A

This section appears for every overall iteration of a run in which any atmospheric model tables, involved in the calculations giving rise to this printout section, are being recomputed, *i.e.* if the option HSE is on, or if the **POPUP** switch has been set. However, if the option ALL is off, then this printout section appears only once, in any case.

Note B

If the option EVERY is off, then this printout section appears for the last subiteration only.

Note C

If the option ALL is off, then this printout section appears for the last overall iteration only.

Note D

If the option ALLY is off, then this printout section appears for the last HSLiteration only.

Output from PHASE 0: Input and Initialization

PROVISIONAL INPUT

appears if STANPRNT is on, and if at least one value of $\mathbf{LZA} > 0$.

STATUS OF OPTION

appears if OPTPRNT is on. (An abbreviated version of this listing appears if AOPTPRNT is on.)

INPUT NOTES

appears always.

CO LINES

appears when CO line absorption is included and CODMP is on.

ATMOSPHERE

appears if ATMOPRNT is on. When ZPRNT is on this print out has two sections, $\underline{\text{ATMOSPHERE-1}}$ and $\underline{\text{ATMOSPHERE-2}}$; the second section gives \mathbf{Z} , \mathbf{TE} , etc., to nine figures.

INPUT NUMBER DENSITY AND DEPARTURE COEFFICIENT

appears if INNBPRNT is on.

$\underline{\text{ATOM}}$

appears if ATOMPRNT is on.

DEPTH-DEPENDENT TRANSITIONS DATA

appears if INRBPRNT is on.

ELEMENTS

appears always.

BACKGROUND

appears always.

INPUT

appears if INDAPRNT is on. (An abbreviated version of this printout appears if AINDPRNT is on.) Many diverse parameters may be printed here. The first page is a bit of a grab bag; the remaining input values are grouped in various subsections dealing with specific topics, shown in the headings. Still, some input parameters could equally well have been included in several of these groups, so, which group a given parameter is printed with may seem somewhat arbitrary. Subsections are printed as needed.

CONSTANTS

appears if STANDARD is on.

HYDROGEN and H2

appear if HNPRNT is on (note input parameter MOPRNT).

CARBON

appears if CARPRNT is on (note input parameter **MOPRNT**).

SILICON

appears if SILPRNT is on (note input parameter **MOPRNT**).

HELIUM

appears if HELPRNT is on (note input parameter $\mathbf{MOPRNT}).$

HELIUM-II

appears if HEL2PRNT is on (note input parameter **MOPRNT**).

ALUMINUM

appears if ALUPRNT is on (note input parameter **MOPRNT**).

MAGNESIUM

appears if MAGPRNT is on (note input parameter **MOPRNT**).

IRON

appears if FEPRNT is on (note input parameter MOPRNT).

SODIUM

appears if SODPRNT is on (note input parameter MOPRNT).

CALCIUM

appears if CALPRNT is on (note input parameter MOPRNT).

OXYGEN

appears if OXYPRNT is on (note input parameter MOPRNT).

OXYGEN2

appears if OXY2PRNT is on (note input parameter MOPRNT).

OXYGEN3

appears if OXY3PRNT is on (note input parameter **MOPRNT**).

SULPHUR

appears if SULPRNT is on (note input parameter $\mathbf{MOPRNT}).$

DIRECTIONS

appears if SPHERE is off and STANDARD is on, and if either GRCONT or GRLINE is on.

SPHERE

appears if SPHERE is on, and if either STANDARD or SPHEGEOM is on.

PARTITION

appears if PARTPRNT is on.

STIMULATED EMISSION FACTORS

appears if STIMPRNT in on. BETA(TR) appears only if CSWITCH is on.

TABLES

appears if STANDARD is on.

INTEGRATION

appears if INTAPRNT is on. (An abbreviated version of this listing appears if AINTPRNT is on.)

DOPPLER

appears if DPDWPRNT is on, for every radiative transition u, ℓ for which **LSFPRINT**^{u,ℓ} = 1 or **PROF**^{u,ℓ} = 1.

CHARGE EXCH.

appears if CHXPRNT is on.

STATISTICAL

appears if KURPRNT is on (note input parameter **LWNT**). This is a parent section, with one subsection as follows:

• dump of unprocessed data: the value of **KUDNT** must be > 0.

COMPOSITE

appears if KOMPRNT is on (note input parameter **LWNT**). This is a parent section, with one subsection as follows:

• dump of unprocessed data: the value of **KODNT** must be > 0.

AVERAGED

appears if AVOPRNT is on (note input parameter **LWNT**).

STANDARD RATES INTEGRATION WAVELENGTHS

appears if both USEWTAB and WTABPRNT are on.

JNU

appears if there is at least one PRD transition, and if $\mathbf{JNUNC} > 0$.

Output from PHASE 1: Iterations

ND, NK and BD

appears at the start of every overall iteration, if ALL is off and MITPRNT is on.

Z-SCALE

appears in a Hydrogen run if values of **TAUKIN** were provided, so that the values of **Z** had to be updated (see also Note A).

CONTINUUM DATA

may appear in every overall iteration of a run which recomputes any of the atmosphere model data needed for continuum calculations (JNU, etc.) — *i.e.* if option HSE is on, if the **POPUP** switch has been set, and/or if **Z** must be updated. In other runs continuum calculations need to be done (and this printout can appear!) in the first overall iteration only. (If such a run has **IOMX** > 1 and option ALL is off, this printout will not appear!)

This is a major parent section whose subsections are related to the various contexts in which continuum calculations arise, as follows:

- for line core wavelengths: LINECOPR or LBDPRNT must be on (when LINECOPR is on, LBDPRNT is superfluous here) (see also Notes A and C);
- for transition rates integrations: RATEPRNT and RATECOPR must both be on and USETRIN must be off (see also Notes A and C);
- for standard background wavelengths: USEWTAB and STANCOPR must both be on (see also Notes A and C);
- for H-minus calculations: HMS and HMSCOPR must both be on (see also Notes A and C);
- for dust opacity wavelengths: DUSTYPE, DUSTEMP, and DUSTCOPR must all be on (see also Notes A and C);
- for 'additional wavelengths': ADDCOPR must be on;
- for additional photoionization: RATEPRNT and APHICOPR must both be on (see also Notes A and C);
- for Composite Line Opacity data wavelengths: appears only if these data are actually used, and if COMPCOPR is on (see also Notes A and C);
- for K-shell wavelengths: KSHLCOPR must be on (see also Notes A and C);
- for FDB wavelengths: FDBCOPR must be on (see also Notes A and C);

- \bullet for CO-lines absorption wavelengths: COCOPR must be on (see also Notes A and C);
- ullet for every wavelength whose corresponding context OPTION is off: output will appear if that wavelength occurs in the ${f SCOW}$ table.

More control information on next page.

These Continuum Data printouts, from all contexts, are grouped as one batch and appear in order of increasing wavelength.

The printout for any particular wavelength consists of several parts, each of which appears only if the appropriate option is on, as follows:

absorbers printout OPAPRNT emitters printout EMIPRNT

CSF printout CSFPRNT (note option ACSFPRNT)

absorbers graph OPAGRAF emitters graph EMIGRAF CSF graph CSFGRAF summary graph CSFGRAF

RATES

is a major parent section; a summary explanation of the calculations, and the printouts available from them, always appears. Substantive printouts appear if RATEPRNT is on. This section may appear both in the first and the last iteration of some runs. The amount of information printed depends on options RATEALL and RATEFULL. It has subsections as follows:

- for CHKI and CHIJ: COLHPRNT must be on;
- for upper-level charge exchange: CHEXUP and CHXPRNT must be on;
- for CIJ: CIJPRNT must be on;
- for PIJ: PIJPRNT must be on;
- for RIJ: RIJPRNT must be on;
- for additional photoionization: APHIPRNT must be on;
- for fast electrons: FELEPRNT must be on.

Note the extensive explanatory text in the regular printout.

RATES GRAPHS

appears if RATEGRAF is on.

AMBIPOLAR DIFFUSION

appears if RATEPRNT is on and if either AMBPRNT or VLGPRNT is on. *Note:* this printout occcurs near the end of the regular RATES printout, if one or both of the options AMDIFF or VELGRAD are on. Options ADN1DMP, AMD-DMP, DIFFANA, and VELGDMP affect this printout.

DIELECTRONIC RECOMBINATION

appears if RCOMPRNT is on.

H MINUS

appears if HMS is on (see also Notes A and C). This is a parent section, with one subsection as follows:

• for JNU: HMSJPRNT must be on.

DUST

appears if DUSTEMP and DUSTYPE are both on (see also Notes A and C).

***** Notes A, B, C, D are explained on page 11.4 *****

Start of Line Source Function printout groups (if any).

Printout can appear if there is at least one radiative transition. At least some part of the printout group for transition u, ℓ appears if **LSFPRINT**^{u,ℓ} = 1, or if option LSFPRNT is on, or if option LSFGRAF is on. (*Note:* **LSFPRINT**^{u,ℓ} and option LSFPRNT are different beasties, but they work together.)

STARTING NUMBER DENSITY AND DEPARTURE COEFFICIENT

appears for the first iteration if default values were computed.

DAMPING

appears if DPDWPRNT is on (see also Notes A and C). It will *not* appear if a) HSE is on and this is not the last overall iteration, or b) HSE is off and this is not the last overall iteration but this is a Hydrogen run.

ANALYSIS

appears if ANALYSIS is on (see also Notes A and C).

LINE (U/L)

always appears; it contains a summary explanation of the various printouts related to the line source function calculations for radiative transitions.

STIM, and TAU

appear if TAUPRNT is on (see also Note B). (See also option PEGTNALL.)

STATISTICAL EQUILIBRIUM

is a major parent section which has three subsections as follows:

- for timing data: SETIME must be on;
- for PE, FE, etc.: SEPRNT must be on;
- for methods comparison: SECOMP or METPRNT must be on.

Note: option DIFFANA also affects this printout (see also Note B).

PRD

Printouts related to PRD calculations appear, for all PRD transitions, if option PRDPRNT is on. The amount of output depends on input parameters **IPRDF** and **IPRDD**. Tables of JNU are printed if option JNUPRNT is on. Printouts from PRD-related background (continuum) calculations, for wavelengths (frequencies, XI-values) selected by **IPRDF**, appear if option PRDCOPR is on (and/or for every PRD wavelength occurring in the **SCOW** table). For the purposes of PRD these "continuum printouts" have been split into two separate parts, but they have the standard format used for 'CONTINUUM DATA,' above, and use the same options for detailed control as described there. If iterations are used with the Hubeny-Lites formulation (i.e. option PRDMETH is on), then only the results of the last iteration are printed unless option PRDITER is on (see also Note B).

LINE SOURCE FUNTION

is a major parent section which has several subsections as follows:

- TNU-analysis is controlled by **KANTNU** (q.v.);
- for Line Source Function details for transition u, ℓ : **LSFPRINT**^{u, ℓ} = 1 or option LSFPRNT must be on (an abbreviated version of this printout appears if option ALSFPRNT is on); a part of this detail printout also depends on option LSFFULL;
- for source function graph for transition u, ℓ : **LSFPRINT**^{u,ℓ} = 1 or option LSFGRAF must be on:
- for radiative force for transition u, ℓ : **LFLUX**^{u,ℓ} = 1, (the full computed Line Flux Distribution appears if LFDPRNT is on).

Note: See also option PESRJALL (see also Note B).

Note: The section 'LINE SOURCE FUNCTION' (if not a PRD transition) will appear twice in a diffusion run with DIFFANA on, concluding with a summary graph comparing the results with and without diffusion terms.

End of Line Source Function printout groups (if any).

* *** ****

LOG PLOT OF TAU SCALES

appears if there is at least one radiative transition and if LSCALE is on, in the very last sub-iteration only.

COLLATED TAU SCALES

appears if there is at least one radiative transition and if SCALE is on, in the very last sub-iteration only.

RHO AND RBD

is a major parent section. An explanation of the available printouts always appears. Substantive results appear if RHBPRNT is on, and subsections may appear as follows:

- for details of each radiative transition: RHBPRDT must be on;
- for details of BDQ calculation: BDQPRDT must be on;
- for complete sets of BDR, BDJ, BDS, and S*: BDPRNT must be on;
- for final sets of Rho and b-ratios: RHBPRSM must be on.

Note that the results printed by RHBPRSM are also printed by RHBPRDT; thus it is not normally necessary to turn both on; (RHBPRSM is intended to provide "minimal" printout).

CONSISTENCY CHECKS

appears if CHKPRNT is on, and is controlled by EVERY (see also Note B).

POPULATIONS

is a major parent section which appears here if LYMAN is on (see also Note D). See detailed description below.

CONTINUUM DATA FOR LYMAN

appears if LYMAN is on, and if either LYMCOPR is on or for every wavelength that occurs in the **SCOW** table (see also Note D). Detailed control of the print-out parts for each Lyman wavelength is as for other 'CONTINUUM DATA', described above.

$\underline{\text{LYMAN}}$

is a major parent section which appears if LYMAN is on (see also Note D). (An abbreviated version of this major parent section is printed if ALYMPRNT is on.) It has three subsections as follows:

- for EP methods comparison: EPCOMP must be on;
- for RK comparison: COMPRK must be on;
- for PIJ: HSE must be off and this must not be the last iteration.

POPULATIONS

is a major parent section which appears here if HSE is on (see also Note D). See detailed description below.

NE

appears if HSE and NESWICH are both off and POPUP has been set.

HSE

appears if HSE is on (see also Note D). (An abbreviated version of this section is printed if AHSEPRNT is on.)

MODEL DATA

is a major parent section which appears if HSE is on (see also Note D); it is a continuation of the HSE section. It has subsections as follows:

- for absorbers at 500 nm: OPAPRNT must be on;
- for HYDROGEN: this always appears;
- recalculated Z-scale appears if values of **TAUKIN** were provided, or if values of **ZMASS** were provided and ZCOMP is on;
- for electrons calculations results (with graphs): ELECPRNT must be on (appears in the last iteration only).

\underline{GAS}

appears if HSE is off and \mathbf{POPUP} equals $\mathtt{HYDROGEN}$ (see also Note D).

POPULATIONS

is a major parent section controlled by ALL (see also Note D). An explanation of the various controls for this section always appears. Substative printout appears if either POPPRNT or POPGRAF are on. There are five subsections as follows:

- for NE results: **POPUP** must equal HYDROGEN and POPPRNT must be on;
- for the full tables: POPPRNT must be on, (the supplementary printout appears if NBPRNT is on), (an abbreviated version of the full tables appears if APOPPRNT is on);
- for graphs of ND: POPGRAF must be on (see Note D);
- for a trace of the Populations Calculations at depth # **IBNVIEW**: PDETPRNT must be on;
- for graph of BD vs. **Z**: BDGRAF must be on (the plots of TAU vs. **Z** appear only if TAUPLOT is on) (see Note D);
- for graph of BDIJ vs. **Z**: BDGRAF must be on and there must be at least one radiative transition (the plots of TAU vs. **Z** appear only if TAUPLOT is on) (see Note D):
- for graph of **TE** vs. log(TAU): TEGRAF must be on and there must be at least one radiative transition (see Note D).

UPDATED POPULATIONS DATA

is a major parent section, controlled by ALLY (see also Note D). Its various subsections are concerned with the various 'population-update ions,' as follows:

- for Hydrogen: HNPRNT must be on and **POPUP** must equal HYDROGEN;
- H2: **POPUP** must equal HYDROGEN and **NHTSW** > 0;
- for Carbon: CARPRNT must be on and **POPUP** must equal CARBON;
- for Silicon: SILPRNT must be on and **POPUP** must equal **SILICON**;
- for Helium: HELPRNT must be on and POPUP must equal HELIUM;
- for Helium-II: HEL2PRNT must be on and **POPUP** must equal HELIUM2;
- for Aluminum: ALUPRNT must be on and **POPUP** must equal ALUMINUM;
- for Magnesium: MAGPRNT must be on and POPUP must equal MAGNESIUM;
- for Iron: FEPRNT must be on and **POPUP** must equal IRON;
- for Sodium: SODPRNT must be on and POPUP must equal SODIUM;
- for Calcium: CALPRNT must be on and **POPUP** must equal CALCIUM;
- for Oxygen: OXYPRNT must be on and **POPUP** must equal **OXYGEN**;
- for Oxygen-II: OXY2PRNT must be on and **POPUP** must equal **OXYGEN2**;
- for Oxygen-III: OXY3PRNT must be on and **POPUP** must equal **OXYGEN3**;
- for Sulphur: SULPRNT must be on and **POPUP** must equal **SULPHUR**.

K-SHELL

appears if a K-shell ionization calculation has been requested in a Carbon run (see Note D).

CHARGE EXCHANGE

appears if upper-level charge exchange has been requested in a Hydrogen run and option CHXPRNT is on (see Note D).

RESTART VALUES OF JNU

appears in a PRD run when option JNUPRNT is on.

DAMPING

appears if PHASE2, PASSPRNT, and DPDWPRNT are all on, and if there is at least one passive transition for which the emergent profile calculation has been turned on.

ANALYSIS

appears if PHASE2, PASSPRNT, and ANALYSIS are all on, and if there is at least one passive transition for which the emergent profile calculation has been turned on.

TAU

appears if PHASE2, PASSPRNT, and TAUPRNT are all on, and if there is at least one passive transition for which the emergent profile calculation has been turned on.

PASSIVES

appears if PHASE2 and PASSPRNT are both on.

DAMPING and ANALYSIS

appear if PHASE2 is on, only for those transitions u, ℓ whose values of $\mathbf{BLCSW}^{u,\ell}$ require this and for which emergent profile calculations are requested. For $\underline{\mathrm{DAMPING}}$, DPDWPRNT must be on, for $\underline{\mathrm{ANALYSIS}}$, ANALYSIS must be on.

TAU

appears if PHASE2, TAUPRNT, LTE and LTEDATA are all on, only for those transitions for which emergent profiles calculations are requested.

LTE DATA

appears if PHASE2, LTE and LTEDATA are all on, only for those transitions for which emergent profiles calculations are requested.

ANALYSIS

appears if PHASE2, ANALYSIS, LTE and LTEDATA are all on, only for those transitions for which emergent profiles calculations are requested.

FREQUENCY-DEPENDENT LINE SOURCE FUNCTION

is a major section, which may appear for the (MS, NS) transition only. It has two subsections, as follows:

- for printout: SLFPRNT must be on;
- for graph: SLFGRAF must be on.

SCATTERING ALBEDO ANALYSIS

appears, for suitable transitions, if LINECOMP is on.

CONTINUUM DATA

appears for all wavelengthe needed for line profile calculations if FBDCOPR is on, or if TRUECONT and TRUECOPR are both on. Detailed control of the printout is as for other 'CONTINUUM DATA', described above.

WAVE SUMM 0

always appears.

WAVE SUMM 1

appears if WAVEPRNT is on. It provides a basic summary of the background (continuum) calculations at each wavelength.

WAVE SUMM 2

appears if WAVEPRNT is on and IWSMD = 1. It provides a basic summary of the contributors to the background (continuum) at each wavelength.

COMPOSITE LINE OPACITY ANALYSIS

appears if COMOPAN is on. (An abbreviated version of this printout appears if \mathbf{KCOAA} is set = 1.)

COOLING

appears if CALCOOL is on. This is a parent section, with one subsection as follows:

• for integrated rates: COOLINT must be on.

HEATING

appears if CALHEAT is on. This is a parent section, with one subsection as follows:

• for integrated rates: COOLINT must be on.

HEATING/COOLING SUMMARY

appears if CALCOOL and CALHEAT are both on.

FUDGERS

appears as needed.

A-TROUBLES

appears as needed.

CHECKS GRAPHS

appears if there is at least one radiative transition and CHKGRAF is on.

ITERATIVE SUMMARIES

is a major parent section which appears as needed and if SUMMARY is on. An Explanation of the various controls for this section appears if either SUMMARY or SUMTREND is on. Its various subsections are controlled by separate options, and are related to various calculated quantities which are obtained by iterative improvement; they appear only in those cases where more than one iterate has been saved so that comparison among successive iterates is possible, as follows:

- for CHECKs: ITERCHK must be on;
- for $S^{u,\ell}$: ITERS must be on, and u,ℓ must be a radiative transition;
- for RHO $^{u,\ell}$: ITERRHO must be on, and u,ℓ must be a radiative transition;
- for $CHI^{u,\ell}$: ITERCHI must be on, and u,ℓ must be a radiative transition;
- for TAU $^{u,\ell}$: ITERTAU must be on, and u,ℓ must be a radiative transition;
- for RK: ITERRK must be on;
- for ND: ITERN must be on;
- for RHOWT $^{u,\ell}$: ITERRWT must be on, and u,ℓ must be a radiative transition;
- for BD: ITERB must be on;
- for NE: ITERNE must be on;
- for Z: ITERZ must be on;
- for TDST: ITERTD must be on.

Iterative Summaries appear in tabular and/or in graphical from, depending on option SUMGRAF and input parameter **ISMSW**.

ITERATION TREND SUMMARY

may appear if there is at least one radiative transition and SUMTREND is on.

Output from PHASE 2: Spectrum and Summaries

None of these sections appear if PHASE2 is off.

EMERGENT CONTINUOUS INTENSITY

appears if EMERINT is on. This is a parent section, with subsections as follows:

- for depths-of-formation: ORIGIN must be on (see option ORSHORT);
- for dI/dh: DIDHC must be on (see also input parameter **ICDIT**;
- for color temperatures: COLTEMP must be on;
- for average continuum intensities: AVCON muts be on.

Note the effect of option WAVENUMB.

CONTINUOUS FLUX

appears if CONFLUX is on. This section includes the integrated flux quantities, and the Rosseland means. It has one subsection as follows:

• for details at each wavelength: FLUXDMP must be on; (which specific details are printed depends on the value of **IFXDS**).

Note the effect of option WAVENUMB.

CONTINUUM ECLIPSE INTENSITIES

appears if EMERINT and ECLIPSE are both on, only for those 'additional wavelengths' and Composite Line Opacity wavelengths for which this was requested explicitly, and for CO lines wavelengths if COCLIPSE is on. Calculations for selected beams of specified widths are done when $\mathbf{NZE} > 0$.

Note the effect of option WAVENUMB.

VELOCITIES

appears if LIGHT is on and $\mathbf{LPVEL} = 1$, but only if there are non-zero velocity tables worth printing. (The corresponding mass-loss rates are printed only if \mathbf{LPVEL} and \mathbf{LPMLR} both = 1.)

Start of Emergent Line Profile printout groups (if any).

These appear, if option LIGHT is on, for every transition (u, ℓ) for which the input parameter $\mathbf{PROF}^{u,\ell} > 0$.

BACKGROUND INTENSITY

computed continuum intensities amd flux needed for residuals calculation will be printed if option PROCPRNT is on.

GRAPH OF S, B VS. Z

appears if LIGHT and INTGRAF are both on, only for those transitions for which emergent profiles calculations were requested. These graphs do not appear if graphs were printed earlier in the LINE SOURCE FUNCTION section.

EMERGENT LINE PROFILES

shows the various versions of the emergent intensity profiles for a given transition, for all values of lookangle (μ) , velocity, and viewing position (front-face (always), back-face (if requested); followed by the flux profiles computed from the intensity profiles. (A somewhat abbreviated version of this printout appears if APRF-PRNT is on.) This parent section has subsections as follows:

- for profile analyses other than those printed earlier: ANALYSIS must be on;
- for depths-of-formation: ORIGIN must be on (note also option ORSHORT);
- for dI/dh: DIDHL must be on;
- for location analysis graph: LOGAS must be > 0;
- \bullet for FNRMLA, FNRMLB: CLNORM must be on in a Hydrogen run. Note the effect of option WAVENUMB.

GRAPH OF RESIDUAL INTENSITY PROFILE

appears if LIGHT and INTGRAF are both on, only for those transitions for which emergent profiles calculations were requested.

Note the effect of option WAVENUMB.

GRAPH OF ABSOLUTE INTENSITY/FLUX PROFILE

appears if LIGHT and INTGRAF are both on, only for those transitions for which emergent profiles calculations were requested.

Note the effect of option WAVENUMB.

ECLIPSE

appears if LIGHT is on, only for those transitions u, ℓ for which $\mathbf{ECLI}^{u,\ell} > 0$. Note the effect of option WAVENUMB.

End of Emergent Line Profile printout groups (if any).

* *** ****

SPECTRUM SUMMARY

appears if SPECSUM is on and if either LIGHT or EMERINT is on.

CONTINUUM CONTRIBUTIONS SUMMARIES

is a major parent section which appears if EMERINT is on. It has three subsections as follows:

for absorbers: OPASUM must be on;
for emitters: EMISUM must be on;
for TAU: TAUSUM must be on.

Performance Data, and Program Version Description

SCRATCH I/O SUMMARY

appears when $\mathbf{IRUNT} > 0$.

TIMING SUMMARY

appears when $\mathbf{IXSTA} > 0$.

VERSION DESCRIPTION

appears always (amount of detail depends on \mathbf{IRUNT}).

(Section 11 – last revised: 2007 Feb 05)

Section 12: Source Functions

PANDORA has three methods for calculating the weight matrices needed for source function calculations:

• **QR** -

the quadratic representation method, which requires an input parameter, Y, the 'damping parameter' (see: SAO Special Report No. 303);

• **RT** –

the ray tracing method, with analytic angle integration (see: E. H. Avrett's program specification '[7/1/71] New Subroutine for Weighting Coefficients');

• GR -

a general ray tracing method based on an integral equation approach, with numerical angle integration (see: E. H. Avrett's program specification '[81 Feb 27] Expansion Velocity in the Source Function Calculations').

When the \mathbf{QR} method is used for the Line Source Function calculation (where \mathbf{KS} or KF weight matrices are required) or for the Level- \mathcal{N} -to-Continuum (*i.e.* Lyman) Source Function calculation (where \mathbf{KK} weight matrices are required), then it can be used in one of two flavors: 'QR-direct' or 'QR-mapped.' When 'QR-direct' is specified, weight matrices (as functions of TNU, mono-chromatic optical depth) are computed directly as needed.

When 'QR-mapped' is specified, a 'standard weight matrix' is computed once (using the standard TAU table **TS**, of length **M**, and the standard value of the damping parameter **YPRE**); the required weight matrices (which are functions of **KS**, KF, or **KK** different TNU tables) are obtained from the standard matrix by an interpolation procedure. *Note*: the purpose of the mapping procedure is to save time; it is less accurate than the direct method. In cases where the **QR** method is chosen, mapping might be appropriate for the early iterations of a calculation, switching to direct calculation of weight matrices when homing in on the final solution.

The input values of the various 'method control parameters' MCP are used to specify which method to use for the various source function calculations to be performed. A value of MCP is interpreted as follows:

```
0 \le MCP \le +1 means: QR-direct;

MCP = -2 means: QR-mapped;

MCP = -1 means: RT;

MCP = -3 means: GR.
```

Note: When MCP selects **QR**-direct, then the value of MCP is also used as the required 'damping parameter' Y = MCP.

Note: **GR** is used automatically for all source function calculations when options SPHERE and/or EXPAND are on.

Note: RT is the default method for stationary plane-parallel cases.

Remember the following input parameters: **TMS**, which affects **RT** and **GR**; **TBAR**, which affects **QR**-mapped only; **TLARGE**, which affects **QR** and **QR**-mapped; and **TSMALL**, which affects all except **GR** (see Section 5).

(*Note* added 2006 Aug 30: The decision to use a single floating point input parameter combining the values of MCP and Y dates from the ancient past. I have long wanted to undo it in favor of using two separate quantities. Today such a

change would require a great deal of work because this ancient convention so pervades PANDORA. It is now much too late for that.)

The following list recapitulates the names of the various method control parameters (single values, or tables – see Section 5) used to select the weight matrix method to be used for the various types of source function calculations:

- **YPRE** for **QR**-mapped, as discussed above;
- YLINE for Line Source Function;
- YL for Level-N-to-Continuum (Lyman) source function;
- **YCONT** for Continuum Source Function at the wavelengths of the cores of radiative transitions;
- YWAVE for Continuum Source Function at 'additional' wavelengths;
- **YRATE** for Continuum Source Function at the wavelengths specified for the rates integrations;
- **YHM** for Continuum Source Function at the wavelengths specified for the H-minus calculation;
- **YLDT** for Continuum Source Function at the wavelengths specified for the Type-2 Dust Temperature calculation;
- YLYM for Continuum Source Function at the wavelengths specified for the Level-N-to-Continuum (Lyman) transfer calculation;
- **YCR** for Continuum Source Function at the wavelengths at which incident coronal radiation is specified;
- YKR for Continuum Source Function at the wavelengths for which additional photoionization is specified;
- **BANDY** for Continuum Source Function at Composite Line opacity wavelengths in a particular band;
- **YRATS** for Continuum Source Function at standard rates integrations wavelengths;
- YCOL for Continuum Source Function at CO-lines absorption wavelengths.

(Section 12 – last revised: 2006 Nov 02)

Section 13: Auxiliary Depth Tables

PANDORA deals with many depth-dependent quantities. When these exist in tabular form, they are specified as functions of the set of discrete geometrical depth values that constitute the standard kilometer depth table $\mathbf{Z}_i, 1 \leq i \leq \mathbf{N}$. However, it may happen that when such a quantity is to be input to PANDORA, it is known only as a function of a different set of depth values. When that is the case, such a different set of depth values may be input as an auxiliary depth table. Upon reading tables corresponding to that auxiliary Z table, PANDORA will perform, during the input reading process, the interpolations necessary to convert such tables to functions of the actual **Z**-scale of the run. After input reading is finished, and before beginning the actual calculations, PANDORA discards the auxiliary Z tables.

The remainder of this section discusses in detail how to introduce and use auxiliary Z tables.

Every auxiliary Z table, **ZAUX**, has a unique identifier $m, 1 \leq m \leq 50$. By definition, the value m = 0 refers to the standard kilometer depth table of the run, **Z**.

To introduce an auxiliary Z table, it is only necessary to specify its length, \mathbf{LZA}_m , in an LZA statement in Part B of the input (see Section 4), and then the table itself, \mathbf{ZAUX}_i^m , $1 \le i \le \mathbf{LZA}_m$, in a ZAUX statement in a subsequent Section of the input file.

There are three ways of referring to (i.e. specifying) a depth table when specifying input values of depth-dependent quantities:

- 1) If none is referrenced explicitly, or if m=0, then the standard kilometer depth table of the run, \mathbf{Z} , is assumed.
- 2) The auxiliary depth table index \mathbf{m} can be specified in the same input statement as the corresponding input quantity itself. Input statements of the Type $\mathbf{2}^*$, $\mathbf{3}^*$ and $\mathbf{5}^*$ (see Section 2) have been provided for this purpose. When the value of m is specified in this manner, then it affects that input statement only.
- 3) A global value of auxiliary depth table identifier m can be specified as the input parameter MAUX. (The default value of MAUX = 0.) Upon encountering a MAUX statement, PANDORA assumes that all depth-dependent quantities that follow (except those that use input statement Types 2^* , 3^* , or 5^*) correspond to the auxiliary depth table whose index was specified in that statement, and will perform the necessary interpolations mentioned above. A value of m as set by a MAUX statement remains in effect until countermanded by a subsequent MAUX statement.

The auxiliary depth table identifier value m=0 is permitted in MAUX statements, but not in LZA or ZAUX statements.

Since the interpolation from **ZAUX** to **Z** is done during the reading of the input statements (as opposed to being done after all the input has been read), it is necessary that a given **ZAUX** table must have already occurred in the input before it is first referred to, and the **Z** table must already have occurred in the input before the first ZAUX-dependent input is read.

Note: It is normally possible (indeed, convenient at times) to use several distinct, non-contiguous input statements to specify the sequence of elements of an input array (using **I**, the explicit facility for specifying the index of the 'array member currently being read into'; see Section 2).

This is not possible with arrays that are functions of auxiliary Z tables. For such arrays (even when PANDORA only needs to 'go through the motions' of interpolation), all elements must be specified in *one* input statement.

Note

Many years' experience with auxiliary Z tables has shown that their use causes

confusion; it seems best only to use them as temporary expedients.

(Section 13 – last revised: 1998 Sep 17)

Section 15: Partial ReDistribution

PANDORA uses either "complete redistribution" (CRD, the default) or "partial redistribution" (PRD, selected by input switch $\mathbf{SCH}^{u,\ell}$) to compute the line source function of transition (u,ℓ) . PRD can be done by one of two methods, depending on the option PRDMETH. When PRDMETH is on, PANDORA uses a procedure based on the formulation of Hubeny & Lites as discussed in ApJ., $\mathbf{455}$, 376. When PRDMETH is off, PANDORA uses a simplified procedure based on the formulation of Kneer & Heasley as discussed in Appendix A of Vernazza, Avrett & Loeser (1981), Astrophys.J.Suppl. $\mathbf{45}$, 635, and in a paper by Avrett & Loeser (1984) appearing in *Methods in Radiative Transfer*, Kalkofen, ed., pp. 341-379. Note that PRDMETH selects the method for all PRD-transitions in a run.

Input Parameters

Set $\mathbf{SCH}^{u,\ell} = 1$ when PRD is to be used for transition (u,ℓ) (see also Note 47 of Section 5), and set option PRDMETH for the desired procedure. The input parameters $\mathbf{GMMA}^{u,\ell}$ and \mathbf{IGMSW} control the calculation of γ and are always required.

When PRDMETH is on the other input parameters are **ITPRD**, **PRDCV** and **IGII**. The iterations limit **ITPRD** and the convergence criterion **PRDCV** control the (JNU: S) iterations. **IGII** determines how the function RII is computed: **IGII** = 1 selects the fast approximations developed by Gouttebroze, while **IGII**

= 2 selects the more accurate calculation of Adams, Hummer & Rybicki.

When PRDMETH is off the other input parameters are: $\mathbf{XC}^{u,\ell}$, $\mathbf{XP}^{u,\ell}$, $\mathbf{XR}^{u,\ell}$, \mathbf{DDR}_k and \mathbf{XDR}_k for $0 \le k \le \mathbf{NDR}$, \mathbf{XCL} , \mathbf{TAUCL} , $\mathbf{LMDL2}$, $\mathbf{LMDL3}$, and \mathbf{DRLIM} , used to compute DR. Note that values of $\mathbf{XC}^{u,\ell}$, $\mathbf{XP}^{u,\ell}$, and $\mathbf{XR}^{u,\ell}$ can be specified for each PRD transition; but there is only one table of \mathbf{DDR} vs. \mathbf{XDR} values, used by all PRD transitions of a run, and only one pair of \mathbf{XCL} and \mathbf{TAUCL} values.

The remainder of this section relates to $Gamma(\gamma)$ and to DR.

Gamma

 $\gamma_i^{u,\ell}$ is the degree of coherent scattering in the wings of the (u,ℓ) line. γ is defined in equation (73) of Avrett & Loeser (1984). γ depends on depth (index i) and is very close to unity for low densities. PANDORA provides three ways of specifying $\gamma_i^{u,\ell}$, selected by the value of input parameter **GMMA**^{u,ℓ}.

When $\mathbf{GMMA}^{u,\ell} = -1$ (the default value), then $\gamma_i^{u,\ell} = \mathbf{CRD}^{u,\ell}/DP_i^{u,\ell}$, where the input parameter $\mathbf{CRD}^{u,\ell}$ is the radiative damping parameter and $DP_i^{u,\ell}$ is the computed total (radiative and collisional) damping parameter.

When $\mathbf{GMMA}^{u,\ell} < 0$, but > -1, (say, $\mathbf{GMMA}^{u,\ell} = -.99$), then the smaller of $(|\mathbf{GMMA}^{u,\ell}|, \mathbf{CRD}^{u,\ell}/DP_i^{u,\ell})$ is used as the value of $\gamma_i^{u,\ell}$.

When $\mathbf{GMMA}^{u,\ell} > 0$, then $\gamma_i^{u,\ell} = \mathbf{GMMA}^{u,\ell}$ (i.e. that constant value at all depths), disregarding $\mathbf{CRD}^{u,\ell}/DP_i^{u,\ell}$.

When **IGMSW**= 1, then the alternate formulas specified in the writeup dated [05 Feb 18] are used for $\gamma^{2,1}$ and $\gamma^{3,1}$ (Lyman alpha and beta) in Hydrogen runs.

DR

When PRDMETH is off one must specify the function DR(x), which describes the change from zero coherent scattering in the Doppler core to partial coherent scattering in the wing. DR(x) is the function f(x) defined by equation (78) of Avrett & Loeser (1984).

PANDORA provides three options for computing values of DR(x), selected by the value of input parameter $\mathbf{XC}^{u,\ell}$.

- 1) When $\mathbf{XC}^{u,\ell} < 0$, then DR(x) is obtained by interpolation from the input table \mathbf{DDR}_k vs. \mathbf{XDR}_k , $1 \le k \le \mathbf{NDR}$. The default values of this input table are the same as Table 33 of Vernazza, Avrett & Loeser (1981).
- 2) When $\mathbf{XC}^{u,\ell} > 0$, PANDORA uses

$$DR(x) = \begin{cases} 1, & x \le x_c, \\ \exp\left[-\left(\frac{x - x_c}{x_c}\right)^p\right], & x > x_c. \end{cases}$$
 (1)

- (c.f. equation (78) in Avrett & Loeser (1984)). Here $x_c = \mathbf{X}\mathbf{C}^{u,\ell}$ and $p = \mathbf{X}\mathbf{P}^{u,\ell}$. Moreover, when DR(x) is computed in this way it may not be less than $drlim^{u,\ell}$ (see below).
- 3) When $\mathbf{XC}^{u,\ell} = 0$, DR(x) is computed from equation (1) but with XXC_i in place of x_c . XXC_i depends on the depth-dependent Voigt function parameter a_i ; on the mean optical depth of the line

$$TAUM_{i} = 10^{5} \int_{Z_{i}}^{Z_{i}} (GTN_{i} + KPC_{i1})dz;$$

and on the input parameters **XCL** (default = 3.5) and **TAUCL** (default = 10^4) as follows. For $TAUM_i \leq TAUCL$, $XXC_i = XCL$. For $TAUM_i \geq 10^6$, $XXC_i = FXC_i$ where

$$FXC_i = \left(\frac{4a_i TAUM_i}{\pi}\right)^{0.3333}.$$

For **TAUCL** $< TAUM_i < 10^6$, linear interpolation is used, so that

$$XXC_i = \frac{(6 - \log_{10}TAUM_i)XCL + (\log_{10}TAUM_i - \log_{10}TAUCL)FXCC_i}{6 - \log_{10}TAUCL}$$

where

$$FXCC_i = \left(\frac{4a_i 10^6}{\pi}\right)^{0.3333}$$
.

However, whenever XXC_i is less than XCL, it is replaced by XCL. Again, when DR(x) is computed in this way it may not be less than $drlim^{u,\ell}$ (see below).

DR limit

The value of $DR(x)^{u,\ell}$ computed from equation (1) above is not allowed to be less than the specified limit $drlim^{u,\ell}$ for that transition. There are two procedures for obtaining the value of $drlim^{u,\ell}$: a) the general case, and b) Hydrogen (u,1) transitions, *i.e.*, the Hydrogen Lyman lines. These procedures use the input parameters $\mathbf{XR}^{u,\ell}$, \mathbf{DRLIM} , $\mathbf{LMDL2}$, and $\mathbf{LMDL3}$.

a) General case

If
$$\mathbf{X}\mathbf{R}^{u,\ell} \neq -1$$
, then

$$drlim^{u,\ell} = \mathbf{X}\mathbf{R}^{u,\ell};$$

but if $\mathbf{X}\mathbf{R}^{u,\ell} = -1$, then

$$drlim^{u,\ell} = \mathbf{DRLIM}$$
.

b) Hydrogen Lyman lines

If
$$\mathbf{X}\mathbf{R}^{u,1} \neq -1$$
, then

$$drlim^{u,1} = \mathbf{X}\mathbf{R}^{u,1};$$

but if $\mathbf{XR}^{u,1} = -1$, then

if u = 2, *i.e.* the Lyman- α line, then

$$drlim^{2,1} = \mathbf{LMDL2}$$
,

if u = 3, *i.e.* the Lyman- β line, then

$$drlim^{3,1} = \mathbf{LMDL3}$$
,

but if $4 \le u \le 15$, then

$$drlim^{u,1} = \frac{\sum_{k=2}^{u-1} A^{u,k}}{A^{u,1} + \sum_{k=2}^{u-1} A^{u,k}},$$

the branching ratio equation, where the $A^{i,j}$ are the computed Einstein A coefficients (see Section 19).

(Section 15 – last revised: 2005 Jun 15)

Section 16: Velocities

PANDORA uses several velocity tables, for various purposes. A velocity table may be specified in the input either as a tabulated function of depth (like other input tables), or by means of parameters appearing in the equation used to generate velocity tables as functions of depth.

This section 1) describes the various velocities, by exhibiting instances of their use in the program, 2) describes input procedures and post-read defaults, and 3) lists additional information about how PANDORA uses these velocities. The descriptions given here are rather sketchy (full information can be found in E. H. Avrett's program specifications and explanatory memoranda); the descriptions and equations appearing in this section are only meant to be illustrative, not exhaustive.

All the velocities treated in this section are arrays of length N.

1) Descriptions of Velocities

a) Broadening velocities V and VR

PANDORA uses two "broadening velocities" to compute doppler widths, depending on the option VSWICH. When VSWICH is off, then one velocity is used: \mathbf{V}_i (in km/s), called the "broadening" velocity or "microturbulent" velocity. When VSWICH is on, then two velocities are used: \mathbf{V}_i (in km/s), called the "tangential" broadening velocity and \mathbf{VR}_i (in km/s), called the "radial" broadening velocity.

The doppler width DW is computed from:

$$DW_{im} = \alpha \sqrt{\beta \times \mathbf{TE}_i + \mathcal{V}_{im}^2}$$

(where α and β are terms specified elsewhere). When VSWICH is off:

$$\mathcal{V}_{im}^2 = \mathbf{V}_i^2 \quad ,$$

but when VSWICH is on:

$$\mathcal{V}_{im}^2 = \mathbf{V}\mathbf{R}_i^2 M U_m^2 + \mathbf{V}_i^2 (1 - M U_m^2) \quad ,$$

where MU_m is cosine of the angle between the direction m and the outward normal.

b) Expansion velocities **VXS** and **VX**

Two "expansion velocities" may be specified: \mathbf{VXS}_i (in km/s, positive outwards), called the "Source Function" expansion velocity, and various tables of \mathbf{VX}_i^m , $1 \le m \le \mathbf{NVX}$ (in km/s, positive outwards), called "additional" expansion velocities. \mathbf{VXS} describes differential mass motion in the atmosphere and is used together with option EXPAND. "Expansion" affects the line source function calculation in fundamental ways: a whole-profile solution must be done (see also Section 18); and WN-matrices (i.e., Λ -operators) must be computed with the general ray tracing method, which uses numerical (explicit) angle integration, in place of the other methods, which use analytic angle integration (and require much less computing). (Note that, for study and testing purposes, $\mathbf{VXS}_i = 0$ is allowed when option EXPAND is on; this forces PANDORA to use the general ray tracing method even in a stationary atmosphere.)

The effect of velocity on the calculated line profile can be studied approximately but economically by computing the line source function statically and then calculating not only the corresponding static line profile but also one or more additional profiles using "additional" expansion velocities $\mathbf{V}\mathbf{X}$.

(Important: tables of VX are used *only* for the line profile calculations, *not* for source function calculations; however, their use does cause all line source function calculations to be whole-profile solutions; see Section 18.)

Line absorption profiles are given by the Voigt function

$$\phi_{ik}^{jm} = \frac{a_i}{\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{\exp(-x^2)dx}{a_i^2 + (U_{ik}^{jm} - x)^2}$$

where $a_i = DP_i/DW_i$ (the doppler width DW_i is given in section (1a) above), and DP_i is the damping parameter. The damping parameter for transition (u, ℓ) is computed from:

$$\begin{split} DP_i^{u,\ell} &= \mathbf{CRD}^{u,\ell} + \mathbf{CVW}^{u,\ell} \left(\frac{\mathbf{HN}_i^1}{10^{16}} \right) \left(\frac{\mathbf{TE}_i}{5000} \right)^{0.3} + \mathbf{CSK}^{u,\ell} \left(\frac{\mathbf{NE}_i}{10^{12}} \right)^{\mathbf{PW}} \\ &+ \mathbf{CRS}^{u,\ell} \left(\frac{\mathbf{ND}_i^1}{10^{16}} \right) + HDP_i^{u,\ell} \quad , \end{split}$$

where HDP is the ion broadening term (upper levels of Hydrogen only). The parameter U is computed from

$$U_{ik}^{jm} = \frac{(DL_k + DV_i^m) - \mathbf{DDL}^j \mathbf{FDDL}_i}{DW_i},$$

where DL_k is wavelength offset ("delta Lambda") computed from \mathbf{XI}_k , DV_i^m is the wavelength shift due to velocity, and \mathbf{DDL}^j is the offset of the jth component of a blended line (most transitions are not "blended lines" and have $\mathbf{LDL} = 1$ and $\mathbf{DDL}^1 = 0$.)

The wavelength shift due to velocity is given by

$$DV_i^m = VP_i^m \left(\lambda^{u,\ell}/c\right) \times 10^5 \,,$$

where VP^m is the velocity projected along direction m, $\lambda^{u,\ell}$ is the "core" wavelength of transition (u,ℓ) , and c is the light speed (in cm/s). The projected velocity is given by

$$VP_i^m = MU^m \times (\mathcal{V}_i - \mathcal{V}^*),$$

where MU^m is the cosine of the angle between direction m and the outward normal, $\mathcal{V}^* = 0$ in the restframe but $\mathcal{V}^* = \mathcal{V}_I$ in the frame comoving with point I, and $\mathcal{V} = \mathbf{VXS}$ or $\mathcal{V} = \mathbf{VX}$, as the case may be.

PANDORA provides two types of VX: "general VX" and "shock VX." This distinction (described below) arises from the different generating formulas used to generate tables of VX_i when such tables were not explicitly given in the input.

c) Flow-brodadening velocities, VXFB, for profiles

When option FLWBROAD is on, a special set of velocities is generated and used to compute a set of line profiles; these profiles are averaged to yield a "flow-broadened" profile. These flow velocities, VXFB, enter the profile calculations just like the "additional" expansion velocities, VX, discussed above.

d) Sobolev velocity VSB

The "Sobolev" velocity VSB_i (in km/s, positive outwards) is needed when the moving escape probability (i.e. Sobolev) solution is selected for one or more transitions. The Sobolev formula for the net radiative bracket is

$$RHO_i^{\text{Sobolev}} = G_i \left(1 - \frac{J_i}{S_i} \right) ,$$

$$G_i = \int_0^1 f_i(x) dx ,$$

$$f_i(x) = \frac{1 - \exp[-H_i(x)]}{H_i(x)} ,$$

$$H_i(x) = \frac{FXI_i}{x^2 \mathbf{VSB}_i' + (1 - x^2)RV_i}$$

where \mathbf{VSB}'_i is the derivative of \mathbf{VSB} with respect to \mathbf{Z} . In the plane-parallel case: $RV_i = 0$; but in the spherical case:

$$RV_i = rac{\mathbf{VSB}_i}{(\mathbf{Z}_N - \mathbf{Z}_i) + \mathbf{R1N}}$$

e) Mass motion velocity **VM**

The "mass motion" velocity \mathbf{VM}_i (in km/s, positive inwards) is needed when the option VELGRAD is on and is further explained in section (2b) below. The mass motion velocity can also be introduced into the hydrostatic equilibrium calculations, depending on the option HSEV. This is illustrated next, in the description of the use of \mathbf{VT} .

f) Turbulent pressure velocity **VT**

 \mathbf{VT} is the "turbulent pressure" velocity (in km/s), (note that when option VTV is on then, if no values of \mathbf{VT}_i were specified in the input, \mathbf{VT}_i will be set equal to \mathbf{V}_i). \mathbf{VT} is used in the hydrostatic equilibrium calculations in the equation for the total pressure.

The hydrostatic equilibrium equation is

$$dp/dx = g\rho$$
,

where p is the total pressure, x is the distance from the outer boundary (in cm), and the density ρ is given by

$$\rho_i = m_{\rm H} \, \mathbf{N} \mathbf{H}_i \, \left(1 + \frac{m_{\rm He}}{m_{\rm H}} \frac{NHE_i}{\mathbf{N} \mathbf{H}_i} \right) \,,$$

where NHE_i is the Helium density. The total pressure is given by

$$p_i = (1 + \gamma)P_i^{\text{gas}} + P_i^{\text{turb}} + P_i^{\text{exp}} \quad .$$

 γ is the input constant **RMAGP** that can be used to simulate the effect of magnetic pressure; $P_i^{\rm gas}$ is the gas pressure

$$P_i^{\text{gas}} = (NHA_i + NHE_i + \mathbf{NE}_i - NH2_i) k \mathbf{TE}_i$$

where NHA_i is the atomic Hydrogen density and $NH2_i$ is the molecular Hydrogen density; P_i^{turb} is the turbulent pressure

$$P_i^{\text{turb}} = 1/2\rho_i (\mathbf{V}\mathbf{T}_i \times 10^5)^2 \quad ;$$

and P_i^{exp} is the expansion pressure

$$P_i^{\text{exp}} = \rho_i (\mathbf{V} \mathbf{M}_i \times 10^5)^2$$

only when the option HSEV is on; when the option HSEV is off, then $P_i^{\text{exp}} = 0$ (note that option HSEV is on by default). Here **VM** is the mass motion velocity, further explained in section (2b) below.

2) Establishing and checking velocity values

After all the input has been read, the values of **V**, **VR**, and **VT**, are accepted as they stand (but note that option VTV is relevant).

a) Values of VSB, VXS, and "general" VX^n may either be input directly as simple arrays, or by means of their corresponding generating parameters CVSB, CVXS, and CVX^n , from which the input tables are computed. "General" VX are computed when $ISSV^1 = 0$; for "shock" VX, see below. (Values of VXFB cannot be input as simple arrays but can only be obtained with generating parameters; see below.)

Such values of velocity V_i are computed from the corresponding generating parameter C as follows:

$$\mathcal{V}_i = \frac{\mathcal{C} \times 10^{10} \times TERM_i}{\mathbf{NH}_i} \times \frac{FMV_i}{FFRS_i^2}$$

(see E. H. Avrett's program specifications "Use of the continuity equation for the fluid velocity," dated 8/9/88, and "Depth-dependent helium abundance," dated 12/31/90, and the further modifications dated 1/25/93 and 4/26/95). Here

$$TERM_i = \frac{(1 + \mu \times a^*)}{(1 + \mu \times a_i)},$$

where $\mu = m_{\text{He}}/m_{\text{H}}$, $a_i = ABD_{\text{He}} \times \text{RHEAB}_i$, and a^* is a reference value of a_i determined as specified in [12/31/90].

The multiplier FMV_i is used to set $V_i = 0$ deep in the atmosphere and is obtained as follows:

$$FMV_i = 0, t_i < \mathbf{FMVLIM},$$

or

$$FMV_i = t_i, \qquad t_i \ge \mathbf{FMVLIM},$$

where

$$t_i = \frac{1}{2}[1 - \tanh(x_i)],$$

and

$$x_i = (\mathbf{Z}_i - \mathbf{CVZ})/\mathbf{CDZ}, \quad \mathbf{CDZ} \neq 0,$$

or

$$x_i = 1,$$
 $\mathbf{CDZ} = 0.$

CDZ (default = 1 km) and **CVZ** (default = the smallest value of \mathbf{Z}_i for which $\mathbf{NH}_i > 10^{11}$), and **FMVLIM** (default = 10^{-4}), are input parameters.

The term $FFRS_i$ is required when spherical geometry has been selected. Thus, when the option SPHERE is off, $FFRS_i = 1$; but when the option SPHERE is on,

$$FFRS_i = \frac{(\mathbf{R}\mathbf{1}\mathbf{N} + \mathbf{Z_N}) - \mathbf{Z}_i}{(\mathbf{R}\mathbf{1}\mathbf{N} + \mathbf{Z_N}) - Z^*},$$

where $Z^* = \mathbf{Z_1}$ when $\mathbf{NH_1} > 10^{10}$; $Z^* = \mathbf{Z_N}$ when $\mathbf{NH_N} < 10^{10}$; but otherwise is obtained by interpolation in the **Z** and **NH** tables so that $\mathbf{NH}(Z^*) = 10^{10}$.

Shock velocity

When input parameter $\mathbf{ISSV}^1 > 0$, then tables of "shock" velocity values \mathbf{VX}_i^m , $1 \leq m \leq \mathbf{NVX}$, are generated from other input parameters as follows: $\mathbf{VX}_i^m = \mathbf{SCVB}$ when $i > \mathbf{ISSV}^m$, but

$$\mathbf{V}\mathbf{X}_i^m = -\mathbf{SCVA} \exp[(\mathbf{Z}_i - \mathbf{Z_{ISSV^m}})/\mathbf{SCVS}]$$

for $i \leq \mathbf{ISSV}^m$. Here \mathbf{ISSV} is the shock velocity depth index, \mathbf{SCVA} is the velocity amplitude, and \mathbf{SCVS} is the velocity scale height.

Flow-broadening velocities, VXFB

VXFBs consist of two groups: the $2 \times \mathbf{NFB}$ isotropic velocities generated with \mathbf{CVXF} . The \mathbf{CVXM} , and the 2 mass-conserving flow velocities generated with \mathbf{CVXF} . The generating procedure discussed above does not produce proper values of the isotropic velocities, which are intended to represent ubiquitous "random" flows in the Sun's upper chromosphere and lower transition region. So these isotropic velocities are edited, after computation, to insure that they are nowhere smaller than values obtained by interpolation from the input table \mathbf{FNH} (a function of \mathbf{HNDF}). These VXFB effectively constitute the \mathbf{VX} -set for this run (with \mathbf{NVX} determined by the program); when option $\mathbf{FLWBROAD}$ is on no other types of "additional" expansion velocities are allowed (and the run will be aborted if an input value of $\mathbf{NVX} > 0$ is provided).

b) Values of **VM** may either be input directly as a simple array, or by means of the generating parameters **CFH** or **CFHE**. These are used to compute **VM** by a procedure that is intimately related to how **VM** is used in the diffusion calculations when the option VELGRAD is on, as follows.

In a Hydrogen run:

$$\mathbf{VM}_i = 10^{-5} \left(\frac{\mathbf{CFH}}{\mathbf{NH}_i} - RS_i \times \mathbf{VBMB}_i \right) \times \frac{FMV_i}{FFRS_i^2},$$

while in a Helium run:

$$\mathbf{VM}_{i} = 10^{-5} \left(\frac{\mathbf{CFHE}}{NHE_{i}} + RH_{i} \times \mathbf{VBMB}_{i} \right) \times \frac{FMV_{i}}{FFRS_{i}^{2}};$$

where

$$RS_i = \mu \times HEND_i/(\mathbf{NH}_i + \mu \times HEND_i)$$
,

while

$$RH_i = \mathbf{NH}_i / (\mathbf{NH}_i + \mu \times HEND_i);$$

where again $\mu = m_{\rm He}/m_{\rm H}$ and $NHE_i,\,FMV_i$ and $FFRS_i$ are as in section (2a), above.

- **c)** When values of velocity tables are established by these procedures, then the following three remarks apply:
- 1) whenever the input value of a generating parameter $\mathcal{C} \neq 0$, then the corresponding \mathcal{V} will be computed from it, regardless of whether or not an input table of values was provided;
- 2) whenever one velocity table is set equal to another (see just below), then the corresponding generating parameters are set equal as well; and
- 3) whenever NH_i is recomputed during a run, those velocity tables whose corresponding generating parameters are $\neq 0$ are recomputed as well.
- d) After these procedures have been applied as needed during post-read input processing, the tables of VM, VXS and VSB are checked for reasonableness and consistency, as follows:

First, the values **VM** are checked. They may = 0, but they must be \neq 0 if VEL-GRAD is.

Next, the values of **VXS** are set up. When there are input values of **VXS**, they are accepted and named VXI (i.e. the "original input" values of **VXS**). The values of VXI must = 0 when EXPAND is off; they may be ≥ 0 when EXPAND is on. [NOTE: the values of **VXS** that are used in the line source function calculations (and the emergent profile calculations) are redetermined from time to time, as needed; normally, however, **VXS** is set = VXI.] Then, when EXPAND is on, the following occcurs. If the values of $VM \neq 0$, then VXI is set = VVM. But if the values of VM = 0, then VXI retains its input values as read; note that these may = 0! After these rules have been enforced, VXS is set = VXI.

Last, the values of **VSB** are checked. If the values of **VM** \neq 0, then **VSB** is set = -**VM**. If the values of **VM** = 0 and the values of **VXS** \neq 0, then **VSB** is set = **VXS**. If the values of **VM** and of **VXS** both = 0, then **VSB** retains its input values as read. Note that **VSB** must \neq 0 if a Sobolev solution is requested!

3) More about how velocities are used

a) As part of every diffusion calculation (*i.e.* when options AMDIFF and/or VELGRAD are on), tables $VADD_i$, $VV1_i$, and $VV2_i$ are computed as follows:

$$VADD_i = VV1_i + VV2_i$$
 ;

where, when AMDIFF is on in a Hydrogen run:

$$VV1_i = -VH_i \times 10^{-5} \quad ,$$

when AMDIFF is on in a Helium I run:

$$VV1_i = -V1_i \times 10^{-5} \quad ,$$

or, when AMDIFF is on in a Helium II run:

$$VV1_i = -V2_i \times 10^{-5} \quad ;$$

and, when VELGRAD is on:

$$VV2_i = -\mathbf{V}\mathbf{M}_i$$
 ;

(see E. H. Avrett's program specification "Use of diffusion velocities in emergent profile calculations," dated 10/25/89). Then, if the option VELS is on, the current values of **VXS** are replaced by the following:

$$\mathbf{VXS}_i = VXI_i + VV1_i \quad .$$

b) Emergent line profile calculations are done with as many velocity tables as possible. (These enter the calculation by way of the "doppler width" DW, given above). A "set" of velocity tables is assembled as follows:

The first velocity is either \mathbf{VXS}_i or \mathbf{VSB}_i , depending on whether or not the Sobolev solution was used for this transition.

If $VADD_i \neq 0$ and \neq the first velocity, then VADD is added to the set as the second velocity.

Thereafter, the tables $\mathcal{V}_i^n = \mathbf{V}\mathbf{X}_i^n + VADD_i$, $1 \leq n \leq \mathbf{N}\mathbf{V}\mathbf{X}$, are added to the set, provided that $\mathcal{V}_i^n \neq 0$ and \neq any of the preceding velocities. Recall that these $\mathbf{V}\mathbf{X}$ are either "additional" expansion velocities (either of type "general" or of type "shock") or flow-broadening velocities.

(Section 16 – last revised: 2005 Aug 17)

Section 17: Ion Abundances

For simplicity, PANDORA treats, in any one run, the levels of a single ionization stage together with the lowest level of the next higher stage. The sum of the populations of these two *ions* at depth i is $\mathbf{ABD} \times \mathbf{RABD}_i \times \mathbf{HND}_i$, where \mathbf{ABD} is the *elemental* abundance relative to hydrogen, \mathbf{HND}_i is the total hydrogen number density (*i.e.*, protons + neutral hydrogen atoms + 2 × hydrogen molecules), and \mathbf{RABD}_i is the fraction of the elemental abundance in the two stages. By default, $\mathbf{RABD}_i = 1$ for all i.

In a hydrogen run, $\mathbf{ABD} = 1$, and \mathbf{RABD}_i is automatically calculated to account for the atomic fraction relative to the total including molecules (input parameter \mathbf{NHTSW}). In carbon and oxygen runs, \mathbf{RABD}_i is automatically reduced to account for the portions of those elements that are in the form of carbon monoxide (input parameter \mathbf{NCOSW}).

Diffusion may render invalid the assumption that \mathbf{ABD} of a particular element is constant throughout the atmosphere (*i.e.*, the elemental abundance itself may be depth-dependent). When the options AMDIFF and HEABD are both on, PANDORA calculates the depth-dependence of the total helium abundance, \mathbf{RHEAB}_i . The product $\mathbf{ABD}_{\mathrm{He}} \times \mathbf{RHEAB}_i$ is then used in that run in place of the constant $\mathbf{ABD}_{\mathrm{He}}$ as appropriate. (By default, $\mathbf{RHEAB}_i = 1$ for all i.)

The quantities $FION_i$ (the fraction of ions) and $FLVS_i$ (the fraction representing the sum of bound-level populations), as they appear in the POPULATIONS printout, are included in output file fort.20 (see Section 8). Note that $FLVS_i$ + $FION_i = \mathbf{RABD}_i$. Sets of FION & FLVS values from the runs with different ionization stages can then be read by a separate program, called CENSUS, which

computes tables of \mathbf{RABD}_i for the different ions. CENSUS is available for general use, as an auxiliary program for PANDORA.

For example, a He I run (He I levels plus the lowest level of He II) and a He II run (He II plus He III) could both be started with default values of **RABD**. The sets of FION & FLVS values obtained from both these runs are then used by CENSUS to compute a table of **RABD**_i values for He I and another table for He II. Values of the He II table will be less than unity because of the He III fraction, and values of the He II table will be less than unity because of the He I fraction. After those initial parallel He I and He II runs starting with **RABD**_i = 1, it is then better to alternate between He I and He II runs, each followed by a CENSUS run to update the **RABD**_i values, instead of making He I and He II runs in parallel before using CENSUS.

The FION & FLVS data from PANDORA output file fort.20 consist of the lines following the marker [CENSUS data start] and up to the marker [CENSUS data end], exclusive (see Section 8). Note that each set includes the \mathbf{Z}_i table, and a number specifying the stage of ionization.

The input file for CENSUS is fort.91. It should contain the FION & FLVS sets from the latest runs with all the ions of the element. The main CENSUS printout file is fort.92. There is also a data output file, fort.93, which contains tables of \mathbf{RABD}_i for all the ions represented in the input, in the form of valid PANDORA input statements.

CENSUS can deal with the case of different \mathbf{Z}_i tables in the various FION & FLVS sets. If the \mathbf{Z}_i tables do differ (in length and/or by value), the program constructs an all-inclusive merged table, Z_m , interpolates all FION and FLVS input tables to Z_m , computes the various \mathbf{RABD}_i tables to correspond to Z_m , and then writes out the individual \mathbf{RABD}_i tables to correspond to the appropriate original input \mathbf{Z}_i tables. This procedure can lead to unwanted results if the various FION & FLVS sets are intended to correspond to, say, identical \mathbf{TE}_i tables, but the different PANDORA runs had assigned different \mathbf{Z} values to the depth slots associated with that same \mathbf{TE}_i table. (Note that PANDORA recomputes \mathbf{Z} in HSE runs for which input values of \mathbf{ZMASS}_i or \mathbf{TAUKIN}_i were provided.) It is important to pay attention to this. The user may need to intervene and edit the data in the CENSUS input file to make sure that the FION & FLVS tables are associated with appropriate \mathbf{Z}_i tables, and that inappropriate interpolations are avoided.

(Section 17 – last revised: 1997 Apr 08)

Section 18: Frequency Tables

Tables of frequency values, ξ of length k, are needed —1) for the calculations performed for every radiative transition (u, ℓ) as follows: a) integration over frequency for the Line Source Function, b) integration over frequency for PRD terms (if needed), c) emergent line profile calculation; and —2) to capture simulated lines in the "background" (continuum). A frequency table can span either a half-profile (which then implies a symmetric whole profile), or a whole profile (which need not be symmetric).

Internally, PANDORA establishes separate complete sets of preliminary frequency tables for every transition (u, ℓ) . Such a complete set consists of: a symmetric half-profile table, a blue-side half-profile table, and a red-side half-profile table. These tables will be set equal to unique transition-specific half-profile input tables if such were provided, otherwise to general-purpose common half-profile input tables.

Full-profile frequency tables are assembled from half-profile tables. However, for every transition (u, ℓ) that is a blended line, a composite full-profile frequency table is specially constructed by combining the full-profile tables of each of the component lines. Full-profile tables are augmented automatically to account properly for "background lines."

The remainder of this section describes the input, the defaults provided when no inputs are specified, how the full-profile table and the composite full-profile table (if needed) are constructed, and which tables are selected for the source function and emergent profile calculations.

Important Note

The lengths of the various input and constructed frequency tables should not exceed the limits explained below for **KMMAX**, and also in Section 5, Note 47.

Input

For historical reasons, only half-profile frequency tables may be specified in the input. All these tables must be specified with their values in ascending order, and
each table's first value must = 0.

One may specify unique half-profile frequency tables for some or all transitions (u, ℓ) , and/or one may specify common half-profile frequency tables to be used for all those transitions for which no unique sets are specified.

1) Common half-profile frequency tables:

The basic *common* half-profile frequency table is **XISYM** of length **KS**. (The defaults are given is Section 5, above.) A *common* blue-side half-profile table, **XIBLU** of length **KB**, and a *common* red-side half-profile table, **XIRED** of length **KR**, may also be specified. After PANDORA has read Part D of the input, defaults will be provided for unspecified tables: **XIBLU** will be set equal to **XISYM** if no values were input, and **XIRED** will be set equal to **XISYM** similarly.

2) Unique half-profile frequency tables:

[The transition-superscripts (u, ℓ) on names ending in 'T' are omitted in the next paragraph.]

The following half-profile frequency tables can be input for transition (u, ℓ) : symmetric **XISYMT** of length **KST**, blue-side **XIBLUT** of length **KBT**, and red-side **XIREDT** of length **KRT**. After PANDORA has read Part D of the input, defaults will be provided for unspecified tables: The *unique* **XISYMT** will be set equal to *common* **XISYM** if no values were input; thereafter, **XIBLUT** will be set equal to **XISYMT** if no values were input, and **XIREDT** will be set equal to **XISYMT** similarly.

Note also the relevant input parameters **KSTMAX**, **KBTMAX**, and **KRTMAX**, which must be specified.

3) Full-profile frequency table:

[The transition-superscripts (u, ℓ) on names ending in 'T' are omitted in the next paragraph.]

After **XIBLUT** and **XIREDT** for transition (u, ℓ) have been established, a whole-profile frequency table XIFULT of length KFT is constructed by concatenating the values of **XIREDT** and the negatives of the values of **XIBLUT**: XIFULT₁ =

 $-XIBLU_{KBT}$, XIFULT_{KBT} = 0.0, XIFULT_{KFT} = $XIREDT_{KRT}$, where KFT = KBT + KRT - 1.

4) Blended line transitions:

A special composite full-profile frequency table XICMPT^{u,ℓ} of length KCT^{u,ℓ} is constructed by merging $\mathbf{LDL}^{u,\ell}$ XIFULT^{u,ℓ} tables, each offset appropriately, with redundant points eliminated as much as possible.

Note: For storage allocation purposes, PANDORA estimates the value of the largest KCT^{u,ℓ} before any have been computed. This estimate may be much too large (in cases when many redundant points can be eliminated). Yet a run could be stopped if this estimate is larger than can be accommodated. The input parameter KMMAX has been provided for such a case: if KMMAX > 0 then, if it is larger than the estimate, KMMAX will be used for storage allocation purposes instead of an internal estimate; if KMMAX < 0 then, if -KMMAX is less than the estimate, -KMMAX will be used for storage allocation purposes instead. A run will still be stopped, however, if ultimately any KCT^{u,ℓ} > |KMMAX|.

Uses

After all these preliminaries, PANDORA is ready to set up the frequency table ξ for each transition. The choice of table depends on whether the range of the Line Source Function frequency integration extends over the whole profile, or only over half a profile:

- 1) If option EXPAND is on, then full-profile integrations are done for all transitions.
- 2) If NVX > 0, then full-profile integrations are done for all transitions.
- 3) If $\mathbf{LDL}^{u,\ell} > 1$ (*i.e.*, if this is a blended line transition), then full-profile integration is used for transition (u,ℓ) .
- 4) If $\mathbf{LSFFDB}^{u,\ell} = 1$ (i.e., if frequency-dependent background is required for this transition), then full-profile integration is used for transition (u,ℓ) . Note that PANDORA sets $\mathbf{LSFFDB}^{u,\ell} = 1$ automatically for every PRD transition.
- 5) In all other cases, half-profile integrations are used.

Then, for every radiative transition (u, ℓ) :

If half-profile integration is used for transition (u, ℓ) , then $k^{u,\ell}$ is set equal to $\mathbf{KST}^{u,\ell}$ and $\xi^{u,\ell}$ is set equal to $\mathbf{XISYMT}^{u,\ell}$.

If full-profile integration is used for transition (u, ℓ) and this is a blended line, then $k^{u,\ell}$ is set equal to $\mathrm{KCT}^{u,\ell}$ and $\xi^{u,\ell}$ is set equal to $\mathrm{XICMPT}^{u,\ell}$.

If full-profile integration is used for transition (u, ℓ) and this is not a blended line, then $k^{u,\ell}$ is set equal to KFT^{u,\ell}} and $\xi^{u,\ell}$ is set equal to XIFULT^{u,\ell</sub>.}

Moreover, if a full-profile ξ -table has been selected:

PANDORA checks whether the centers of any simulated "background lines" occur in the wavelength band corresponding to the range ξ_1 to ξ_k . If yes, then the ξ -table is augmented with enough additional values to resolve such lines properly. The Hydrogen Lyman lines are handled as a special case. All other background lines cause all or part of a set of frequency values—obtained by constructing a full-profile frequency table from the input table **BXI** of length **KBX**—to be inserted in the ξ -table. (*Note*: **BXI** is also used for inserting "background line wavelengths" in the standard Rates Integrations wavelengths table constructed and used when option USEWTAB is on.)

(Section 18 – last revised: 2004 Jul 07)

Section 19: Atomic Models

PANDORA uses the numeric parameters of a model of the ion-of-the-run to compute the line source functions and emergent line profiles of interest. The user must see to it that the minimum required set of atomic model parameters is specified in the input. Some of these atomic parameters (in the case of Hydrogen: most) can take on default values supplied by the program.

Over the years, and with the help of many people, we have compiled and collected several dozen atomic model data sets. These data sets are known as "atomic model files" and are available for general use.

The purpose of this section is to provide some general guidance for setting up an atomic model and to describe the available defaults. Please refer to Section 5 for complete details about the various parameters mentioned here.

Note that PANDORA-supplied default parameter values are written to file fort.20 (i.e., .msc) when option ATOMSAV is on (see Section 8).

There now follow: 1) General Information; 2) Defaults For Ions Other Than Hydrogen; 3) Defaults for Hydrogen; and 4) More About Collision Rates.

1) General Information

An atomic model consists of a set of energy levels, a continuum level, specifications of the properties of levels, and specifications of the properties of transitions between levels and between levels and the continuum. (As well, PANDORA uses many other atomic model-related parameters that pertain to the details of various specific computational and organizational procedures.)

Levels

The number of energy levels ('regular levels') is \mathbf{NL} , ($\mathbf{NL} \geq 2$). Additional higher levels can be included in the calculations in an approximate way as 'supplementary levels' by setting $\mathbf{NSL} > \mathbf{NL}$. (Normally these are not used, and the program sets $\mathbf{NSL} = \mathbf{NL}$.)

The principal quantum numbers n and ℓ for each level are specified by means of the **NLPAIR** statement. (Another parameter **QNL**, the "number of $n\ell$ electrons," must be specified for each level if default **CI** values [see below] are used.) The value of \mathbf{NU}^j , $1 \leq j \leq \mathbf{NSL}$, is the energy of level j in frequency units (in units of 10^{15} Hz); the convention $\mathbf{NU}^1 = 0$ is enforced. The value of \mathbf{NUK} , similarly, is the energy of the continuum. If the higher level(s) of the ion model are 'autoionizing' level(s), then auxiliary continuum energies, $\mathbf{NUC}^j > \mathbf{NUK}$, can be specified (the default value of $\mathbf{NUC}^j = \mathbf{NUK}$).

Other parameter values needed for each level include: **P**, statistical weight; **CP**, photoionization cross-section; and values of **ELSYM** and **IONSTAGE** (e.g., for Mg-II, **ELSYM** = MG and **IONSTAGE** = 2).

The collisional ionization rate is $\mathbf{CI}_i^j \times \mathbf{NE}_i \times \exp(-h\,\mathbf{NU}^j \times 10^{15}/k\,\mathbf{TE}_i)$, where \mathbf{CI} is the collisional ionization coefficient. Values of \mathbf{CI} can also be provided in the input. \mathbf{CI} can be given as functions of a specified short temperature table \mathbf{TER}_k , $1 \leq k \leq \mathbf{NTE}$. When values of \mathbf{CI}_i^j at particular depths i (i.e., for particular values of \mathbf{TE}_i) are required as the calculation proceeds, they are then obtained by interpolation from these given tables of $\mathbf{CI}^j(\mathbf{TER}_k)$, $1 \leq j \leq \mathbf{NSL}$, $1 \leq k \leq \mathbf{NTE}$. When $\mathbf{NTE} = 1$, then the constant value \mathbf{CI}^j is used for all temperatures.

However, CI can also be computed "on-the-fly" for the specific value of TE_i (and NC_i in a Hydrogen run) at every depth i; see (4), below.

Transitions between levels

PANDORA computes the collisonal transitions, both due to electrons and due to hydrogen, between all levels, and from all levels to the continuum (thus providing rates between levels via the continuum). However radiative transitions are computed only between specified pairs of levels (u, ℓ) , $u > \ell$. There are **NT** such pairs, which are specified by means of the **INPAIR** statement. The "radiative" transitions so specified, depending on how PANDORA should treat them, can be of five different types as indicated by the parameter **KTRANS**^{u,ℓ}: RADIATIVE, PASSIVE, THICK, THIN, and 2-PHOTON. Note that RADIATIVE transitions can be designated as 'blended lines'; this is triggered by setting **LDL**^{u,ℓ} > 1 (see also input parameter **LDLMAX**).

Values of the Einstein parameter $\mathbf{A}^{u,\ell}$ are required for all RADIATIVE and PASSIVE transitions, and may be specified for THICK transitions. Values of the broadening parameters $\mathbf{CRD}^{u,\ell}$ (radiative), $\mathbf{CVW}^{u,\ell}$ (van der Waals), $\mathbf{CSK}^{u,\ell}$ (Stark) and $\mathbf{CRS}^{u,\ell}$ (resonance) may be specified for RADIATIVE and PASSIVE transitions.

The collisional de-excitation rate is $\mathbf{CE}_i^{u,\ell} \times \mathbf{NE}_i \times (\mathbf{P}^u/\mathbf{P}^\ell)$, while the excitation rate is $\mathbf{CE}_i^{u,\ell} \times \mathbf{NE}_i \times \exp[-h\left(\mathbf{NU}^u - \mathbf{NU}^\ell\right) \times 10^{15}/k\,\mathbf{TE}_i]$; here \mathbf{CE} is the excitation coefficient. Values of \mathbf{CE} may also be provided in the input. \mathbf{CE} can be given as functions of the short temperature table \mathbf{TER}_k , $1 \leq k \leq \mathbf{NTE}$, mentioned above. When values of $\mathbf{CE}_i^{u,\ell}$ at particular depths i (i.e., for particular values of \mathbf{TE}_i) are required as the calculation proceeds, they are then obtained by interpolation from these given tables of $\mathbf{CE}^{u,\ell}(\mathbf{TER}_k)$, $2 \leq u \leq \mathbf{NL}$, $1 \leq \ell < u$, $1 \leq k \leq \mathbf{NTE}$. When $\mathbf{NTE} = 1$, then the constant value $\mathbf{CE}^{u,\ell}$ is used for all temperatures.

However, **CE** can also be computed "on-the-fly" for the specific value of \mathbf{TE}_i (and \mathbf{NC}_i in a Hydrogen run) at every depth i; see (4), below.

Minimum input

Values for at least the following atomic model parameters are required in order to be able to do anything at all: **NL**, **NU**, **NUK**, **P**, **CP**, **NT**, **A**, and values of **CI** and **CE** for one value of **TER** (for, say, the default value 4000 K).

2) Defaults For Ions Other Than Hydrogen

a) Unspecified values of $\mathbf{CI}^{j}(\mathbf{TER}_{k})$, $1 \leq j \leq \mathbf{NSL}$, $1 \leq k \leq \mathbf{NTE}$ are replaced by computed ones. Three different methods are available; the (set of) method(s) to be used can be specified in a CIMETHOD statement. The

CIMETHOD statement lists methods by codename as follows:

CLARK: Clark, Abdallah, and Mann (1991), ApJ **381**, 597;

AR: Arnaud and Rothenflug (1985), A&A **60**, 425;

VORONOV: Voronov (1997), Atomic Data and Nuclear Tables 65, 1.

AR and VORONOV can only be used for level j=1, of some ions; CLARK can be used in all cases.

The default methods set is: AR for j=1 if possible, and CLARK otherwise.

- b) Unspecified values of **KTRANS**^{u,ℓ}, for all (u,ℓ) pairs mentioned in **INPAIR**, are set equal to RADIATIVE.
- c) If **CP** is not specified, then for level 1 a default value is computed according to Verner *et al.* (1996), ApJ, **465**, 487 if they list data for this ion. If not, and for other levels, default values are obtained from the hydrogenic approximation.
- d) Unspecified values of $\mathbf{CE}^{u,\ell}(\mathbf{TER}_k)$, $2 \leq u \leq \mathbf{NL}$, $1 \leq \ell < u$, $1 \leq k \leq \mathbf{NTE}$ are replaced by computed ones. Two different methods are available; the (set of) method(s) to be used can be specified in a CEMETHOD statement. The CEMETHOD statement lists methods by codename as follows:

SEATON: Seaton (1962), Proc.Phys.Soc. **79**, 1105;

VREGE: van Regemorter (1962), ApJ **136**, 906.

SEATON can only be used for transitions with nonzero **A**-values, of neutral atoms; VREGE can be used for all cases. The VREGE method needs **A**-values. If $\mathbf{A}^{u,\ell} = 0$ then theoretical values of $\mathbf{A}^{u,\ell}$ for such 'forbidden' transitions are computed assuming that the oscillator strength of the transition is given by the parameter **FROSCE** (whose default value = 0.01).

The default methods set is: SEATON for neutral atoms, and VREGE otherwise.

- e) Unspecified values of $\mathbf{CRD}^{u,\ell}$, $\mathbf{CVW}^{u,\ell}$, and $\mathbf{CSK}^{u,\ell}$ are updated with computed ones. The calculation of \mathbf{CRD} -vales uses all available \mathbf{A} -values.
- f) If all values of **RRCP** for any level are unspecified, default sets for such levels are computed either according to Verner *et al.* (see (c), above), or using $1/\nu^3$.

3) Defaults For Hydrogen

a) Unspecified values of $\mathbf{N}\mathbf{U}^j$, \mathbf{P}^j and $\mathbf{C}\mathbf{P}^j$, $1 \leq j \leq \mathbf{NSL}$, and of $\mathbf{N}\mathbf{U}\mathbf{K}$ are replaced by computed ones.

b) Unspecified values of $\mathbf{CI}^{j}(\mathbf{TER}_{k})$, $1 \leq j \leq \mathbf{NSL}$, $1 \leq k \leq \mathbf{NTE}$ are replaced by computed ones. Five different methods are available; the (set of) method(s) to be used can be specified in a CIMETHOD statement. The

CIMETHOD statement lists methods by codename as follows:

CLARK: Clark, Abdallah, and Mann (1991), ApJ **381**, 597;

AR: Arnaud and Rothenflug (1985), A&A **60**, 425;

JOHNSON: Johnson (1972), ApJ 174, 227;

VS: Vriens and Smeets (1980), Phys.Rev.A **72**, 940;

SHAH: Shah, Elliott, and Gilbody (1987), J.Phys.B 20, 3506.

AR and SHAH can be used for level j=1 only; the others can be used in all cases. The default methods set is: SHAH for j=1, and CLARK otherwise.

c) Unspecified values of $\mathbf{CE}^{u,\ell}(\mathbf{TER}_k)$, $2 \leq u \leq \mathbf{NL}$, $1 \leq \ell < u$, $1 \leq k \leq \mathbf{NTE}$ are replaced by computed ones. Six different methods are available; the (set of) method(s) to be used can be specified in a CEMETHOD statement. The CEMETHOD statement lists methods by codename as follows:

SEATON: Seaton (1962), Proc. Phys. Soc. **79**, 1105;

VREGE: van Regemorter (1962), ApJ **136**, 906;

SCHOLZ: Scholz et al. (1990), MNRAS 242, 692;

PB: Przybilla and Butler (2004), ApJ **609**, 1181;

AGGRWL: Aggarwal et al. (1991), J.Phys.B 24, 1385;

VS: Vriens and Smeets (1980), Phys.Rev.A 22, 940;

JOHNSON: Johnson (1972), ApJ 174, 227.

SCHOLZ can be used for transition (2/1) only; PB works for all transitions (u, ℓ) , $u \leq 7$; AGGRWL works for all transitions (u, ℓ) , $u \leq 5$; the others can be used for all cases.

The default methods set is: AGGRWL for all transitions it works for, and JOHNSON otherwise.

d) Unspecified values of $\mathbf{A}^{u,\ell}$, for all (u,ℓ) pairs mentioned in **INPAIR**, are computed according to Johnson (1972), ApJ **174**, 227 (uses 'lowering of the ionization potential when **IXNCS** = 1). All unspecified values of **KTRANS**^{u,ℓ}, for all

- (u,ℓ) pairs mentioned in **INPAIR**, are set equal to RADIATIVE.
- e) Unspecified values of $\mathbf{CRD}^{u,\ell}$, $\mathbf{CVW}^{u,\ell}$, $\mathbf{CSK}^{u,\ell}$, and $\mathbf{CRS}^{u,\ell}$ are updated with computed ones. The calculation of \mathbf{CRD} -values uses all available \mathbf{A} -values; the calculation of \mathbf{CSK} -values uses the method of Sutton (1978), JQSRT **20**, 233.

4) More About Collision Rates

When PANDORA computes values of **CI** and/or **CE**, as described in (2) and (3) above, such raw computed values are modified before use, as follows:

$$CI_{default}^{j} = ACI^{j} + MCI^{j} \times CI_{raw}^{j}$$

$$CE_{default}^{u,\ell} = ACE^{u,\ell} + MCE^{u,\ell} \times CE_{raw}^{u,\ell}$$

(The default values of the input parameters **ACI** and **ACE** are all 0, and of the input parameters **MCI** and **MCE** are all 1.)

Before any input or computed CI and CE values are used in the calculations, they are all multiplied by input parameter RFAC (default = 1).

When option CEFACTS is on and any values of $\mathbf{PCE}^{u,\ell} > 0$, then sets of $\mathbf{FCE}^{u,\ell}_i$ are computed and adjusted to prevent $S_i^{u,\ell} \leq 0$. Such \mathbf{FCE} values are saved for use in restart runs.

If ONTHEFLY was specified for **CI** in a CIMETHOD statement, and/or for **CE** in a CEMETHOD statement, then the tabulated values in the ATOM printout section are for information only. Actual values of **CI** and/or **CE** will be computed at every depth as needed.

In a Hydrogen run computed default \mathbf{CI} and \mathbf{CE} values using JOHNSON or VS also depend on \mathbf{NC} when the value of the input parameter $\mathbf{IXNCS} = 1$ (the default is $\mathbf{IXNCS} = 0$, *i.e.* the \mathbf{NC} -dependent factor is set = 1). When the \mathbf{NC} -dependent factor is computed explicitly it is intended to account for the 'lowering of the ionization potential.'

A comparison of the various default CI and CE values appears in the printout section INPUT NOTES. These sample values are computed using TE_i , where i is the input parameter INCEI.

(Section 19 – last revised: 2007 Apr 18)

Section 20: Statistical Equilibrium Equations

This section supplements the derivation and discussion given in the paper "Iterative Solutions of Multilevel Transfer Problems" by Avrett & Loeser in *Numerical Radiative Transfer*, ed. W. Kalkofen (Cambridge University Press, 1987), pp. 135–161.

The single-rate and net-rate statistical equilibrium equations are equations (10) and (14), respectively, in the paper cited above. To change from a net rate to a single rate for the u, ℓ transition, $u > \ell$, $\rho_{u,\ell}$ is replaced by $1 + (\bar{J}_{u,\ell}/\alpha_{u,\ell})$ where $\alpha_{u,\ell} = 2h\nu_{u,\ell}^3/c^2$, and $A_{u,\ell}(\bar{J}_{u,\ell}/\alpha_{u,\ell})(p_u/p_\ell)$ is added to the collisional excitation rate $C_{\ell,u}$. (Here $A_{u,\ell}$ is the Einstein emission coefficient and p_u/p_ℓ is the ratio of statistical weights.) These equations are written in terms of the bound-level number densities n_m . The continuum number density was eliminated by the use of equation (2).

Equation (10) or (14) for $m=2,3,\cdots,M$ when divided by n_1 each form a set of M-1 equations for $n_2/n_1,n_3/n_1,\cdots,n_M/n_1$ given the \overline{J} values in the first case and the ρ values in the second. (Here M, the number of bound levels, corresponds to the input parameter \mathbf{NL} .) These equations can be expressed in terms of the departure coefficient ratios $b_2/b_1,b_3/b_1,\cdots,b_M/b_1$ if the rate coefficients are multiplied by γ_m/γ_1 where $\gamma_m=p_m\exp(-h\nu_{m1}/kT)$.

If we specified all transitions as "single," PANDORA would use the set of equations (10) to obtain "b-ratios from \bar{J} ." If we specified all transitions as "net," PANDORA would use equations (14) to obtain "b-ratios from ρ ." When PANDORA starts a calculation from scratch with no input ρ values (i.e., all input $\mathbf{RHO}_i^{u,\ell} = 0$) and no input \bar{J} values (i.e., all input $\mathbf{JBAR}_i^{u,\ell} = 0$) the "b-ratios

from ρ " equations are used regardless of any transitions specified as "single." We include a "b-ratios from \bar{J} " calculation in each iteration mainly as a consistency check regardless of transitions specified as "net."

Otherwise, transitions are consistently treated as net or single according to the input transition rate selector $\mathbf{KRATE}^{u,\ell} = 1$ or $\mathbf{KRATE}^{u,\ell} = 2$, respectively. Some experimentation may be required in any given situation to determine which rate selector value to use for which transitions; we have found that best results are obtained by choosing 1 for strong lines and 2 for weak lines.

(Section 20 – last revised: 1996 Apr 02)

Section 21: The Hydrogen Lyman Lines in the Continuum Calculations

1. Theory

The Hydrogen Lyman lines are transitions between any upper level U and the lower level L=1. The absorption coefficient for a line transition between levels U and 1 is

$$\kappa_{\nu} = n_1 \frac{h\nu_{U1}}{4\pi} \mathcal{B}_{1U} \frac{\phi(a, x)}{\Delta\nu_D} \tag{1}$$

where n_1 is the number density of the lower level,

$$\phi(a,x) = \frac{a}{\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{\exp^{-z^2}}{a^2 + (z-x)^2},$$
 (2)

and where $x = \Delta \nu / \Delta \nu_D$, $\Delta \nu = \nu - \nu_{U1}$, and $a = \delta / \Delta \nu_D$. In equation (1) we have ignored stimulated emission since it is negligible at Lyman line wavelengths. Here ν_{U1} is the line-center frequency, and the Doppler width $\Delta \nu_D$ is given by

$$\Delta\nu_D = \frac{\nu_{U1}}{c} \sqrt{\frac{2kT}{M} + V^2} \tag{3}$$

where M is the mass of the atom and V is the line-broadening or microturbulent velocity.

The damping parameter is the sum

$$\delta = \delta_{\text{Nat}} + \delta_{\text{Res}} + \delta_{\text{Stark}} + \cdots \tag{4}$$

and here we consider only the natural, resonance and Stark components

$$\delta_{\text{Nat}} = \frac{1}{4\pi} \sum_{k=1}^{U-1} A_{Uk}$$
 (5)

and

$$\delta_{\text{Res}} = \frac{1}{4\pi} \frac{3e^2}{m} \sqrt{\frac{g_L}{g_U}} \frac{f_{1U}}{\nu_{U1}} n_1 \,, \tag{6}$$

and

$$\delta_{\text{Stark}} = 7.06 \times 10^{-6} \, \text{PMSK} \, a^{U1} \frac{U^4}{U^2 - 1} \left(\frac{NE}{10^{12}}\right)^{2/3}$$
 (7)

where

$$a^{U1} = \begin{cases} 0.642 & \text{if } U = 2\\ 1.0 & \text{otherwise} \end{cases}$$
, (8)

and **PMSK** is an input parameter (default = 1). This expression for Stark damping is from Sutton, K., 1978, J.Q.S.R.T., 20, 333. (Including δ_{Stark} is optional in PANDORA; see below.)

In equation (6) n_1 represents the number density of perturbing atoms of the same ionization stage. The Einstein coefficients in equations (1) and (5) are related by the equations $A_{U1} = (2h\nu_{U1}^3/c^2)\mathcal{B}_{U1}$ and $g_U\mathcal{B}_{U1} = g_1\mathcal{B}_{1U}$, where g_U and g_1 are the statistical weights of the upper and lower levels. A_{U1} and the oscillator strength f_{1U} are related by

$$A_{U1} = \frac{g_1}{q_U} \frac{8\pi^2 e^2 \nu_{U1}^2}{mc^3} f_{1U} \tag{9}$$

where e and m are the electron's charge and mass, respectively. When a=0 in equation (2) the profile function reduces to

$$\phi(0,x) = \frac{1}{\sqrt{\pi}} \exp^{-x^2} . \tag{10}$$

For x larger than 3 (typically), and a > 0,

$$\phi(a,x) \to \frac{a}{\pi x^2} \,, \tag{11}$$

or

$$\frac{\phi(a,x)}{\Delta\nu_D} \to \frac{\delta}{\pi(\Delta\nu)^2} \,. \tag{12}$$

Thus in the line wings we can write equation (1) as

$$\kappa_{\nu} = n_1 \frac{h\nu_{U1}}{4\pi^2} \mathcal{B}_{1U} \frac{\delta_{\text{Nat}} + \delta_{\text{Res}} + \delta_{\text{Stark}}}{(\Delta\nu)^2} \,. \tag{13}$$

In PANDORA we use equation (1) to determine κ_{ν} in the line core and equation (13) for larger $\Delta\nu$ in the line wings.

In the line core the source function is the frequency-independent line source function

$$S_{U1} = \frac{2h\nu_{U1}^2/c^2}{\frac{g_U}{g_1}\frac{n_1}{n_U} - 1}.$$
 (14)

In the line wings, however, photons can be scattered (changing only their direction by the encounter with the atom) with no change in frequency, rather than being absorbed and the re-emitted with $\phi(a,x)$ frequency distribution. For those scattered photons the source function (i.e., the ratio of emission to absorption coefficients) is the mean intensity J_{ν} .

The transfer equation then is written as

$$\mu \frac{dI_{\nu}}{dz} = \kappa_{\nu}^{\text{abs}} (I_{\nu} - S_{U1}) + \kappa_{\nu}^{\text{sct}} (I_{\nu} - J_{\nu}). \tag{15}$$

We introduce a scattering albedo α_{ν} and let

$$\kappa_{\nu}^{\text{abs}} = (1 - \alpha_{\nu})\kappa_{\nu} \,, \tag{16}$$

and

$$\kappa_{\nu}^{\text{sct}} = \alpha_{\nu} \kappa_{\nu} \,. \tag{17}$$

We specify α_{ν} as a function of $x = \Delta \nu / \Delta \nu_D$. (Note that $\Delta \nu_D$, a function of T and V, varies with depth.) We define $(1 - \alpha_{\nu}) = DR(x)$, which is determined as described below. DR(x) must not be less than the allowed lower limit which, for $3 \leq U \leq 15$ is given by the branching ratio equation

$$drlim^{u,1} = \frac{\sum_{k=2}^{U-1} A_{Uk}}{\sum_{k=1}^{U-1} A_{Uk}}.$$
 (18)

Equation (13), which we use in the line wings (i.e., when $x \geq XLIM$; see below), is written as

$$\kappa_{\nu} = \kappa_{\nu}^{\text{Nat}} + \kappa_{\nu}^{\text{Res}} + \kappa_{\nu}^{\text{Stark}} \tag{19}$$

where

$$\kappa_{\nu}^{\text{Nat}} = \begin{cases} n_1 \frac{h\nu_{U1}}{4\pi^2} \mathcal{B}_{1U} \frac{\delta_{\text{Nat}}}{(\Delta\nu)^2} & \lambda < 142.5 \text{ nm} \\ 0 & \lambda \ge 142.5 \text{ nm} \end{cases}$$
(20)

and

$$\kappa_{\nu}^{\text{Res}} = \begin{cases}
n_1 \frac{h\nu_{U1}}{4\pi^2} \mathcal{B}_{1U} \frac{\delta_{\text{Res}}}{(\Delta\nu)^2} & U > 2 \\
10^{-17} n_1^2 \pi f_{12} r_{\text{el}} F(\lambda, T) & U = 2
\end{cases}$$
(21)

(where $r_{\rm el} = 2.818 \times 10^{-13}$ cm is the classical electron radius), and

$$\kappa_{\nu}^{\text{Stark}} = n_1 \frac{h\nu_{U1}}{4\pi^2} \mathcal{B}_{1U} \frac{\delta_{\text{Stark}}}{(\Delta\nu)^2} \,. \tag{22}$$

We set $\kappa_{\nu}^{\text{Nat}} = 0$ for $\lambda \geq 142.5$ nm in equation (20) since this is a component of the Rayleigh scattering opacity which we determine separately according to

$$\sigma_{\nu}^{\text{Ray}} = \begin{cases} 0 & \lambda < 142.5 \text{ nm} \\ n_1 R(\lambda) & \lambda \ge 142.5 \text{ nm} \end{cases}$$
 (23)

The values of $R(\lambda)$ are given by: M. Gavrila, 1967, Phys.Rev., 163, 147, Table I. The standard formula for $\kappa_{\nu}^{\rm Res}$ in equation (21) is used only for the U>2 Lyman lines. For the wings of Lyman alpha we can use values of $F(\lambda,T)$ calculated by N. F. Allard (private communication, October 2002), based on general unified theory, including all the transitions contributing to Lyman alpha, taking into account the variation of the dipole moment during the collision, averaging over velocity. (HH potentials from: T. Detmer, P. Schmelcher, L. S. Cederbaum, 1998, J.Chem.Phys., 109, 9694; dipole moments from: I. Drira, 1999, J.Mol. Spectrosc., 198, 52.) $F(\lambda,T)$ has been tabulated for two values of temperatures, T=5000 K and T=8000 K, and for the wavelength range 261.3429 nm $\geq \lambda \geq 110.1760$ nm (the actual values can be found in the listing of subroutine reaper; for example, $F(140.1269,8000)=9.7522\times10^{-11}$). We obtain any value of $F(\lambda,T)$ by linear interpolation/extrapolation between 4000 K and 10,000 K; we use $F(\lambda,4000)$ for T<4000 K and $F(\lambda,10000)$ for T>10,000 K. We set $F(\lambda,T)=0$ for values of λ outside the tabulated wavelength range.

While we use equation (1) in the line core and equation (13) in the line wings for $1 \leq U \leq 15$, for U > 15 only the line core equation is used. At wavelengths near the $U = \infty$ Rydberg limit (911.75347...Å) there are contributions from

many overlapping Lyman lines. As many of these contributions are computed and summed as seem significant.

For $U > \mathbf{NQLYM}$ linear combinations of the Lyman line and Lyman continuum absorption coefficients and source functions can be used to avoid a discontinuity at the Rydberg limit; when $\mathbf{NQLYM} = 0$, however, such linear combinations are not used (and $\mathbf{NQLYM} = 0$ is the default).

2. Practice

A simulation of the H Lyman- α line has been used in PANDORA as one of the contributors to the background (or "continuum") absorption for a long time. (In the 1960s Yvette Cuny's work, revealing the enormous wings of this line, had shown this to be an important opacity in the sun.) From the beginning H Ly- α absorption and scattering have been treated separately. Recently further incremental additions were made to the treatment of background H Lyman lines simulations.

This incremental development has resulted in five different contributors to the background absorption and emission calculations, as shown in the printout section BACKGROUND:

```
11 — H Ly alpha Abs. = H(2/1) Line absorption 16 — H Ly alpha Sct. = H(2/1) Line scattering 34 — H Ly 3-15 Abs. = H(u,1), 3 \le u \le 15, Lines absorption 36 — H Ly 3-15 Sct. = H(u,1), 3 \le u \le 15, Lines scattering 37 — H Ly>15 Abs. = H(u,1), u > 15, Lines absorption
```

(See printout section BACKGROUND for more information regarding these background contributors.)

The following input parameters control these calculations: \mathbf{NLY} ; \mathbf{LMXX}_j , \mathbf{LMDR}_j , $1 \le j \le \mathbf{LLY}$; \mathbf{LMXC} , \mathbf{LMXP} , $\mathbf{LMDL2}$; $\mathbf{LMDL3}$; \mathbf{LMZ} , \mathbf{LMH} ; and \mathbf{NQ} - \mathbf{LYM} , \mathbf{IFALL} , \mathbf{JHLSK} , \mathbf{PMSK} . These are briefly discussed below; their values for the run are listed in printput section INPUT, under the subheading "Hydrogen Lyman alpha opacity."

If the additional input parameter **LYODS** > 0, then extensive printouts of computational details, for every **LYODS**'th depth, will be printed for every wavelength for which dumps of the background calculation details have been turned on (input table **DWAVE**; see Section 5, Note 65).

For the lines $(u, 1), 2 \le u \le 15$, PANDORA's simulation needs values of XLIM (the boundary beween core and wing) and of DR(x) (which describes the change from zero coherent scattering in the Doppler core to partial coherent scattering in

$$XLIM = \begin{cases} \mathbf{LMXC} & \mathbf{LMXC} > 0 \\ \mathbf{LMXX}_1 & \text{otherwise} \end{cases}.$$

DR(x) is computed by the same procedure as that used for calculating PRD terms in PANDORA's detailed line source function calculations. (In many Hydrogen runs the (2,1)-line and the (3,1)-line are computed with PRD.) This calculation of DR(x) is described in subsections (3.) and (4.) of Section 15. The input parameters **LMXC**, **LMXP**, **LMDL2**, and **LMDL3**, and the input tables **LMXX**_j, **LMDR**_j, $1 \le j \le$ **LLY**, are used for this. (Note that **LMXC** = 0 is not allowed.)

When "H Ly 3-15" (the "higher Lyman lines") are simulated, the upper limit is the value of **NLY** (default = 15). "H Ly>15" (the "highest Lyman lines") are done only when **NLY** = 15; in that case, as many of the converging lines are computed as "make a difference" to the total absorption (or emission) resulting from many overlapping line wings (this calculation uses the built-in upper limit 500).

Values of the contributions to the background absorption or emission due to the cores and wings of the Lyman- α and the higher Lyman lines are computed only at wavelengths less than **LMZ** Å(default = 1682); values of the highest Lyman lines are computed only at wavelengths less than **LMH** Å(default = 950). The lower wavelength limit for all these simulations is the head of the Lyman continuum (the Rydberg wavelength, ≈ 911 Å).

The Lyman- α line simulation can use N. F. Allard's experimental values of $F(\lambda, T)$, as mentioned earlier. These data are used only when **IFALL** = 1 (the default); otherwise $F(\lambda, T) = 0$ is used.

Stark broadening can be included in the simulations, as mentioned earlier. This is done only when $\mathbf{JHLSK} = 1$ (the default). \mathbf{PMSK} is a parameter for computing Stark damping.

NQLYM controls the provision for avoiding absorption and emission discontinuities at the Lyman continuum edge.

(Section 21 – last revised: 2004 Nov 09)

Section 99: Tutorial — How to Run PANDORA

This section describes the input files and output files for four PANDORA demonstration runs. I hope that first-time users will find this helpful. By way of background: when we first began work on PANDORA, we envisioned a 'Dial-an-Atom' program; thus PANDORA's original raison d'être was the coupled line source function calculation, and the statistical equilibrium calculations required for them, with arbitrary model ions. Over the years the program has grown to do many more and different things, but PANDORA's primary purpose remains the calculation of line source functions and emergent line profiles. Before reading this section: be sure you have become familiar with the main body of this handbook, what kind of information it contains, and how it is organized.

Any PANDORA run requires input from four 'logical data Groups': 1) atmosphere model data; 2) atom (ion) model data; 3) levels- and transition-related restart data (*i.e.*, partially-converged solutions) from the preceding run (which may be omitted for runs starting from scratch); and 4) run-specific numeric and control data. Items from any of these 'groups' may/will occur in each of the four major structural parts of PANDORA's input: Parts B, D, F and H. Also, all runs require a run-specific **HEADING** line as the first line of the input file. (PANDORA runs that use PRD for one or more transitions may also require JNU restart values.)

A basic minimum of Group-1 data and Group-2 data normally *must* be supplied, since there are no appropriate default values for them. Group-3 data normally are not supplied for runs beginning from scratch (*i.e.*, the defaults are used); however, sometimes it makes sense to supply output from a related run as input for a

new run. Restart runs normally use Group-3 data that were written in an output file (a 'restart' file) by the preceding run. Group-4 data need not be supplied (especially for runs beginning from scratch) since the automatic defaults should be applicable to a variety of situations. As a calculation progresses through a series of restarts, it should become clear what switch settings, option settings, alternative numerical methods, and numerical control parameter values are most appropriate for any particular case.

There are six Types of PANDORA runs: 1) population-update runs with Hydrogen; 2) population-update runs with ions other than Hydrogen; 3) regular runs; 4) no-ion runs; 5) continuum-only runs; and 6) input-only runs.

The distinction between population-update and regular runs arises from the following. PANDORA computes both 'line' absorption and 'continuum' (more properly: 'background') absorption. Many 'absorbers' can be included in the total computed 'continuum' opacity, including the bound-free absorption of H, He-I, He-II, C-I, Si-I, Al-I, Mg-I, Fe-I, Na-I, Ca-I, O-I, and S-I. The calculations of the contributions of these absorbers require values of number densities and departure coefficients as functions of depth; computed non-LTE values will be used if they are provided. (If none are provided, then LTE default values of number densities will be computed, and/or default values of departure coefficients will be computed from whatever values of number density are available.) Consider a run with, say, Si-I. At the end of every overall iteration, new values of the number densities and departure coefficients of the 'ion-of-the-run' (in this case, Si-I) are computed. These values can be used when the 'continuum' opacity is recomputed at the start of the next iteration (i.e., PANDORA can be instructed that new values of number densities and departure coefficients for Si-I are available, and that therefore Si-I's contribution to the opacity must be recomputed). For this purpose, the new data must be copied from their 'ion-of-the-run' slots into the appropriate 'population-ion-data' slots (i.e., into the 'Si-I-population-data' slots). PANDORA will do this 'updating' if the **POPUP** switch is set. (If the population-ion-data are not updated at the end of each overall iteration, then they will retain their initial values.) (These population ion data can be printed by turning on the appropriate population-ion-data print option – in this case, SILPRNT.) Moreover, when the **POPUP** switch is set, then the latest recomputed population-ion-data will be written in one of the restart files, for later use. Thus, any PANDORA run for one of the 12 ions listed above may be (but need not be) a population-update run. A run with a valid **POPUP** statement among

the input is a 'population-update' run; runs without the **POPUP** switch set are 'regular' runs. (In Type-4 and Type-5 runs the **POPUP** switch is not used.) (The input table **RUNTOPOP** is important for population update runs. The parameters describing the built-in population-ion-models are printed as part of the population ion data for a particular population-update ion -e.g. with SILPRNT on. Note the input parameters **POPION**, **POPXLM**, and **POPRCP**, provided for emergency use.)

Hydrogen runs are special because PANDORA does certain things only when Hydrogen is the ion-of-the-run. These include: recomputation of **Z**, of **NH**, and of **NE**. Such recomputed tables will be written in restart files, and normally should be used in subsequent runs. (Population-update runs also recompute **NE** and write it out – however, we generally ignore such **NE** values, preferring to rely on those produced by Hydrogen runs.)

Type-5, continuum-only, runs are about as far removed from PANDORA's basic purpose as one can imagine. Only 'continuum' source functions, and emergent continuum emission (depending on specific option settings), are computed. This is done at specific wavelengths only, as controlled by the switch **JSTCN**.

Type-4, no-ion, runs resemble continuum-only runs in that no line transfer is computed. In any run with the option DOION off, all those things, but only those things, that specifically concern an ion-of-the-run are omitted. Thus a no-ion run does more things (such as, hydrostatic equilibrium calculation, Dust temperature recalculation) than a continuum-only run.

Type-6, input-only, runs are useful for checking whether the input data being supplied for a run are what they should be. An input-only run only reads and massages the raw input, and does some other input-related initializations, and then stops -i.e., its output file (provided it ran to completion) exhibits the **Phase 0** output (see Section 11), and the input JNU values (if there were any). After this output has been inspected and found satisfactory, the statement "DO (JSTIN)" can be removed from the input, and the run resubmitted as a normal run.

Tutorial Runs

DEMO1 is a type-1 run from scratch, using a single input file; DEMO2 is identical to DEMO1 except for using multiple input files; DEMO3 is a restart, with changes, of DEMO2; and DEMO4 is a type-3 run from scratch.

In this section I refer to the various files by the file "extension codes" used with schema (see Section 7). The complete file names of these demonstration runs are constructed with these extensions; thus: demol.dat, demol.jnr, etc.

(*Please note:* PANDORA's input provisions are very flexible, and users are free to adopt a variety of conventions for organizing input data. I will describe what I have found convenient; feel free to establish different procedures.)

DEMO1

This run uses a single input file, .dat. This file first contains the **HEADING** line (Part A); then Group-1 data, Group-2 data, and Group-4 data in Part B (before the first **GO**); then more Group-1 data, Group-2 data, and Group-4 data in Part D (before the second **GO**); Part F and Part H are empty (*i.e.*, defaults will be used).

Group-1, atmosphere model, data comprise the statements: $\underline{\mathbf{N}}$, \mathbf{NVH} , $\mathbf{R1N}$, \mathbf{CGR} , $\underline{\mathbf{Z}}$, $\underline{\mathbf{TE}}$, $\underline{\mathbf{NH}}$, $\underline{\mathbf{NE}}$, and \mathbf{BDHM} . The underlined ones constitute the basic minimum that must be provided; if any of these are missing, the run will fail. (However, as a special case, when \mathbf{ZMASS} , \mathbf{TE} , and \mathbf{NE} are provided then \mathbf{Z} and \mathbf{NH} need not be.) (Note: I have to set $\mathbf{NVH} = 0$ because I want to have $\mathbf{V} = 0$.)

Group-2, atom model, data comprise the statements: NL, NTE, NT, INPAIR, NAME, ELSYM, IONSTAGE, MASS, PART, ABD, PW, P, CP, TER, CI 1, CI 2, CI 3, CE 2 1, CE 3 1, A 3 2, CE 3 2, CRD 3 2, CVW 3 2, CSK 3 2, and CRS 3 2. Again, the underlined ones represent the basic minimum that must be provided, or the run will fail (Note: see Section 19.) These model atom data constitute a basic three-level Hydrogen atom, with the (2,1) and (3,1) lines in detailed balance. A value of PW is provided because a CSK statement appears. If the temperature-dependence of CI and CE were not known, then NTE and TER would not appear, and only single, constant values of CI and CE would have to be provided. (But note that while the foregoing is true generally, there is much more to it for Hydrogen, which is a special case—see Section 19.) The PART statement is not really needed (since 0 is the default); I like to use it to remind me that depth-dependent partition functions will be used (the default state of PARTVAR is on).

Group-4 data comprise: **DO**, **OMIT**, **IOMX**, **POPUP**, **RUNTOPOP** and **TRN**. PANDORA provides defaults for all of them – but this run wants the val-

ues appearing in .dat. The **TRN** statements appear because the option USETRIN is on. The **POPUP** switch is on, for the purpose described earlier. **RUNTOPOP** appears because values other than the defaults are required in this case.

To execute this run, I submit the run-specific script demo1, which uses the general script schema. The main purpose of these scripts is to connect actual files to the files that Fortran I/O expects by default.

Between them, pandora and schema send a slew of messages to standard output (the screen; these messages can be redirected to a "log" file in the usual manner—it is useful to do that). These messages consist of 'computation progress reports,' relevant directory listings, and other information that is useful for the record. The last message that comes from pandora is "PANDORA done"; this is the *only* reliable indication that a run completed properly.

The main output file ('printout' file) from PANDORA is the file .aaa; here, demol.aaa. A few of the printout sections in this output file always appear; the remaining printouts are controlled by option settings, as described in Section 11.

If option LSFPRNT = off in addition to **LSFPRINT**^{3,2} = 0, then the printout headed "LINE (3/2)" would not have appeared, leaving only the subsequent "Plot of logs of ST ..." as a record of the line source function calculation. In a converged solution the values of "S(n)" and "S" would be more nearly equal.

The printed values of "Consistency CHECKs," at the end of the printout "RHO AND RBD," look pretty good. If these tables do not have almost all values close to 1, then the calculation has not converged and needs to be iterated further.

The printout "LEVEL 1 TO K" appears because the option LYMAN is on and **KOLEV** = 1. The fact that the printed values of "Old/New" for RK-1 (on the page just before "NE") are rather far from unity is an indication that this calculation has not converged.

While the sections "WAVE SUMM 0" and "WAVE SUMM 1" can be turned off with option WAVEPRNT, I do not recommend doing that.

The various "Iterative Ratio" plots show significant changes from iteration to iteration, another strong indication that the calculation has not yet converged. NE has settled down in the outer half of the atmosphere.

"Execution Data" always appears (the amount of printout is controlled by option IRUNT). Before signing off, the program version identifies itself.

The remaining files produced by this run are .msc, .pop and .rst; their contents are described in Section 8. Most of these data are needed in order to restart this

run for additional iterations – DEMO3 is an example of such a restart.

DEMO2

This run uses the same input parameters as DEMO1, and thus produces the same output files — what is different is that the input, instead of being all contained in .dat, is now distributed over four files: .mod, .atm, .res, and .dat. (These four files correspond to the four 'logical data Groups' described earlier.)

I do this because I find this a convenient way to organize my data. My conventions are: .atm contains the data specifying the physical parameters of an atom or ion model; .mod contains the data specifying the physical parameters of a model atmosphere; .res contains the same data as the output file .rst, i.e., the restart data for the line source function calculations, and the 'Lyman' calculation (if any); and .dat contains the heading and the various run-specific processing and numerological control parameters, and the GO statements that define the structure of the input.

PANDORA always begins reading from .dat; thereafter, **USE** statements tell it which file to read from next.

Input reading begins at the **HEADING** in demo2.dat. 'USE (MODEL)' then switches reading to .mod (i.e., demo2.mod – recall that demo2 and schema set up this connection), and reading of Part B data then continues there until 'USE (INPUT)' switches reading back to .dat. 'USE (ATOM)' then immediately switches reading to .atm (i.e., atom2.atm), and reading of Part B data then continues there until 'USE (INPUT)' switches reading back to .dat. Reading of Part B data from .dat then continues until the first GO, which terminates Part B. Then reading is again switched to .mod and .atm for Part D data, and then to .res (i.e., demo2.res) which, you will note, is empty. Thereupon the last of the Part D data are read from .dat, until the second GO, which terminates Part D. As with DEMO1, Part F is empty; and so is Part H, even though reading of Part H is switched to .mod (the reason why I do this may become clear with DEMO3). When PANDORA first reads from a given file, it starts at the beginning of the file. When it reads from a partially-read file again, it resumes right after the last statement previously read.

The .mod files, in general, are convenient when you wish to calculate solutions for various ions in the same atmosphere – all those runs can be set up to use the same .mod file. The .atm files, in general, are convenient when you wish to cal-

culate solutions for the same ion in different atmospheres – all those runs can be set up to use the same .atm file. Over the years we have accumulated many .atm files for a variety of atom and ion models (e.g. there are many different Hydrogen models, using different numbers of levels and transitions; we also have various models of atoms and ions important in the Sun; plus some odds and ends). All these are available for general use.

DEMO3

This run shows how I go about setting up a restart of DEMO2.

DEMO3 needs the files: .dat, .mod, .atm, and .res. (Normally, the files for a restart of DEMO2 would have 'DEMO2-names' – these would be edited versions of the previous DEMO2 input files. However, for tutorial purposes, here I have given them new 'DEMO3-names'.) I obtained the DEMO3 input files from the input and output files of DEMO2 as follows:

.res is simply a copy of DEMO2's *output* file .rst. (If I were restarting DEMO2 'normally', without changing names from DEMO2 to DEMO3, I would: first delete demo2.res, and then change the name of demo2.rst to demo2.res.) .mod is an edited copy of DEMO2's .mod, with the following changes:

- old values of **NE** were removed, and replaced by those in demo2.pop;
- values of NP, HN 1 ... HN 15 and BDH 1 ... BDH 15, from demo2.pop, were added after the second 'USE (INPUT)' to Part H of .mod, where they will be read when the third occurrence of 'USE (MODEL)' in .dat switches reading back to this .mod file. To alert PANDORA to the existence of these 'Hydrogen-population-data', I had to add 'NLH (15)' near the beginning, in Part B of .mod. (If DEMO2 had calculated FNRMLA,FNRMLB, then I would have used the updated values of these tables, found in demo2.msc, to update any previous values in demo2.mod.)

I also introduced some further changes into Part D of this atmospheric model (not for restart purposes, but because I wanted to change the calculation):

- a set of values of **V** is added;
- the molecular Hydrogen abundance calculation is turned off (NHTSW);
- the He-II-lines and X-ray absorptions are turned off (NABS).

Atomic model data normally do not need to be changed for a *restart* run, and so demo2.atm could (and normally would) have been used for this run. However, I wanted a more elaborate atomic model for DEMO3, which I obtained by copying

demo2.atm and adding 'rates integrations' data: the MR, WRAT and RRCP statements. (Note: none for level 1 because the 'Lyman' calculation is done for level 1; starting values for the the level-1 rates RL 1 and RK 1 are in .res, having been computed by DEMO2.)

Finally, .dat for DEMO3 is a modified version of demo2.dat. Only one of these modifications is strictly for *restart* purposes: the **HEADING** line. The other modifications change the details of the calculation itself, and the contents of the 'printout' file:

- a value of **LF** that differs from the default;
- different option settings (note that the options PHASE2 and USETRIN now revert to their default settings, which are 'on' and 'off', respectively);
- the option IRUNT is changed to the 'prolix' setting;
- ullet a value of $\mathbf{YLINE}^{3,2}$ that differs from the default;
- the emergent profile calculation for the (3,2) line is turned on (**PROF**);
- sets of values of **TRN** are omitted, since they are no longer needed;
- and the other parameter changes that you see there.

DEMO3 produces the same output files as DEMO2, but the contents differ. In .aaa, you will note the following (among others):

- "ATMOSPHERE" has different values of 'Electron density'; 'Broadening velocity' appears;
- "ND, NK, + BD" now has nonzero values (from .res);
- "ATOM" has different 'Line source function method' and 'Show computed line profile'; it no longer has 'Radiation Temperature';
- the list of contributors in "BACKGROUND" is different;
- "INPUT" has data for "Rates Integrations"; non-zero input values of **RKWT** 1, **EP1**, and **EP2** appear (from .res); "He II Lines Opacity data" is gone; data for "Spectrum Calculations" appears;
- "CONSTANTS" and "TABLES" are gone (why?);
- "HYDROGEN" population data now have input values, and no longer their approximate (i.e., LTE) default values;
- "RATES" (through "RIJ") appears (option RATEPRNT), "Details of Recombination Calculation" is gone (why?);
- "Results of TAU Calculation, ..." appears (option TAUPRNT);
- "NE" and the printed tables in "POPULATIONS" are gone (option POP-PRNT);
- "Old/New" for RK-1 are closer to unity, overall;

- "WAVE SUMM 0" shows that DEMO3 computed more continuum solutions than did DEMO2 (why?);
- "Iterative behavior ..." printouts are gone (why?);
- "Background Intensity" (for **LF** values of **MUF**) appears (why?, and why does "Background Flux" not appear?);
- "Profile of the 3/2 Line" (for **L=LF** values of **MU**) appears;
- "Scratch I/O ..." appears (option IRUNT);
- "Execution Data", and program version description, give more details (option IRUNT).

DEMO3's output files .msc and .pop contain the same amounts of data as those of DEMO2; .rst has a bit more (because **RHOWT**^{3,2} now has some non-zero values).

DEMO3 could now be restarted further, just as before. If this were the kind of Hydrogen run that produces new values of **Z** (say, because values of **TAUKIN** are specified), or of **NH** (say, because of option HSE), or of **BDHM** (option HMS), then these new sets would also have to be edited into .mod, to replace the old sets.

DEMO4

This is an Mg-II run, 'from scratch' like DEMO1, except that it is a 'regular' type of run and it is a PRD run.

The .atm file for this run contains a simple Mg-II model with two levels and one radiative transition. The .atm file does not contain the specifications of the PRD parameters, since this ion model does not require the PRD treatment. Instead, I consider the PRD parameters to be run-specific, and provide them in .dat. Since JNUNC is mentioned neither in .mod nor in .dat, it retains its default value 0, and a .jnu input file is not required.

(By the way, regarding $\mathbf{GMMA}^{2,1} = -0.999$: this value might put too severe a strain on a 'from scratch' calculation. One might instead begin with, say, $\mathbf{GMMA}^{2,1} = \mathbf{I} -0.8$ and then, through a series of restarts, gradually work up to the 'desired' value -0.999.)

The .mod file contains 8 levels worth of 'population-ion-data' for H, He-I, He-II, C-I, and Si-I. Values of departure coefficients are specified for levels 1 - 5 of H only; default values (see the 'printout') will be set up for everything else. .mod also contains five auxiliary depth tables and illustrates their use; note that .mod

does not contain **Z**, the depth table of the run (*cf.* Section 13). .mod also contains some **DO** statements affecting the 'printout' only; one can debate whether these belong here, or in .dat.

As with DEMO2, .res is empty (why?).

The .dat file is relatively simple; note that it contains the N and Z statements, these being run-specific in this case. Of course, there is no POPUP statement (that makes this a 'regular' run). The YLINE statement is superfluous (see next paragraph), but does no harm. (By the way, a .dat file for most runs—other than H runs—might contain a table of RABD or RABDL values [see Section 17]; a .dat file for a He-II run with diffusion might contain tables of PALBET and PBETAL.)

In the 'printout' file .aaa, note that "ATOM" now has 'Partial Redistribution' and several parameters for P.R.D.; moreover, 'Line source function method' is '(not used)' because the 'Background source function method' specification applies to both calculations. Output from rates integrations is short (RATEPRNT and RATESUMM are off), consisting of graphs only (RATEGRAF is on). The "LINE (2,1)" printouts here have only very abbreviated PRD calculation results, because PRDPRNT and PRDCOPR are both off, and only JNUPRNT is on. Notice that the 'normal' line source function calculation output states (between the lines of dashes) that this is a 'Solution with partial redistribution'. (Note option PRDMETH; often it makes sense to use PRD-METH off initially, until the solution is nearly converged, and then use PRD-METH on.) No "Consistency Checks" are computed for a 2-level ion model. Since LF is greater than 1, a line flux profile was also computed from the calculated intensity profiles (however, with only two MUF values, this is not much of a calculation). Since this line is computed with PRD ($\mathbf{SCH}^{2,1} = 1$), a whole profile, rather than a half profile, was computed. Moreover, a PRD calculation computes the background continuum for every point in the line, and that is why the "Line-Free" continuum was also computed for every point in the line. The other output files produced by this run are .jnr, .msc, and .rst; of course there is no .pop output file (why?).

Restarting this run is simple. Delete .res, and change the name of .rst to .res; change the name of .jnr to .jnu (first deleting the previous .jnu, if any). Update the **HEADING** in .dat, and make any other desired changes. Make sure

that the value of **JNUNC** > 0 (Part D of the input, in .dat). Again, this run only *uses*, but does not *affect*, the atmospheric model data. (At least, not directly. In principle, values of **RABD** for a Mg-I run could be affected by these Mg-II results, and that would change the 'Mg-I-population-data' which are part of the atmospheric model — but DEMO4 treats Mg-I in LTE. For **RABD** see Section 17.)

(Section 99 - last revised: 2007 Feb 05)