Atomic Data and Analysis Structure

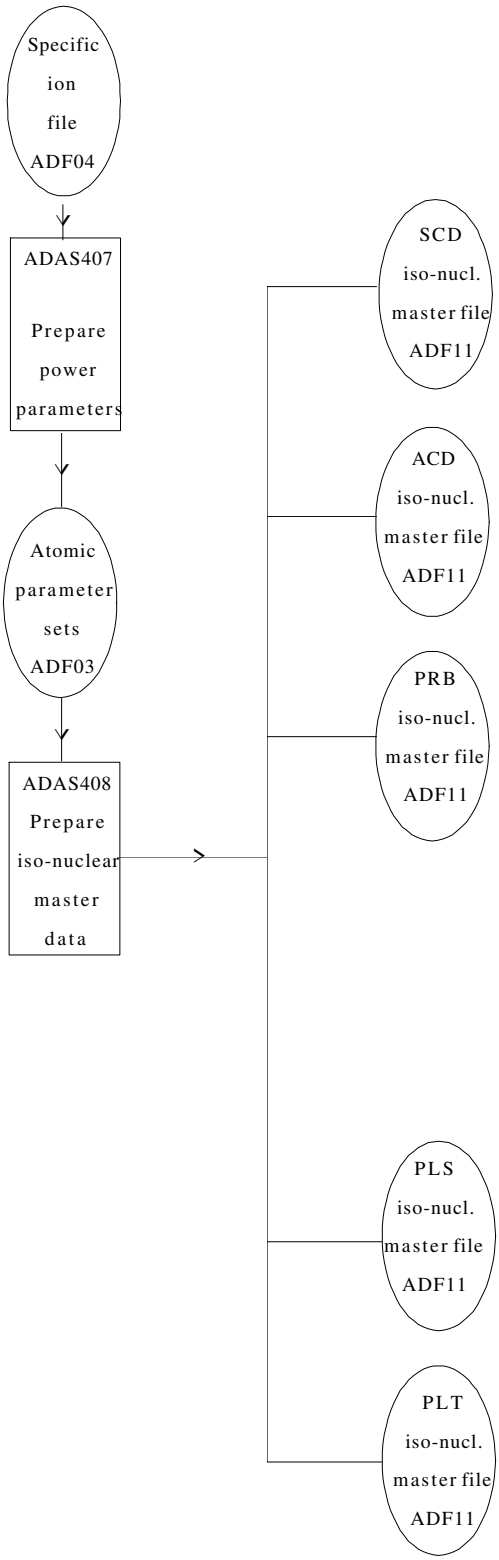
Calculating a simple ionisation balance

In the previous section, we have described the *iso-nuclear master files* in ADAS of type ADF11 including collisional radiative ionisation coefficients (SCD), free electron recombination coefficients (ACD), charge exchange recombination coefficients (CCD), free electron recombination + cascade + bremsstrahlung power coefficients (PRB), charge exchange recombination + cascade power coefficients (PRC) and low level line power coefficients (PLT). Formerly simple analytic approximate forms, applying only to the unresolved picture were used to generate such data rapidly in each plasma transport calculation. For complex atoms with many ionisation stages and quick but less precise studies, these methods remain useful. The programs ADAS407 and ADAS408 allow rapid preparation of unresolved, state to stage ADF11 coefficients of the above types using such approximate methods.

Specific ion files of type ADF04 provide the fundamental collections of energy levels, transition probabilities and collisional rate coefficients which allow detailed excited population calculations and then production of collisional radiative coefficients. The ADAS database contains many such files however complete coverage of all possible species at the highest accuracy levels is not possible. As a background to ADAS, particular atomic structure and collision codes have been set up to mass produce specific ion files. These automatically generated files are less accurate than individually prepared and assessed files. However they are highly structured with special alphanumeric conventions for configurations etc. recognisable by ADAS407. ADAS407 can glean extra information from such specific ion files to obtain parameters of the approximate forms mentioned in the first paragraph which it stores in ADAS data format ADF03 by iso-nuclear sequence. Incidentally, the automatically generated specific ion files can be recognised in the central ADAS database since they have directory names like */../adas/adf04/copmm#..* and */../adas/adf04/copss#.*

ADAS408 simply accesses the ADF03 iso-nuclear parameter collection for an element and generates the ADF11 data over requested temperature and density ranges. It also allows the calculated radiated power functions to be modified by particular filters which might be present in actual radiated power measurements of the plasma.

Figure 3.0


Specific ion file ADF04
ADAS407 Prepare power parameters
Atomic parameter sets ADF03
ADAS408 Prepare iso-nuclear master data
SCD iso-nucl. master file ADF11
ACD iso-nucl. master file ADF11
PRB iso-nucl. master file ADF11
PLS iso-nucl. master file ADF11
PLT iso-nucl. master file ADF11

ADAS407: Iso-nuclear parameter sets - prepare optimised power parameters

The code analyses specific ion files to obtain moderate accuracy numerical zero density recombination, ionisation and radiated power loss coefficient data. It deduces parameters of approximate forms for these coefficients which may be used to generate standard iso-nuclear master files.

Background theory:

In section 3, the population processing codes of ADAS series 2 make use of *specific ion files*. These provide the complete fundamental collections of energy levels, transition probabilities and collisional rate coefficients required in detailed excited population and generalised collisional radiative calculations. The ADAS database contains many such files however complete coverage of all possible species at the highest accuracy levels is not possible. There remains the need to perform simpler analysis and provide more approximate coefficients which can be used easily in less critical areas and for data fill-in. As a background to ADAS, particular atomic structure and collision codes have been set-up to generate specific ion files automatically. These automatically generated files are less accurate than individually prepared and assessed files but can form the basis for satisfying the above need.

The two paths for moderate quality automatic specific ion file creation available at present are:

SUPERSTRUCTURE + IMPACT PARAMETER rate coefficients

COWAN STRUCTURE + BORN rate coefficients

giving files of group names

COPSS#<elem. nucl. charge>.DATA(SM#<ion>)

and

COPMM#<elem. nucl. charge>.DATA(LS#<ion>)

respectively.

The specific ion files created by these two methods have two special features, namely, the electron configuration for each indexed term is given as a symbolic string (called in ADAS the 'Eissner notation') equivalent to

$$n_1 l_1^{\zeta_1} n_2 l_2^{\zeta_2} \ldots\ldots n_m l_m^{\zeta_m}$$

Also, the field for the energies of individual orbitals used in the configurations under study must be present (see Appendix B4). These orbital energies are denoted by

$$\{\varepsilon_k : k = 1,..,m\}$$

Apart from this enhanced rigidity in the use of the optional term naming character field, these files are of the standard ADF04 format.

With this supplementary information, analysis of two such specific ion files corresponding to adjacent ionisation stages z (called the 'ionising' or 'recombined' ion) and $z+1$ (called the 'ionised', 'recombining' or 'parent' ion) allows extraction of a wide range of useful numerical rate coefficient data and parameters of approximate forms for them. Parameters are allowed in two forms, namely cases A and B. Further details are given in the description of ADAS408. A summary is given below as follows:

Total line radiated power analysis

With designation of a particular metastable, i_m, of the ionising ion, all collisional excitation transitions may be isolated from the specific ion file and their excitation rate coefficients, $q_{i_m \to j}(T_e)$ and transition energies $\Delta E_{i_m,j}$ deduced. At low density, it may be assumed that

all collisional excitations lead to radiative decay back to the initial metastable level (possibly indirectly) so that the total line radiated power coefficient is

$$P_{i_m;LT}(T_e) = \sum_j \Delta E_{i_m,j} q_{i_m \to j}(T_e) \qquad 3.7.1$$

This is obtained as a set of numerical values at the temperatures of the ionising specific ion file. Approximate forms for this (see section 5.8) assume that it can be represented by up to five dipole allowed, effective transition energy weighted excitation rates of simplified (Gaunt factor or Van Regemorter) form. The ionising specific ion file is analysed to obtain the oscillator strengths, transition energies and effective Gaunt factor of *allowed* transitions originating with the metastable i_m. These are associated into groups according to transition wavelength and a mean transition energy, summed oscillator strength and mean Gaunt factor for each group obtained as

$$\begin{aligned} f_{i_m \to B} &= \sum_{j \in B} f_{i_m \to j} \\ \Delta E_{i_m,B} &= (\sum_{j \in B} \Delta E_{i_m,j} f_{i_m \to j}) / f_{i_m \to B} \\ \overline{g}_{i_m,B} &= (\sum_{j \in B} \overline{g}_{i_m,j} f_{i_m \to j}) / f_{i_m \to B} \end{aligned} \qquad 3.7.2$$

The approximate radiated power coefficient for the group is

$$\begin{aligned} P_{i_m,B;LT}(T)_e &= \Delta E_{i_m,B} q^{(e)}_{i_m \to B}(T_e) \\ &= 2.18^{-18} (\Delta E_{i_m,B} / I_H) \\ &\quad 4.28^{-6} (I_H / kT_e)^{1/2} (I_H / \Delta E_{i_m,B}) f_{i_m \to B} \overline{g}_{i_m,B} e^{-\Delta E_{i_m,B}/kT_e} \quad Wcm^3 \end{aligned} \qquad 3.7.3$$

in case A and

$$\begin{aligned} P_{i_m,B;LT}(T)_e &= \Delta E_{i_m,B} q^{(e)}_{i_m \to B}(T_e) \\ &= 2.18^{-18} (\Delta E_{i_m,B} / I_H)\, 4.28^{-6} (I_H / kT_e)^{1/2} \\ &\quad (I_H / \Delta E_{i_m,B}) f_{i_m \to B} P(\Delta E_{i_m,B} / kT_e) e^{-\Delta E_{i_m,B}/kT_e} \quad Wcm^3 \end{aligned} \qquad 3.7.4$$

in case B with $P(\Delta E / kT_e)$, the Van Regemorter factor.

The whole approximate power coefficient is assembled as

$$P^{approx}_{i_m;LT}(T_e) = C \sum_B c_B P_{i_m,B;LT}(T_e) \qquad 3.7.5$$

In initial fit, C = 1 and c_B = 1 for all B; in simple fit, c_B = 1 for all B and C is adjusted to equal the exact power at a designated temperature; in optimum fit, C = 1 and the c_B are adjusted to give a least square deviation using a functional weighted to a designated temperature. In case A , the C and c_B coefficients are combined with the Gaunt factors to give revised effective Gaunt factors for each group.

Collisional ionisation analysis

The code obtains the ionisation rate coefficient for the lowest term, indexed by i_{sys}, of each spin system of the ionising ion associated with a particular parent metastable, indexed by i_{prt}, of the recombining ion. The Eissner configuration specification for level i_{sys}, is parsed to give the occupancies of each shell which are combined with the orbital energies to give the set

$$\{\zeta_k, \varepsilon_k : k = 1,..,m_{i_{sys}}\} \qquad 3.7.6$$

The ionisation energy of the outer shell is improved to

$$\overline{\varepsilon}_{m_{i_{sys}}} = E^{(z+1)}_{i_{prt}} - E^{(z)}_{i_{sys}} + I^{(z)} \qquad 3.7.7$$

with $I^{(z)}$ the ionisation potential of the ionising ion.

In case A, the ionisation rate coefficient is evaluated from the expression of Lotz as

$$S^{(z\to z+1)}_{i_{sys}\to i_{prt}}(T)_e = C\sum_{k=k_0}^{m_{i_{sys}}} 1.42^{-6}(I_H/kT_e)^{3/2} a_k \zeta_k [E_1(\varepsilon_k/kT_e)/(\varepsilon_k/kT_e) - b_k e^{c_k} E_1(\varepsilon_k/kT_e + c_k)/(\varepsilon_k/kT_e + c_k)] \quad cm^3 s^{-1} \qquad 3.7.8$$

The parameters a,b,c,ζ and range of the sum k are taken Lotz , when available, otherwise b=c=0 and ζ is taken from the analysis summarised in 4.7.6 above

In case B, the ionisation rate coefficient is evaluated from the expression of Burgess & Chidichimo as

$$S^{(z\to z+1)}_{i_{sys}\to i_{prt}}(T_e) = C\sum_{k=1}^{m_{i_{sys}}} 2.1715^{-8}\ \zeta_k (I_H/\varepsilon_k)^{3/2}(\varepsilon_k/kT_e)^{1/2} E_1(\varepsilon_k/kT_e)\, w \quad cm^3 s^{-1} \qquad 3.7.9$$

with

$$w = \{\ln(1.0 + kT_e/\varepsilon_k)\}^{\beta/(1.0+kT_e/\varepsilon_k)}$$

$$\beta = 0.25[\{(100z+91)/(4z+3)\}^{1/2} - 5] \qquad 3.7.10$$

In both cases A and B, the adjustable scale factor C = 1.

Radiative recombination analysis

The code obtains the recombination rate coefficient for a particular parent metastable, indexed by i_{prt}, of the recombining ion and a spin system of the recombined ion. For a specified parent metastable term, there is at most two recombined ion spin systems indexed by sys. Recombined ion terms of permissible spin system and of configuration differing from the parent metastable configuration by one electron are identified. The principal quantum shell of the additional electron in the recombined ion term is obtained by cross-matching of Eissner configuration specifications. This gives the sets

$$\{n_k, I^{(z)}_{k,i_{prt}}, w_k : k = 1,.., K_{sys,i_{prt}}\} \qquad 3.7.11$$

where $I_{k,i_{prt}}$ and w_k denote the binding energy with respect to the parent and the statistical weight of the term k. The fraction of principal quantum shells of the recombined ion not occupied by bound electrons, prior to recombination, called the *phase space availability factor*, is obtained as

$$Ph_{n,sys,i_{prt}} = 1 - (\sum_{k:n_k=n} w_k)/w_{i_{prt}} n^2 \qquad 3.7.12$$

and an effective principal quantum number for the lowest accessible n-shell, $n_{sys,i_{prt}}$

$$\nu_{n,sys,i_{prt}} = \sqrt{(\sum_{k:n_k=n} w_k) z_1^2 I_H / (\sum_{k:n_k=n} w_k I_{k,i_{prt}})} \qquad 3.7.13$$

The recombination coefficient is then evaluated from the expression

$$\alpha_{i_{prt}}^{(z+1\to z)}(T_e) = scale(z_1^2 I_H / kT_e \nu_0^2)^{edisp}\, \alpha^H(\nu_0) + \sum_{n>n_0+1} \alpha^H(n_n)$$

$$= [2.6^{-14}] z_1 (z_1^2 I_H / kT_e)^{1/2} \{ \frac{2\, phfrac}{\nu_0} (z_1^2 I_H / kT_e \nu_0^2)\, EEI(z_1^2 I_H / kT_e \nu_0^2)$$

$$+ \sum_{n>n_0+1} \frac{2}{n} (z_1^2 I_H / kT_e n^2)\, EEI(z_1^2 I_H / kT_e n^2) \} \quad cm^3 s^{-1}$$

3.7.14

where ν_0 denotes $\nu_{n,sys,i_{prt}}$, n_0 denotes $n_{sys,i_{prt}}$ and $phfrac$ denotes $Ph_{n,sys,i_{prt}}$.

The scale factor adjustment, *scale*, and energy displacement adjustment, *edisp*, are set to 1 and 0 respectively. The above coefficients are multiplied by a spin system weight factor to give the final coefficients as

$$\alpha_{i_{prt}\to sys}^{(z+1\to z)}(T_e) = [(2S_{sys}+1)/2(2S_{i_{prt}}+1)]\alpha_{i_{prt}}^{(z+1\to z)}(T_e) \qquad 3.7.15$$

For case A parameters, expression 3.7.14 is simplified with *scale*=1, *edisp*=0 and n_0 replacing ν_0. For recombination of metastable parents other than the lowest, auto-ionisation of the recombined ion is energetically allowed for sufficiently excited states. The auto-ionisation cut-off n-shell is obtained from the differences of the parent energy and that of the ground parent as

$$n_{cut,i_{prt}} = INT\{\sqrt{z_1^2 I_H / (E_{i_{prt}}^{(z+1)} - E_1^{(z+1)})}\} + 1 \qquad 3.7.16$$

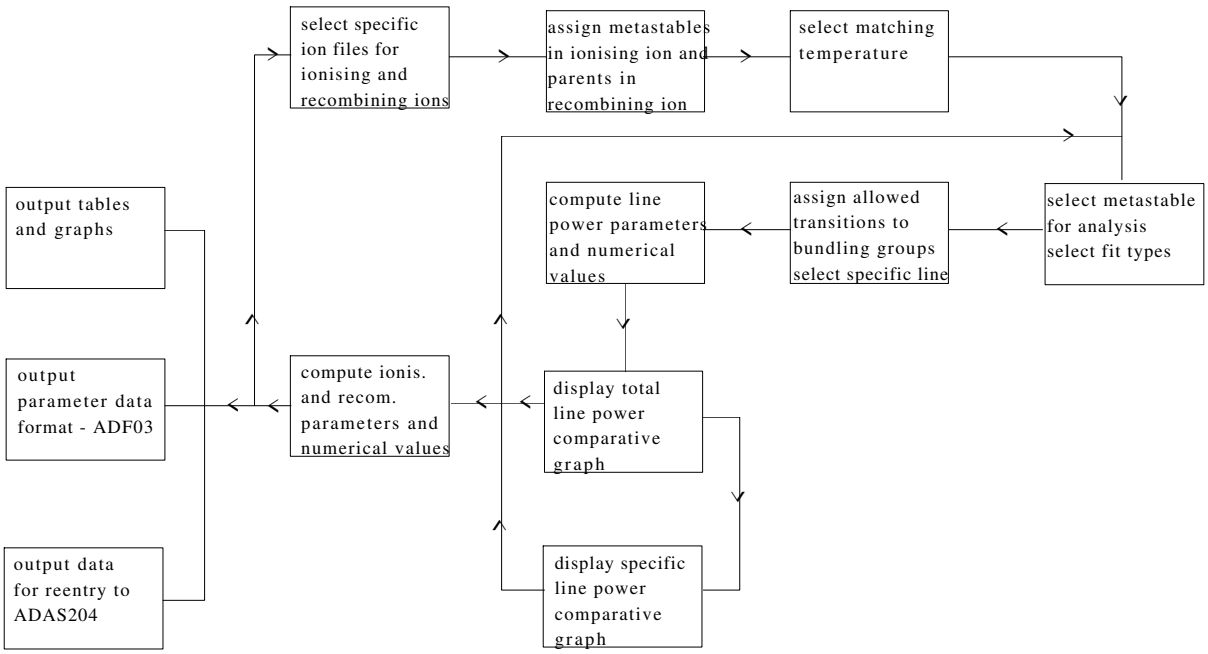
Dielectronic recombination analysis

With designation of a particular parent metastable, i_{prt}, of the ionising ion, all dipole allowed transitions from that metastable may be isolated from the recombining specific ion file, and the oscillator strengths $f_{i_{prt}\to k}$ and transition energies $\Delta E_{i_{prt},k}$ deduced. From examination of the configurations of the upper and lower terms using the Eissner specifications (cf. ADAS103), the parent transition type
is obtained.

Program steps:

These are summarised in figure 3.7.

Figure 3.7



Interactive parameter comments:

The **file selection window** appears first as illustrated below. *adf04* is the appropriate format for use by the program ADAS407 (ADAS User Manual, *appxb-04*). ADAS407 requires two such files, namely, for the 'Ionising Ion' and the 'Ionised Ion'. If you wish to use personal data of this type, then as usual it should be held in a similar file structure to central ADAS with your identifier replacing the first *adas*, but in addition it must have the configuration fields in 'Eissner' notation and the orbital binding energy fields not empty.

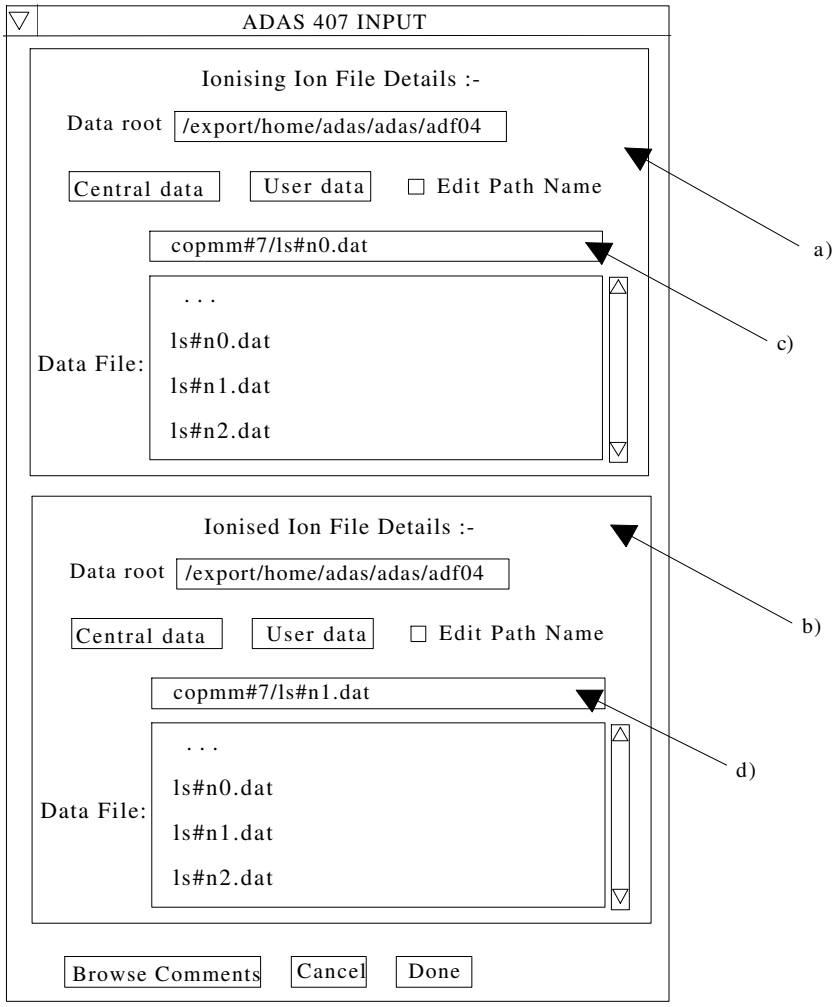
1. The sub-window for the ionising ion a) is upper one. A Data root path to the correct data type *adf04* appears automatically a). Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data.

2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

3. Available sub-directories are shown in the large file display window. Scroll bars appear if the number of entries exceed the file display window size.

4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual data-files are presented for selection. Data-files all have the termination *.dat*. Note that data-sets in sub-directories of the form */copss* and */copmm* are the only ones guaranteed to work.

5. When an ionising ion has been chosen, then the corresponding ionised ion has to be chosen in sub-window b). ADAS407 creates the expected file name and displays it at c) if it exists. This name can be over-ridden in the usual manner.



The **processing options window** has the appearance shown below

6. At the top of the window, an arbitrary title may be given for the case being processed. Sub-windows for the ionising and ionised ions appear side by side below this at b) and c). Summary data of the ions and the files opened are given first. The button *Browse Comments* in each sub-window again allows display of the information field section at the foot of the named ion file, if it exists.

7. The states of the ionising and ionised ions to be treated as metastable must then be decided. For the ionising ion, we call these the metastables and for the ionised ion, the parents. Click on the *Selection* button to see the full level list available for the ion. Click the toggle button opposite each level you wish switch on (or off) as a metastable. Notice the appearance of the configuration specification part of the level designation at b) and c). The '21522533' at b) means $1s^2 2s^2 2p^3$ in 'Eissner notation' (see the ADAS User Manual for more details).

8. At b) click on the particular driving metastable whose associated radiated power loss is to be analysed and displayed. In the lower group of sub-windows, this choice appears at d). In this sub-window, below the metastable index information a display window and associated selection window is present. The display window e) shows all the dipole collisional transitions in the ionising ion *adf04* file linked to selected metastable. The oscillator strength and wavelength of each transition is given.

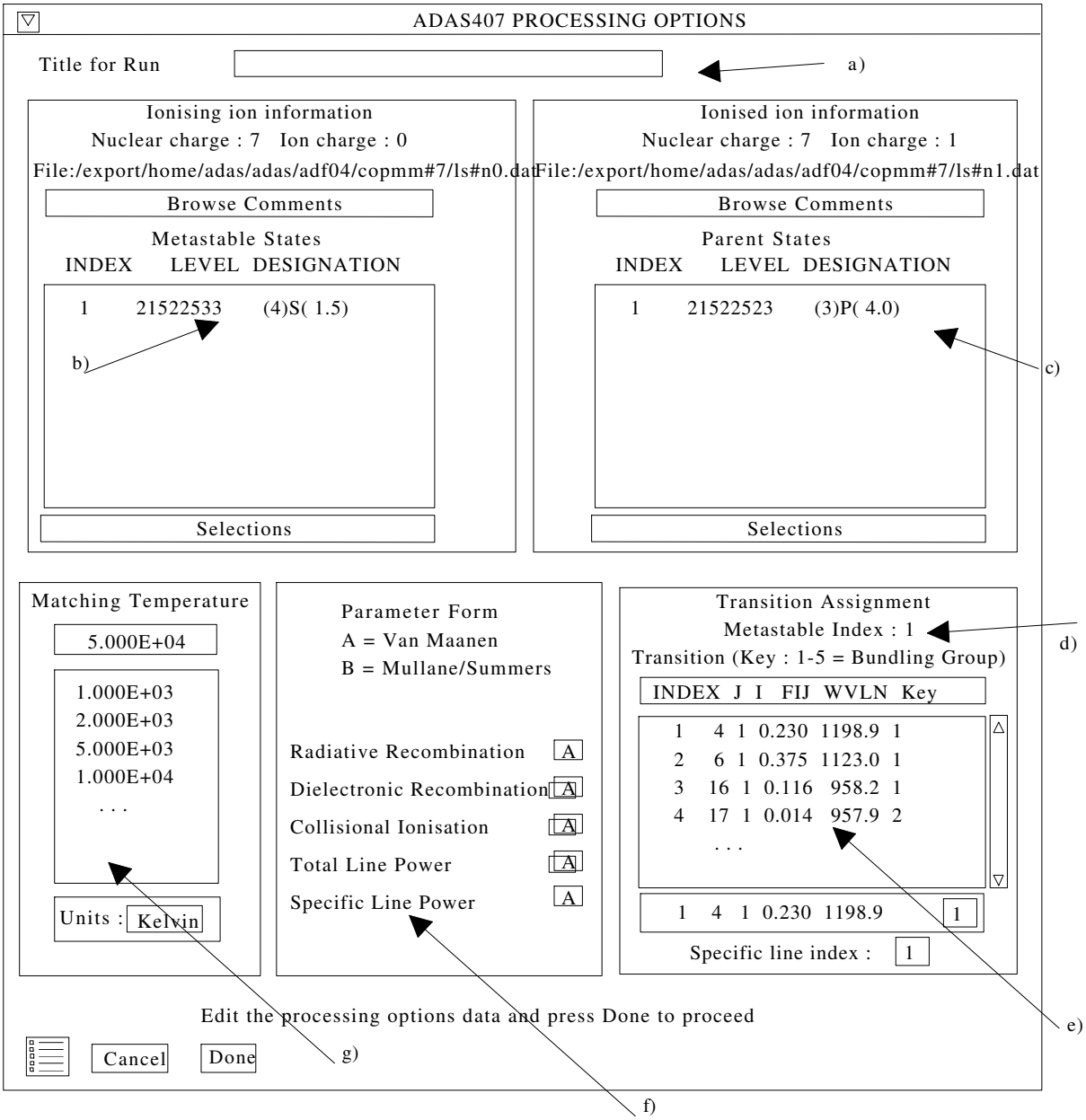
9. ADAS407 seeks to represent the total radiated power driven by the selected metastable by that from up to five effective dipole transitions, called bundling groups. You must associate each transition in the display window with a bundling group. This is usually done by grouping those of similar wavelength. Mostly one or two bundling groups is sufficient. Click on a transition. It appears in the selection window below the display window. Enter the bundling group index in the small editable box at the right side and press *return*. The group index ('Key') appears in

the display window along side the transition and the next transition appears in the selection window ready for assignment to a group.

10. The index of a specific line may be entered below the transition selection window. This is a line whose individual contribution to the total line radiated power you wish.

11. The various pieces of information obtainable from the pair of adjacent *adf04* files include the zero density radiative recombination coefficient, zero-density dielectronic recombination coefficient, the direct collisional ionisation coefficient, total zero-density line power radiative loss coefficient and the radiated power coefficient for the one selected transition (cf. 2.3.6 above). These are listed in the sub-window at f). Simple approximate forms are used to obtain these coefficients. For most of the coefficients an 'A' and 'B' choice of approximate forms are available. The 'A' forms have been used quite widely in fusion historically. The 'B' forms are better but may sometimes be unstable in fitting. We are in the process of tightening these up. Click on the selection button to the right of the type of coefficient at f) to drop down the A or B choice menu.

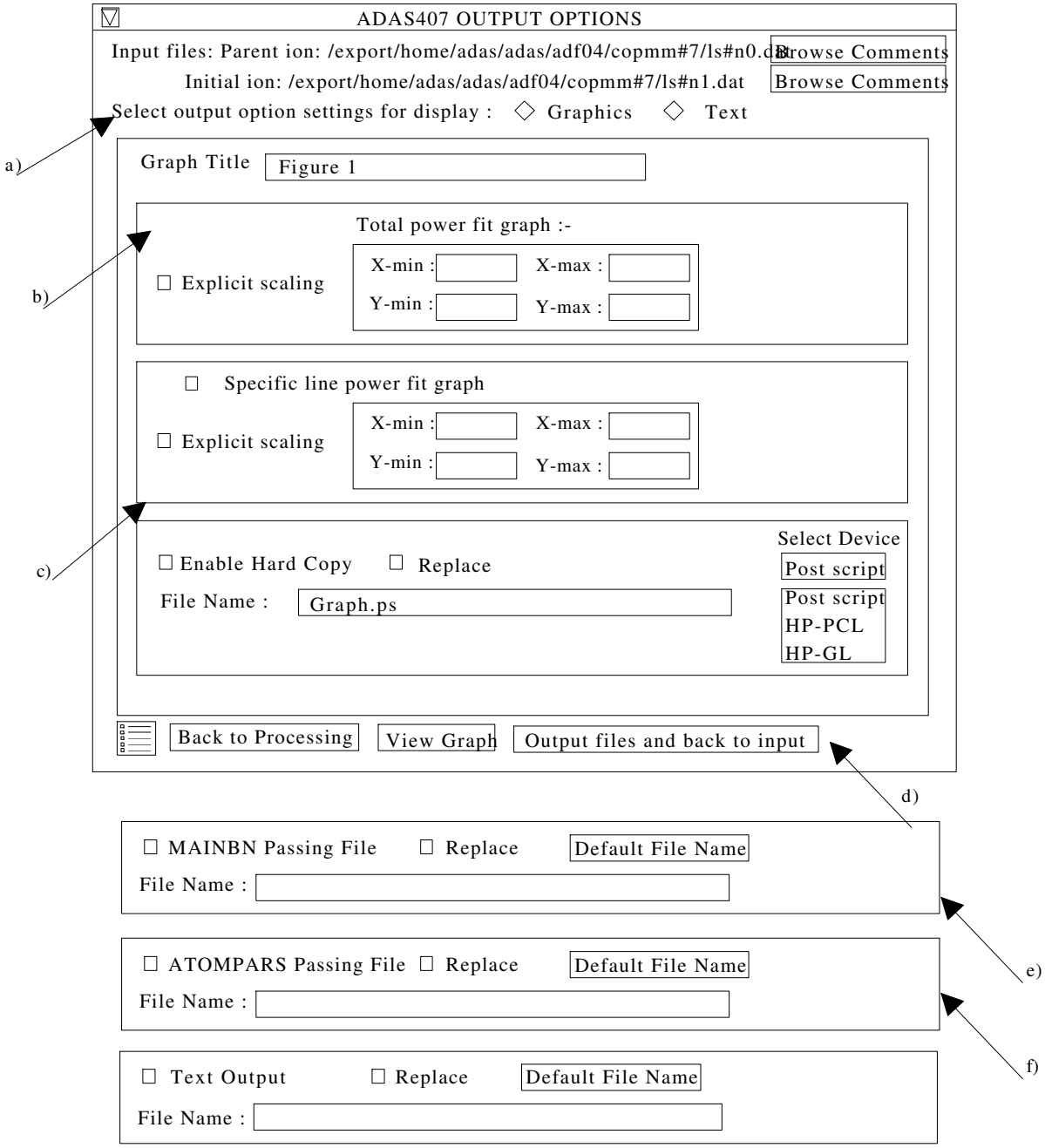
12. For the total zero density line radiated power, the specific ion files allow quite an accurate numerical estimate. Choose an electron temperature in the sub-window g) at which you wish the approximate form and accurate numerical values to agree.



13. The *Exit to Menu* icon is present in ADAS407. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **output options window** is shown below. Broadly it follows the pattern of other ADAS interrogation codes. However since a number of graphs and text outputs are possible, the window has been designed to avoid too much complexity on screen.

14. As usual, the input specific ion files under analysis are shown and can be browsed. Two buttons have been added at a), namely, *Graphics* and *Text*. Activate *Graphics* and the standard graphical output sub-window appears. Activate *Text* and the standard text file output sub-windows appears instead.



15. In the Graphics case, there are two types of graph, namely, the total radiated power fit graph b) and the specific line power graph c). The former is mandatory and the latter optional. Click the appropriate box in window c) if you wish the specific line power fit graph. Default scaling of the chosen graph may be over-ridden by appropriate selections. Below this the usual hard copy may be enabled and a choice of type of output device made.

16. In the Text case, three output files are permitted, namely, the standard line printer text output file summarising the interrogation, the 'MAINBN' file at e) and the 'ATOMPARS' file at f). These are passing files which are placed by default in your */pass* directory as *mainbn.pass* and *atompars.pass*. The MAINBN file is the driving file for ADAS204. The ATOMPARS file is for use by ADAS408 and is of standard *adf03* type. The usual *Replace* and *Default File Name* buttons are present for all the output files.

17. Various completion buttons are available at d). Click the *View Graph* button to show the graph. *Back to Processing* returns you to the previous window for choice of another transition for analysis. Note that the settings from analyses carried out by you are accumulated. Click the *Output files and back to input* button to write the

MAINBN and ATOMPARS passing file and then return to the input options window. In practise, this is the most convenient option since we usually carry on and process all of the ions of an iso-nuclear sequence in succession, assembling thereby a complete ATOMPARS file for an element in one go. The *Exit to Menu* icon takes you directly to the ADAS4 series menu.

Illustration:

Figure 3.7a

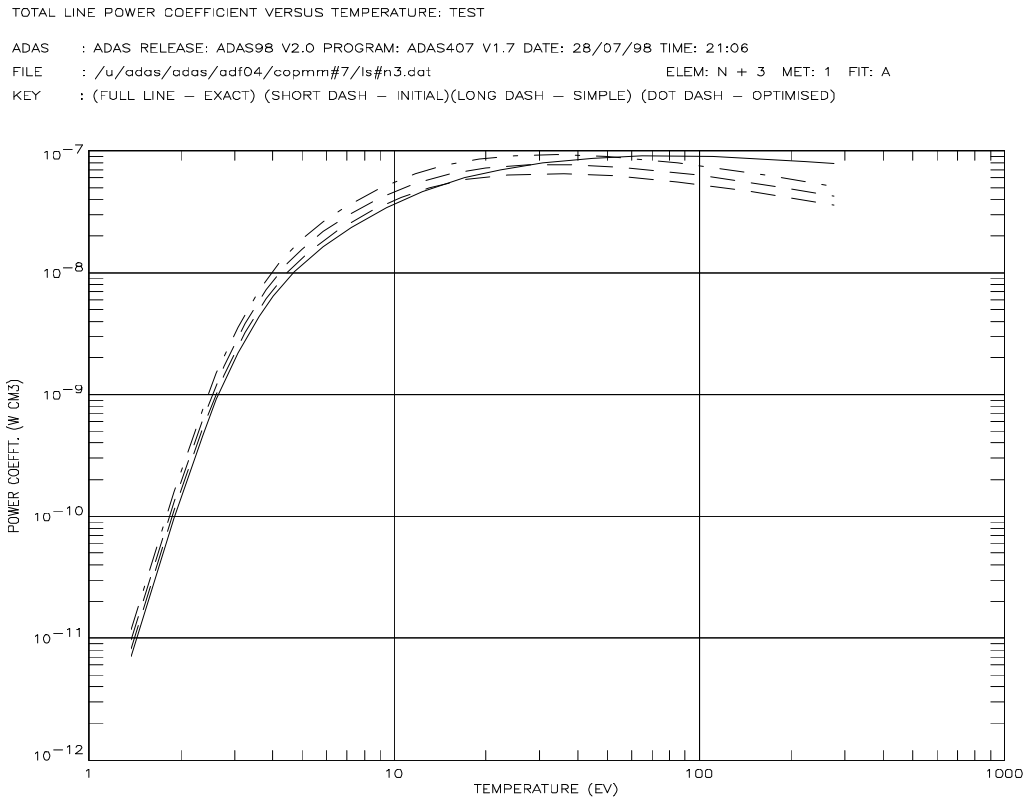


Figure 3.7b

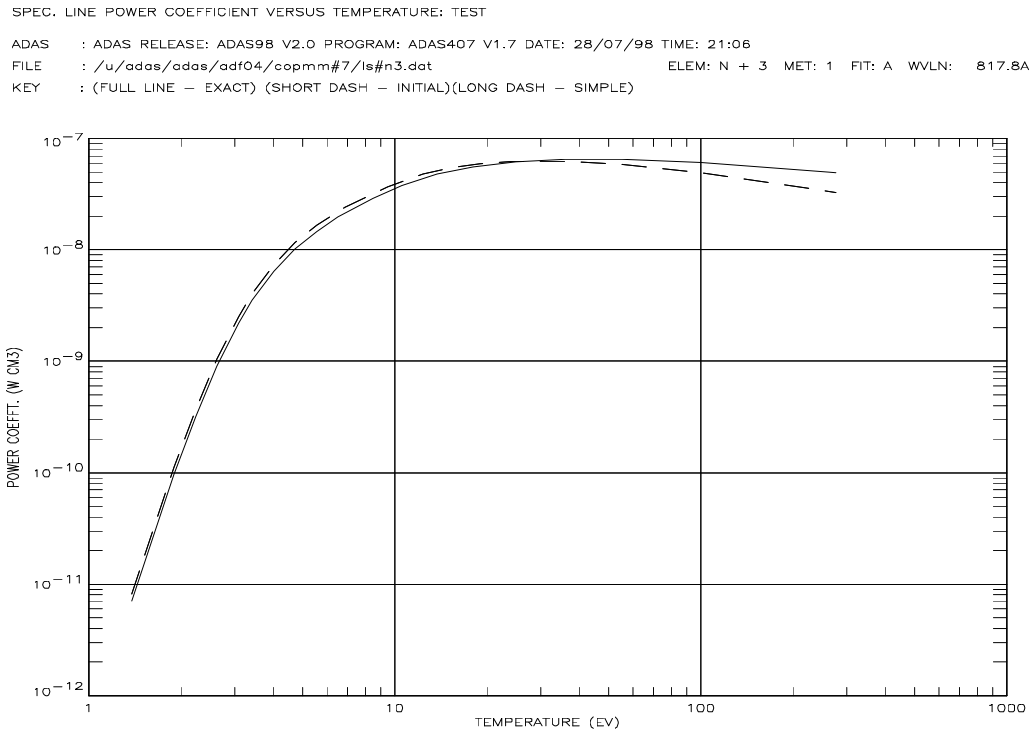


Table 3.7a

```
******************** TABULAR OUTPUT FROM  PARAMETER GENERATION  PROGRAM: ADAS407 - DATE: 28/07/98 ********************


INPUT INITIAL ION COPASE FILE NAME: /u/adas/adas/adf04/copmm#7/ls#n2.dat
 INPUT PARENT  ION COPASE FILE NAME: /u/adas/adas/adf04/copmm#7/ls#n3.dat


 ION      NUCLEAR         RECOMBINING      ------- IONIZATION POTENTIAL -------
         CHARGE (Z0)     ION CHARGE (Z1)    (wave number <cm-1>)      (rydbergs)
 ---------------------------------------------------------------------------
 N + 2         7                3                  382704.           3.4874611



------------------------------------------------------- ENERGY LEVELS ------------------------------------------------------------
  INDEX    CONFIGURATION    (2S+1)L(J)       ----- ENERGY RELATIVE TO LEVEL 1 ------    ENERGY RELATIVE TO IONISATION POTENTIAL
                                             (wave number <cm-1>)     (rydbergs)        (wave number <cm-1>)     (rydbergs)
 ---------------------------------------------------------------------------------------------------------------------------------
    1  22513               (2)1(   2.5)                  0.            .0000000              382704.           3.4874611
    2  12523               (4)1(   5.5)              65997.            .6014129              316706.           2.8860482
                    .          .      .
   30  12513516            (2)3(   6.5)             389676.           3.5509948               -6972.           -.0635337
   31  12513516            (2)2(   4.5)             389938.           3.5533887               -7235.           -.0659276
   32  12513516            (2)1(   2.5)             395110.           3.6005140              -12406.           -.1130529


-- INPUT COPASE FILE TEMPERATURES: (TE=TP=TH) --
 INDEX    (kelvin)         (eV)         (reduced)
 ------------------------------------------------
   1      9.00D+03      7.76D-01      1.00D+03
   2      1.80D+04      1.55D+00      2.00D+03
   3      4.50D+04      3.88D+00      5.00D+03
   4      9.00D+04      7.76D+00      1.00D+04
   5      1.80D+05      1.55D+01      2.00D+04
   6      4.50D+05      3.88D+01      5.00D+04
   7      9.00D+05      7.76D+01      1.00D+05
   8      1.80D+06      1.55D+02      2.00D+05


INPUT COPASE FILE INFORMATION:
 ------------------------------

NUMBER OF ELECTRON IMPACT TRANSITIONS    = 488
 NUMBER OF PROTON   IMPACT TRANSITIONS    =   0
 NUMBER OF CHARGE EXCHANGE RECOMBINATIONS =   0
 NUMBER OF FREE   ELECTRON RECOMBINATIONS =   0


SELECTED PARENT/SPIN SYSTEM COMBINATIONS FOR N + 2
```

RECOMBINING ION				RECOMBINED ION		
PARENT INDEX	LEVEL INDEX	PARENT TERM	PARENT MULTIPLICITY	SYSTEM INDEX	SYSTEM MULTIPLICITY	SPIN WT. FRACTION
1	1	1S	1	1	2	1.000
2	2	3P	3	1	2	.333
2	2	3P	3	2	4	.667

ORBITAL ASSIGMENTS AND ENERGIES FOR N + 2

ORBITAL INDEX	EISSNER SYMBOL	N	L	EFFECTIVE PRINC.QU.NO.
1	1	1	0	.515
2	2	2	0	1.397
3	3	2	1	1.581
4	4	3	0	2.554
5	5	3	1	2.750
6	6	3	2	3.062

TRANSITION AND POWER ANALYSIS FOR METASTABLE 1 LEVEL INDEX = 1

					TRANSITION ANALYSIS							
I1	I2	OSCIL STREN	WVLN (A)	BNDL INDX	TE(K)= 9.00D+03	1.80D+04	4.50D+04	9.00D+04	1.80D+05	4.50D+05	9.00D+05	1.80D+06
					G-BAR							
1	3	.146	967.7	1	.664	.667	.678	.698	.737	.832	.936	1.070
1	4	.087	807.5	1	.601	.604	.612	.628	.661	.743	.842	.969
1	5	.394	716.2	1	.583	.583	.590	.605	.635	.709	.802	.924
1	8	.045	428.2	2	.143	.144	.147	.152	.162	.198	.251	.334
1	11	.502	355.3	2	.223	.224	.226	.231	.241	.275	.328	.409
1	16	.073	315.9	2	.084	.084	.085	.087	.092	.110	.143	.200
1	18	.093	307.5	2	.101	.101	.102	.105	.109	.128	.160	.218
1	19	.012	302.5	2	.160	.160	.161	.163	.168	.186	.218	.276
1	27	.005	269.5	2	.366	.366	.366	.367	.369	.378	.398	.438
1	28	.009	268.1	2	.203	.204	.205	.206	.211	.228	.260	.316
1	29	.008	265.1	2	.042	.043	.043	.045	.048	.061	.085	.131

NUMBER OF TRANSITION BUNDLES = 2
TYPE OF FITTING APPROXIMATION = A
TEMPERATURE INDEX FOR MATCH = 4

	TOTAL LINE POWER ANALYSIS							
APPROXIMATION	TE(K)= 9.00D+03	1.80D+04	4.50D+04	9.00D+04	1.80D+05	4.50D+05	9.00D+05	1.80D+06
	POWER COEFFICIENT (RYD CM3 S-1)							
EXACT VALUE	8.76D-15	2.89D-11	4.34D-09	2.34D-08	5.48D-08	8.74D-08	9.42D-08	8.99D-08
INITIAL FIT	5.74D-16	1.22D-11	3.76D-09	2.15D-08	4.56D-08	5.92D-08	5.42D-08	4.38D-08
SIMPLE FIT	6.26D-16	1.33D-11	4.10D-09	2.34D-08	4.97D-08	6.46D-08	5.91D-08	4.77D-08
OPTIMUM FIT	9.39D-16	2.00D-11	6.15D-09	3.48D-08	7.27D-08	9.22D-08	8.34D-08	6.69D-08

SCALING FOR ATOMPARS FILE = SIMPLE FIT
ERROR AT 7.755D-01 eV = -92.85%
ERROR AT 1.551D+02 eV = -46.88%

SCALING SUMMARY							
BNDL INDX	DE-POW (eV)	F-POW	G-POW	SCALE INITIAL	SCALE SIMPLE	SCALE OPTIM.	G-SCLD
1	15.993	.626	.630	1.000	1.090	1.635	.686
2	36.066	.745	.194	1.000	1.090	1.196	.211

COLLISIONAL IONISATION PARAMETERS FOR N + 2 TO N + 3

PARENT INDEX	SYSTEM INDEX	IONIS. GRP. MULTIPLIER	ORBITAL INDEX	ION. ENER. (RYD)	EQUIV. ELECTRONS
1	1	1.00000	1	33.930	2
			2	4.610	2
			3	3.487	1
2	1	1.00000	1	33.930	2
			2	4.610	1
			3	3.113	2
2	2	1.00000	1	33.930	2
			2	4.610	1
			3	3.454	2

PARENT INDEX	SYSTEM INDEX	TE(K)= 4.50D+03	6.30D+03	9.00D+03	1.35D+04	1.80D+04	2.70D+04	4.50D+04	6.30D+04	9.00D+04	1.35D+05
		IONISATION COEFFICIENT (CM3 S-1)									
1	1	4.18D-63	7.62D-48	2.24D-36	1.99D-27	6.18D-23	2.04D-18	9.29D-15	3.74D-13	6.54D-12	6.71D-11
2	1	5.26D-57	2.25D-43	3.98D-33	3.97D-25	4.13D-21	4.54D-17	8.44D-14	2.24D-12	2.74D-11	2.03D-10

```
     2       2                          2.78D-62 3.61D-47 8.25D-36 6.02D-27 1.69D-22 5.05D-18 2.09D-14 7.88D-13 1.26D-11 1.16D-10


RADIATIVE RECOMBINATION PARAMETERS FOR N + 3 TO N + 2

-------------------------------------------------------------------------------
  PARENT  SYSTEM  LOWEST  EFFECTIVE  PHASE SPACE  ENER. DISP.      SCALE     CUT-OFF
  INDEX   INDEX      N         N         FACTOR        (RYD)        FACTOR       N
 -------------------------------------------------------------------------------
     1       1       2      1.60662         .750         .000       1.000     1000
     2       1       2      1.73729         .750         .000       1.000        4
     2       2       2      1.61443         .750         .000       1.000        4

-------------------------------------------------------------------------------------------------------------------------------
   PARENT  SYSTEM  NOTES           TE(K)= 4.50D+03 6.30D+03 9.00D+03 1.35D+04 1.80D+04 2.70D+04 4.50D+04 6.30D+04 9.00D+04 1.35D+05
   INDEX   INDEX                          -------------------------- RECOMBINATION COEFFICIENT (CM3 S-1) --------------------------
 -------------------------------------------------------------------------------------------------------------------------------
     1       1    N=NMIN *               1.28D-12 1.08D-12 9.01D-13 7.30D-13 6.27D-13 5.05D-13 3.80D-13 3.13D-13 2.53D-13 1.96D-13
     1       1    N>NMIN *               6.22D-12 4.88D-12 3.75D-12 2.75D-12 2.19D-12 1.58D-12 1.03D-12 7.66D-13 5.54D-13 3.78D-13
     1       1    TOTAL                  7.51D-12 5.96D-12 4.65D-12 3.48D-12 2.82D-12 2.09D-12 1.41D-12 1.08D-12 8.07D-13 5.74D-13
     2       1    N=NMIN *               1.19D-12 9.98D-13 8.31D-13 6.72D-13 5.77D-13 4.63D-13 3.48D-13 2.85D-13 2.29D-13 1.76D-13
     2       1    N>NMIN *               1.56D-12 1.30D-12 1.07D-12 8.47D-13 7.13D-13 5.54D-13 3.94D-13 3.10D-13 2.37D-13 1.71D-13
     2       1    TOTAL                  9.15D-13 7.66D-13 6.33D-13 5.06D-13 4.30D-13 3.39D-13 2.47D-13 1.98D-13 1.55D-13 1.16D-13
     2       2    N=NMIN *               1.28D-12 1.08D-12 8.96D-13 7.26D-13 6.24D-13 5.02D-13 3.78D-13 3.11D-13 2.51D-13 1.94D-13
     2       2    N>NMIN *               1.56D-12 1.30D-12 1.07D-12 8.47D-13 7.13D-13 5.54D-13 3.94D-13 3.10D-13 2.37D-13 1.71D-13
     2       2    TOTAL                  1.89D-12 1.58D-12 1.31D-12 1.05D-12 8.91D-13 7.04D-13 5.15D-13 4.14D-13 3.25D-13 2.43D-13


DIELECTRONIC RECOMBINATION PARAMETERS FOR N + 3 TO N + 2

-------------------------------------------------------------------------------------------------------------------------------
  PARENT  NO. OF  TRANS.  TRANS.  LOWEST  EFFECTIVE  PHASE SP.  CUT-OFF    EIJ        FIJ     ENER. DISP.    SCALE   BETHE COR.
  INDEX   TRANS.  INDEX    TYPE      N         N        FACTOR       N      (RYD)                    (RYD)       FACTOR    FACTOR
 -------------------------------------------------------------------------------------------------------------------------------
     1       2       1       4       3      3.06186      1.000   1000     1.11425      .64076      .00000     1.00000      .00000
                     2       2       2      1.58114       .875   1000     3.69380      .34765      .00000     1.00000      .00000
     2       4       1       4       3      3.06186      1.000      4      .97681      .24400      .00000     1.00000      .00000
                     2       3       3      2.55377       .944      4     2.82299      .01547      .00000     1.00000      .00000
                     3       2       3      2.55377       .944      4     3.20875     1.02377      .00000     1.00000      .00000
                     4       2       3      2.55377       .944      4     3.82270      .16602      .00000     1.00000      .00000

-------------------------------------------------------------------------------------------------------------------------------
   PARENT  SYSTEM  TRANS.  NOTES   TE(K)= 4.50D+03 6.30D+03 9.00D+03 1.35D+04 1.80D+04 2.70D+04 4.50D+04 6.30D+04 9.00D+04 1.35D+05
   INDEX   INDEX   INDEX                  -------------------------- RECOMBINATION COEFFICIENT (CM3 S-1) --------------------------
 -------------------------------------------------------------------------------------------------------------------------------
     1               1          *        3.52D-13 9.98D-13 1.87D-12 2.57D-12 3.04D-12 6.68D-12 2.58D-11 4.42D-11 5.76D-11 5.89D-11
     1               2          *        6.81D-12 1.05D-11 1.25D-11 1.17D-11 1.00D-11 7.19D-12 4.16D-12 2.82D-12 2.23D-12 3.08D-12
     1                    TOTAL  *        7.16D-12 1.15D-11 1.43D-11 1.43D-11 1.31D-11 1.39D-11 3.00D-11 4.70D-11 5.99D-11 6.19D-11
     1       1                           7.16D-12 1.15D-11 1.43D-11 1.43D-11 1.31D-11 1.39D-11 3.00D-11 4.70D-11 5.99D-11 6.19D-11
     2               1          *        1.28D-11 9.15D-12 6.09D-12 3.71D-12 2.63D-12 1.67D-12 9.92D-13 7.00D-13 4.72D-13 2.92D-13
     2               2          *        1.18D-33 1.36D-27 4.11D-23 1.03D-19 4.57D-18 1.71D-16 2.53D-15 7.28D-15 1.47D-14 2.21D-14
     2               3          *        1.34D-37 7.41D-30 4.06D-24 9.76D-20 1.33D-17 1.54D-15 5.64D-14 2.39D-13 6.44D-13 1.21D-12
     2               4          *        1.36D-47 3.54D-37 1.96D-29 1.71D-23 1.40D-20 9.79D-18 1.50D-15 1.18D-14 5.03D-14 1.36D-13
     2                    TOTAL  *        1.28D-11 9.15D-12 6.09D-12 3.71D-12 2.63D-12 1.67D-12 1.05D-12 9.58D-13 1.18D-12 1.66D-12
     2       1                           4.27D-12 3.05D-12 2.03D-12 1.24D-12 8.75D-13 5.58D-13 3.51D-13 3.19D-13 3.94D-13 5.55D-13
     2       2                           8.53D-12 6.10D-12 4.06D-12 2.48D-12 1.75D-12 1.12D-12 7.01D-13 6.39D-13 7.88D-13 1.11D-12

NOTES:  * ==> EXCLUDES SPIN WT. FACTOR
```

Table 3.7b

```
&FILINFO  NUCCHG= 7, NPARNT=2, SEQ='b ', XRMEMB='n2n     ',  &END
   24   24  9.00D+06  0.00D+00  3.00D+00  1.00D+00  1.00D+00  1.00D+00
    0    4    1    0
  2.19D+04  2.19D+05  2.19D+06  2.19D+07  2.19D+08  2.19D+09  6.56D+09
  2.19D+10  6.56D+10  2.19D+11  6.56D+11  2.19D+12  6.56D+12  2.19D+13
  6.56D+13  2.19D+14  6.56D+14  2.19D+15  6.56D+15  2.19D+16  6.56D+16
  2.19D+17  6.56D+17  2.19D+18
  4.50D+03  6.30D+03  9.00D+03  1.35D+04  1.80D+04  2.70D+04  4.50D+04
  6.30D+04  9.00D+04  1.35D+05  1.80D+05  2.70D+05  4.50D+05  6.30D+05
  9.00D+05  1.35D+06  1.80D+06  2.70D+06  4.50D+06  6.30D+06  9.00D+06
  1.35D+07  1.80D+07  2.70D+07
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  0.00D+00  0.00D+00  0.00D+00
  4.50D+03  6.30D+03  9.00D+03  1.35D+04  1.80D+04  2.70D+04  4.50D+04
  6.30D+04  9.00D+04  1.35D+05  1.80D+05  2.70D+05  4.50D+05  6.30D+05
  9.00D+05  1.35D+06  1.80D+06  2.70D+06  4.50D+06  6.30D+06  9.00D+06
  1.35D+07  1.80D+07  2.70D+07
  2.50D 04  0.00D 00
    1  520   24
    1    2    3    4    5    6    7    8    9   10   12   15   20   30
   40   50   70  100  150  200  250  300  400  500
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  0.00D+00  0.00D+00  0.00D+00
-------------------------------------------------------------------------
```

```
PRT= 1  TRMPRT=  (1S)   SPNPRT= 1  NCTPRT=1000 SYSG= 1  SPNSYS= 2
NMIN= 2   JDEF= 5     .472  .147  .082  .052  .036
    2   1.60662    .75000    .00000   1.00000
    2
 4    3   3.0619   1.0000 1000    .06964    .64076    .00000  0.00D+00
 2    2   1.5811    .8750 1000    .23086    .34765    .00000  0.00D+00
              FIT PARAMETERS FOR GP                  .00000   1.00000
    1    0    IBSEL1= 0
    JPRT= 1   PRTWHT= 1.000   IBSEL=  0
    JPRT= 2   PRTWHT=  .000   IBSEL=  0
    3
1.000    2   3.77000    2    .51222    1    .38749
  1.47D-11  1.75D-11  1.90D-11  1.78D-11  1.59D-11  1.60D-11  3.14D-11
  4.81D-11  6.07D-11  6.25D-11  5.74D-11  4.57D-11  3.01D-11  2.14D-11
  1.43D-11  8.68D-12  5.96D-12  3.44D-12  1.68D-12  1.03D-12  6.15D-13
  3.39D-13  2.22D-13  1.22D-13
  4.18D-63  7.62D-48  2.24D-36  1.99D-27  6.18D-23  2.04D-18  9.29D-15
  3.74D-13  6.54D-12  6.71D-11  2.27D-10  8.06D-10  2.34D-09  3.77D-09
  5.43D-09  7.21D-09  8.27D-09  9.41D-09  1.02D-08  1.04D-08  1.03D-08
  9.98D-09  9.63D-09  9.02D-09
----------
PRT= 2  TRMPRT=  (3P)   SPNPRT= 3  NCTPRT=   4 SYSG= 1  SPNSYS= 2
NMIN= 2   JDEF= 5     .472  .147  .082  .052  .036
    2   1.73729    .75000    .00000   1.00000
    4
 4    3   3.0619   1.0000 1000    .06105    .24400    .00000  0.00D+00
 3    3   2.5538    .9444 1000    .17644    .01547    .00000  0.00D+00
 2    3   2.5538    .9444 1000    .20055   1.02377    .00000  0.00D+00
 2    3   2.5538    .9444 1000    .23892    .16602    .00000  0.00D+00
              FIT PARAMETERS FOR GP                  .00000   1.00000
    1    0    IBSEL1= 0
    JPRT= 1   PRTWHT=  .000   IBSEL=  0
    JPRT= 2   PRTWHT= 1.000   IBSEL=  0
    3
1.000    2   3.77000    1    .51222    2    .34594
  5.18D-12  3.82D-12  2.66D-12  1.74D-12  1.31D-12  8.97D-13  5.98D-13
  5.18D-13  5.49D-13  6.70D-13  7.35D-13  7.22D-13  5.61D-13  4.27D-13
  2.99D-13  1.88D-13  1.32D-13  7.76D-14  3.87D-14  2.42D-14  1.46D-14
  8.17D-15  5.40D-15  3.00D-15
  5.26D-57  2.25D-43  3.98D-33  3.97D-25  4.13D-21  4.54D-17  8.44D-14
  2.24D-12  2.74D-11  2.03D-10  5.72D-10  1.67D-09  4.08D-09  6.07D-09
  8.20D-09  1.03D-08  1.16D-08  1.27D-08  1.34D-08  1.35D-08  1.32D-08
  1.27D-08  1.21D-08  1.13D-08
----------
PRT= 2  TRMPRT=  (3P)   SPNPRT= 3  NCTPRT=   4 SYSG= 2  SPNSYS= 4
NMIN= 2   JDEF= 5     .472  .147  .082  .052  .036
    2   1.61443    .75000    .00000   1.00000
    4
 4    3   3.0619   1.0000 1000    .06105    .24400    .00000  0.00D+00
 3    3   2.5538    .9444 1000    .17644    .01547    .00000  0.00D+00
 2    3   2.5538    .9444 1000    .20055   1.02377    .00000  0.00D+00
 2    3   2.5538    .9444 1000    .23892    .16602    .00000  0.00D+00
              FIT PARAMETERS FOR GP                  .00000   1.00000
    1    0    IBSEL1= 0
    JPRT= 1   PRTWHT=  .000   IBSEL=  0
    JPRT= 2   PRTWHT= 1.000   IBSEL=  0
    3
1.000    2   3.77000    1    .51222    2    .38375
  1.04D-11  7.68D-12  5.37D-12  3.52D-12  2.64D-12  1.82D-12  1.22D-12
  1.05D-12  1.11D-12  1.35D-12  1.48D-12  1.45D-12  1.13D-12  8.58D-13
  6.01D-13  3.79D-13  2.65D-13  1.57D-13  7.83D-14  4.90D-14  2.96D-14
  1.66D-14  1.10D-14  6.13D-15
  2.78D-62  3.61D-47  8.25D-36  6.02D-27  1.69D-22  5.05D-18  2.09D-14
  7.88D-13  1.26D-11  1.16D-10  3.64D-10  1.18D-09  3.17D-09  4.90D-09
  6.82D-09  8.81D-09  9.97D-09  1.12D-08  1.19D-08  1.20D-08  1.19D-08
  1.14D-08  1.10D-08  1.02D-08
-------------------------------------------------------------------------
&FILINFO  NUCCHG=-1, NPARNT=0, SEQ='??', XRMEMB='????????',  &END
```

Table 3.7c

```
7   ??   ??              1    0    0                                  ADF03
----------
    3    3    2    2    2
     RRC#A    0    0
              2    2
     DRC#A    2    0
              15.159      .641      .000    0    0
              50.253      .348      .000    1    1
     CIO#A    2    0    0
              47.446     4.500      .200      .600    1
              62.718     4.500      .200      .600    2
     PLT#A    2    0
              15.993      .626      .686    0
              36.066      .745      .211    1
     PLS#A    1    0   967.67
              12.812      .146      .698    0
----------
    4    4    3    3    3
     RRC#A    0    0
              2    1
```

```
     DRC#A    2    0
              59.612      .235      .000    1    1
              76.678      .068      .000    1    1
     CIO#A    2    0    0
              77.468     4.500      .000      .000    2
             491.677     4.500      .000      .000    2
     PLT#A    2    0
              15.159      .641      .911    0
              53.310      .465      .146    1
     PLS#A    1    0    817.83
              15.159      .641      .771    0
C-------------------------------------------------------------------------------
C
C  INFORMATION
C  -----------
C
C  PROCESSING CODE:  ADAS407
C  USER IDENTIFIER:  hps
C  DATE           :  28/07/98
C
C  RECOMBINED ION DATA SETS :
C                              1  /u/adas/adas/adf04/copmm#7/ls#n2.dat
C  RECOMBINED ION DATA SETS :
C                              2  /u/adas/adas/adf04/copmm#7/ls#n3.dat
C  RECOMBINING ION DATA SETS:
C                              1  /u/adas/adas/adf04/copmm#7/ls#n3.dat
C  RECOMBINING ION DATA SETS:
C                              2  /u/adas/adas/adf04/copmm#7/ls#n4.dat
C
C-------------------------------------------------------------------------------
```

Notes:

ADAS408: Iso-nuclear master data - prepare from iso-nuclear parameter sets

The program uses parametric forms for zero density recombination, ionisation and radiated power loss coefficients to prepare standard (unresolved, stage to stage) iso-nuclear master files for a particular element. The iso-nuclear master files may be prepared over arbitrary ranges of electron temperature and electron density

Background theory:

The practice in the past in fusion research has been to adopt a substantially simpler and more approximate approach to acquiring the atomic data for plasma models than that which forms the basis of the Atomic Data and Analysis Structure. This is the parametric approximate form approach. It assumes that

1. Simple parametric forms for atomic processes, which apply to any ion of any element, are available.
2. The low density coronal limit may be assumed in all circumstances.
3. Each ionisation stage of an element may be represented by its ground state alone.
4. Each ion may be assumed to experience two effective electron collisional excitations which can be used to represent adequately radiant power losses and dielectronic recombination.

These assumptions and approximations can not be sustained in modern fusion device studies. However the earlier procedures do have the merit of providing atomic data for modelling codes for virtually any element desired (unlike the selective nature of more refined data) as long as too searching questions are not asked. For this reason such data is still widely used. It is necessary that such data can still be generated for comparative purposes and low quality data fill-in. The Atomic Data and Analysis Structure is based on absolute numerical data and interpolation rather than parametric databases, since thereby no data constraint or precision limit is intrinsic to the structure and best available data of whatever type may be used. The ADAS408 code creates data sets of standard iso-nuclear master file organisation from the old parametric forms. The access subroutines to the iso-nuclear master files provided with ADAS allow a seamless switch to the Atomic Data and Analysis Structure with older calculations and assumptions still reproducible.

The following classes of data of standard type are generated:- the collisional-dielectronic recombination coefficient (ACD),the collisional-dielectronic ionisation coefficient (SCD), the collisional-radiative charge exchange recombination coefficient (CCD), the collisional-dielectronic recombination / cascade / bremsstrahlung radiated power coefficient (PRB), the collisional-radiative charge exchange recombination / cascade power coefficient (PRC), the collisional-radiative excitation total line power coefficient (PLT) and the collisional-radiative excitation specific line power coefficient (PLS). However, the data does not constitute true collisional-radiative coefficients. For the various classes, the most prevalent assumptions forced by the parametric forms are summarised below.

Mnemonic	Class simplification	Forms
ACD	zero density radiative + representative dielectronic parent transitions with a finite density cut-off	S
SCD	zero density ground state ionis. coefft.	S
CCD	total zero density coefft.	S
PRB	zero density recom./brems. + two dielectronic transition contributions with simplified energy loss per recombination	S
PRC	zero density with simplified energy loss per recombination.	S
PLT	effective excitations in coronal approximation.	S
PLS	single resonance line in coronal approximation	S

The parametric approximate forms for the above coefficient classes used historically are called here the (A) forms. From the considerations of section 2 of this manual and provided more accurate numerical data is available, some improvement both of the parametric forms and of the actual values of parameters used may be made. The improved parametric forms, called here the (B) forms are those which provide the basis for comparative assessment of new data is the ADAS series 1 codes. Both (A) and (B) parametric forms are allowed by the ADA407 code. They are as follow:

ACD: the coefficient is composed of a sum of radiative and dielectronic recombination parts

$$\alpha^{(z+1\to z)}(T_e, N_e) = \alpha_r(T_e, N_e) + \alpha_d(T_e, N_e) \qquad 3.8.1$$

(A) Hydrogenic formulae are used for radiative recombination with Gaunt factors unity. The ground principal quantum shell is adjusted with an effective principal number ν_0 and lowest shell occupancy factor $phfrac$. The Burgess zero density general formula is used for dielectronic recombination including two parent transitions only.

$$\begin{aligned}\alpha_r &= \alpha^H(n_0) + \sum_{n\geq n_0+1}^{n_G}\alpha^H(n_0) \\ &= [2.6^{-14}]z_1(z_1^2 I_H/kT_e)^{1/2}\{\frac{2\,phfrac}{n_0}(z_1^2 I_H/kT_e n_0^2)\,EEI(z_1^2 I_H/kT_e n_0^2) \\ &\quad + \sum_{n\geq n_0+1}^{n_G}\frac{2}{n}(z_1^2 I_H/kT_e n^2)\,EEI(z_1^2 I_H/kT_e n^2)\} \quad cm^3 s^{-1}\end{aligned}$$

3.8.2

where $z_1 = z+1$, n_0 is the principal quantum number of the valence shell of the ion of the recombined ion, $phfrac$ is the statistical weight fraction of the valence shell unoccupied before recombination and $EEi(x) = e^x E_1(x)$ with E_1 the first exponential integral. The principal quantum shell sum is terminated at

$$n_G = 126.0\{z_1^{12}(kT_e / I_H)(cm^{-6} / N_e^2)\}^{1/17} \qquad 3.8.3$$

The dielectronic recombination part is given by

$$\begin{aligned}\alpha_d &= [4.78^{-11}](z_1^{1/2}(z_1+1)^{5/2} / (z_1^2+13.4)^{1/2})(I_H / kT_e)^{3/2} D(T_e, N_e) \\ &\quad \sum_{j=1}^{2} f_j A(y_j) e^{-\overline{\Delta E_j}/kT_e} \quad cm^3 s^{-1}\end{aligned}$$

3.8.4

where the sum is over at most two parent transitions with oscillator strengths f_j and effective transition energies $\overline{\Delta E_j} = \Delta E_j / a$ with ΔE_j the transition energy and $a = 1.0 + 0.015\{z_1^3 / (z_1+1)^2\}$. The factor A and finite density reduction D depend on whether the parent transition is of '$\Delta n = 0$' type

$$D = n_t / (200 + n_t) \quad , \quad A(y) = y^{1/2} / (1 + 0.105y + 0.015y^2) \qquad 3.8.5$$

or of '$\Delta n = 1$' (excluding 1s initial parent states) type

$$\begin{aligned}&D = 0.0015[(z_1+1)n_t]^2 / (1 + 0.0015[(z_1+1)n_t]^2) \quad , \\ &A(y) = y^{1/2} / (2 + 0.41y + 0.06y^2)\end{aligned} \qquad 3.8.6$$

with $n_t = [5.57^{17}(cm^{-3} / N_e) z_1^6 (kT_e / I_H)^{1/2}]^{1/7}$ and $y_j = (\Delta E_j / I_H) / (z_1 + 1)$.

(B) The hydrogenic expression for radiative recombination to the lowest principal quantum shell uses the effective principal quantum number ν_0 for the shell and is improved by factors *scale* and *edisp* obtained from improved sources. The density dependent n-shell cut-off is not applied. The dielectronic coefficient is based on the Burgess zero density

general formula as for the $\Delta n = 0$ case above, adjusted to fit improved data with factors $scale_1, edisp_1, scale_2, edisp_2$. An extended set of parent transitions but combined into at most two groups.

$$\alpha_r = scale(z_1^2 I_H / kT_e \nu_0^2)^{edisp}\, \alpha^H(\nu_0) + \sum_{n \geq n_0+1} \alpha^H(n_n) \qquad 3.8.7$$

$$\begin{aligned}\alpha_d &= scale_1 \exp(-edisp_1/akT_e) D(T_e, N_e) \sum_{i_1 \in grp_1} \alpha^{GF}(g \to i_1) \\ &+ scale_2 \exp(-edisp_2/akT_e) D(T_e, N_e) \sum_{i_2 \in grp_2} \alpha^{GF}(g \to i_2)\end{aligned} \qquad 3.8.8$$

SCD: The coefficient is a zero density coefficient from the ground state of the ion obtained as a sum over contributing shells. It may include direct ionisation (*shd*) or excitation auto-ionisation (*excit*)

$$S^{(z \to z+1)}(T_e) = S^{approx}_{shd}(T_e) + S^{approx}_{excit}(T_e) \qquad 3.8.9$$

(A) The expressions of Lotz are used for direct ionisation. Only two shells are allowed and there is no excitation auto-ionisation part.

$$S^{approx}_{shd}(T_e) = \sum_{i=1,2} S^{LOTZ}(z, \chi_i, \zeta_i, T_e) \qquad 3.8.10$$

where

$$\begin{aligned}S^{Lotz}_{shd} &= 1.42^{-6} (I_H / kT_e)^{3/2} a\zeta [E_1(\chi / kT_e) / (\chi / kT_e) \\ &\quad - be^c E_1(\chi / kT_e + c) / (\chi / kT_e + c)] \quad cm^3 s^{-1}\end{aligned} \qquad 3.8.11$$

The a, b, c are constants given for each shell, ζ is the number of equivalent electrons in the shell and χ is the ionisation energy of the shell.

(B) The expressions of Burgess & Chidichimo are used together with a contribution from excitation / auto-ionisation.

$$S^{approx}_{shd}(T_e) = \sum_I c_I \sum_{i \in I} S^{BCHID}(z, \chi_i, \zeta_i, T_e) \qquad 3.8.12$$

where

$$S^{BCHID} = 2.1715^{-8}\, c\zeta (I_H / \chi)^{3/2} (\chi / kT_e)^{1/2} E_1(\chi / kT_e)\, w \quad cm^3 s^{-1} \qquad 3.8.13$$

with

$$w = \{\ln(1.0 + kT_e / \chi)\}^{\beta/(1.0+kT_e/\chi)}$$

$$\beta = 0.25[\{(100z + 91)/(4z + 3)\}^{1/2} - 5] \qquad 3.8.14$$

and

$$S^{approx}_{excit}(T_e) = \sum_R c_R \sum_{r \in R} 1.45\, WT_r\, (I_H / \Delta E_r)(I_H / \varepsilon)\, \pi a_0^2 \qquad 3.8.15$$

CCD: Only charge transfer from neutral hydrogen in its ground state is included. The total charge exchange cross-section is used at a mean hydrogen collision speed to obtain the rate coefficient.

(A) A constant cross-section for total charge transfer is used except for the ions of carbon, nitrogen and oxygen

$$\alpha^{(z+1 \to z)}_{CX}(T_i) = 3.07^{-9} ((kT_i / I_H)(m_H / m_i))^{1/2}\, z_1^{1.07} \quad cm^3 s^{-1} \qquad 3.8.16$$

(B) There is no separate expression

$$\alpha_{CX}^{(z+1\to z)}(T_i) = 3.07^{-9}((kT_i / I_H)(m_H / m_i))^{1/2}\ z_1^{1.07} \quad cm^3 s^{-1} \qquad 3.8.17$$

PRB: The power coefficient is a zero density coefficient obtained as a sum of radiative recombination, dielectronic recombination and bremsstrahlung parts

(A) A radiative recombination is assumed to release energy equal to ground state ionisation energy of the recombined ion. Dielectronic recombination energy loss is summed over the two parent transitions and each is assumed to release an energy equal to the parent transition energy together with the ionisation energy of the ground state of the recombined ion. Bremsstrahlung is taken to be hydrogenic with free-free Gaunt factor set to unity.

$$P_{RB}^{(z+1\to z)} = 1.6^{-19}\{\alpha_r^{(z+1\to z)}\ \chi + \sum_{j=1}^{2}[\alpha_d^{(z+1\to z)}(\Delta E_j + \chi)]\} \\ +5.68^{-32} z_1^2 (kT_e / I_H) \quad Wcm^3 \qquad 3.8.18$$

(B) A radiative recombination is assumed to release energy equal to ground state ionisation energy of the recombined ion. Dielectronic recombination energy loss is summed over the two parent transitions and each is assumed to release an energy equal to the parent transition energy together with the ionisation energy of the ground state of the recombined ion. Bremsstrahlung is taken to be hydrogenic with free-free Gaunt factor set to unity.

$$P_{RB}^{(z+1\to z)} = 1.6^{-19}\{\alpha_r^{(z+1\to z)}\ \chi + \sum_{j=1}^{2}[\alpha_d^{(z+1\to z)}(\Delta E_j + \chi)]\} \\ +5.68^{-32} z_1^2 (kT_e / I_H) \quad Wcm^3 \qquad 3.8.19$$

PRC: The coefficient is a zero density coefficient based on the total charge exchange recombination coefficient

(A) A recombination is assumed to release an amount of energy equal to the ionisation energy of the ground state of the recombined ion..

$$P_{RC}^{(z+1\to z)}(T_e) = 1.60^{-19}\,\chi\,\alpha_{CX}^{(z+1\to z)}(T_e) \quad Wcm^3 \qquad 3.8.20$$

(B) There is no separate expression

$$P_{RC}^{(z+1\to z)}(T_e) = 1.60^{-19}\,\chi\,\alpha_{CX}^{(z+1\to z)}(T_e) \quad Wcm^3 \qquad 3.8.21$$

PLT: The coefficient is a zero density coefficient obtained by assuming a coronal picture and represented by effective collisional excitations from the ground state of the ion.

(A) A $\overline{g}$ dipole approximation is assumed, specified by an oscillator strength and a constant effective Gaunt factor

$$P_{LT}^{(z)}(T_e) = \sum_{j=1}^{2} \Delta E_j q_{g\to j}^{(e)}(T_e) \qquad 3.8.22$$

where

$$\Delta E_j q_{g\to j}^{(e)} = 2.18^{-18}(\Delta E_j / I_H) \\ 4.28^{-6}(I_H / kT_e)^{1/2}(I_H / \Delta E_j) f_j \overline{g}_j e^{-\Delta E_j / kT_e} \quad Wcm^3 \qquad 3.8.23$$

(B) Similar expressions are used but with the $\overline{g}$ replaced with the $P(\Delta E / kT_e)$ of Van Regemorter. The expressions are based on two effective transitions with mean transition energies and oscillator strengths. Multipliers c_j are chosen to optimise the fit to best available data at one temperature

$$P_{LT}^{(z)}(T_e) = \sum_{j=1}^{2} c_j \overline{\Delta E}_j \bar{q}_{g\to j}^{(e)}(T_e) \qquad 3.8.24$$

where

$$\overline{\Delta E}_j \bar{q}_{g\to j}^{(e)} = 2.18^{-18}(\overline{\Delta E}_j / I_H) \; 4.28^{-6}(I_H / kT_e)^{1/2}(I_H / \overline{\Delta E}_j)\bar{f}_j P(\overline{\Delta E}_j / kT) e^{-\overline{\Delta E}_j / kT_e} \quad Wcm^3 \qquad 3.8.25$$

PLS: The coefficient is a zero density coefficient for the power in a resonance line excited from the ground state of the ion.

(A) A $\bar{g}$ dipole approximation is assumed, specified by an oscillator strength and a constant effective Gaunt factor

$$P_{LS}^{(z)}(T_e) = \Delta E \; q^{(e)}(T_e) \qquad 3.8.26$$

where

$$\Delta E \; q^{(e)} = 2.18^{-18}(\Delta E / I_H) \; 4.28^{-6}(I_H / kT_e)^{1/2}(I_H / \Delta E) f\bar{g} e^{-\Delta E / kT_e} \quad Wcm^3 \qquad 3.8.27$$

(B) A similar expression is used but with the $\bar{g}$ replaced with the $P(\Delta E / kT_e)$ of Van Regemorter. The expression is based on an effective dipole excitation with the transition energy and oscillator strength specified. A multiplier c is chosen to optimise the fit to best available data at one temperature

$$P_{LS}^{(z)}(T_e) = c \; \Delta E \; q^{(e)}(T_e) \qquad 3.8.28$$

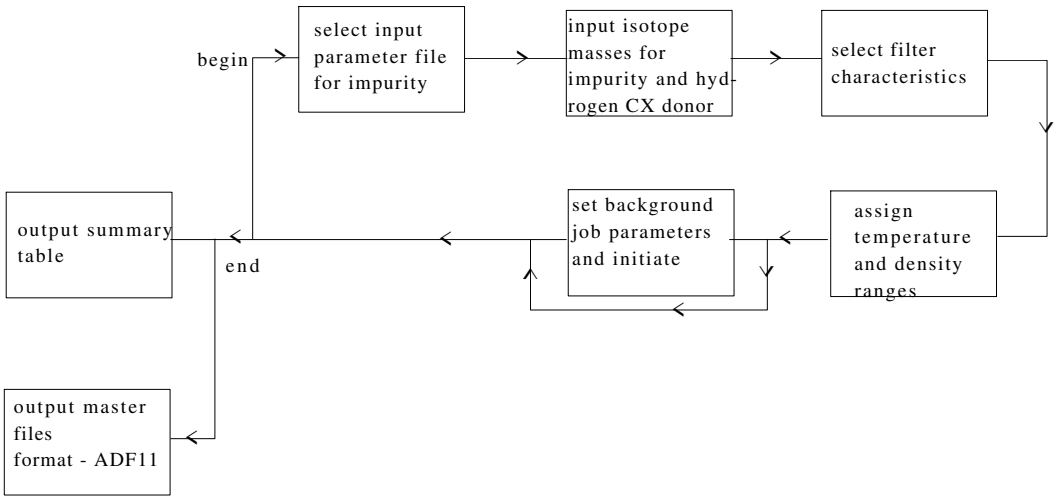
where

$$\Delta E \; q^{(e)} = 2.18^{-18}(\Delta E / I_H) \; 4.28^{-6}(I_H / kT_e)^{1/2}(I_H / \Delta E) f \; P(\Delta E / kT) e^{-\overline{\Delta E}_j / kT_e} \quad Wcm^3 \qquad 3.8.29$$

Program steps:

These are summarised in figure 3.8.

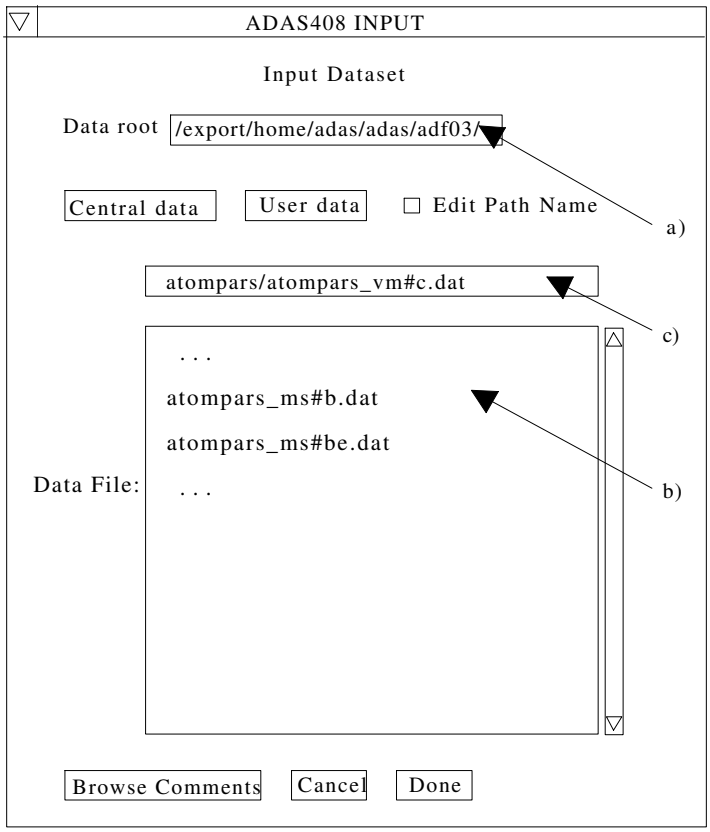
Figure 3.8



Interactive parameter comments:

The program uses parametric forms for zero density recombination, ionisation and radiated power loss coefficients, type *adf03*, to prepare standard (unresolved, stage to stage) iso-nuclear master files for a particular element of type *adf11*. The iso-nuclear master files may be prepared over arbitrary ranges of electron temperature and electron density

The **file selection window** has the appearance shown below



1. Data root a) shows the full pathway to the appropriate data sub-directories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. The appropriate ADAS data format for input to this program is *adf03* ('atompars files'). Click the *User Data* button to insert the pathway to your own

data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas,* to use this facility.

2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

3. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.

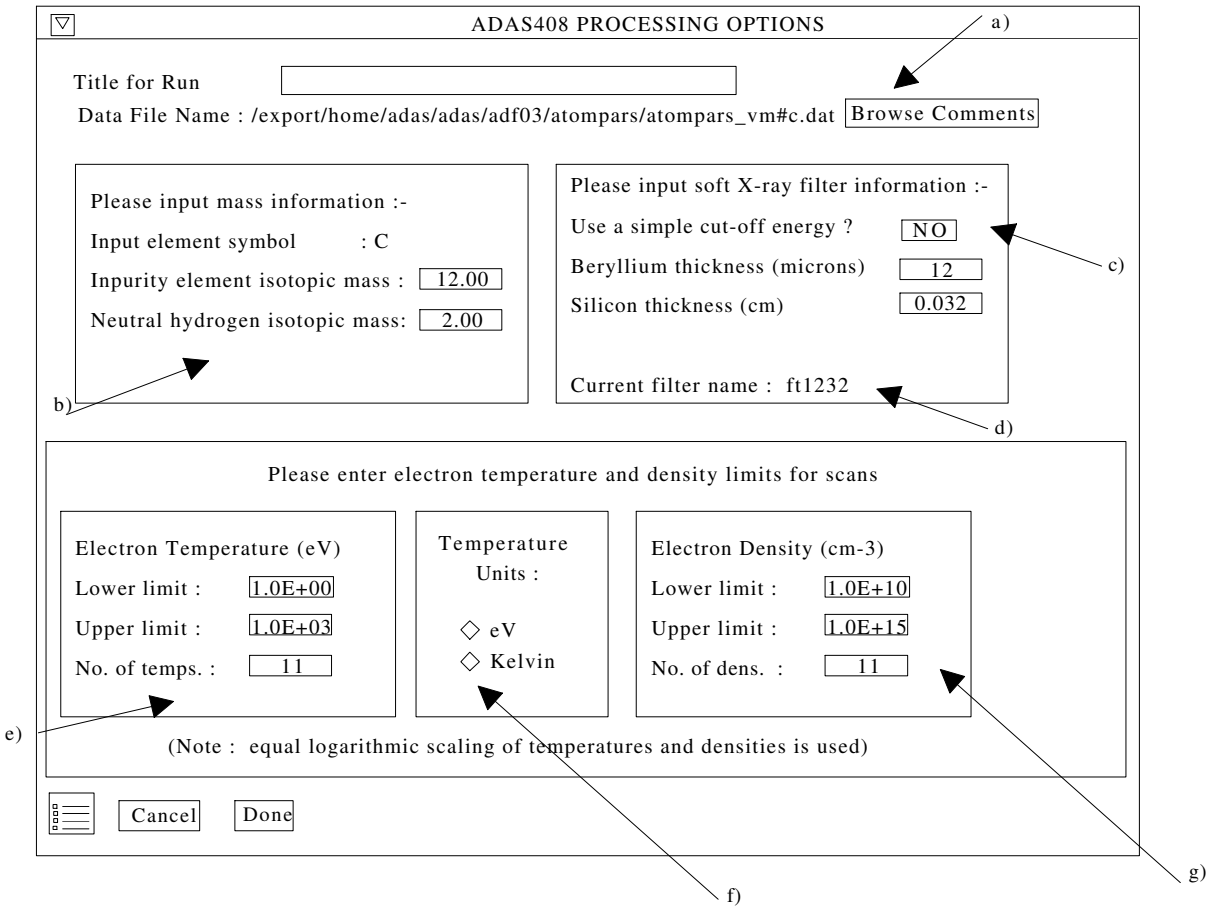
4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual data-files are presented for selection. Data-files all have the termination *.dat*.

5. Once a data file is selected, the set of buttons at the bottom of the main window become active.

6. Clicking on the *Browse Comments* button displays any information stored with the selected data-set. It is important to use this facility to find out what is broadly available in the data-set. The possibility of browsing the comments appears in the subsequent main window also.

7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

The **processing options window** has the appearance shown below



8. At the top of the window, an arbitrary title may be given for the case being processed. The name of the data file under analysis is shown. The button *Browse*

Comments allows display of the information field section at the foot of the named atompars file, if it exists.

9. At b), the mass number for the actual isotope of the element of the atompars file present in the plasma is entered. For information the element chemical symbol is displayed. Likewise, the mass number of hydrogen isotope constituting the primary plasma species is sought. Type the values in the editable boxes and press return.

10. In the adjacent window, a capability is given for modifying the output file of total radiated line power to include the attenuation through a soft-x-ray filter. Two choices are available, namely, a simple cut-off and a more elaborate representation of the characteristics of beryllium/silica windows. Click in the box at c) to drop down a standard choice menu. In the beryllium/silica case thicknesses must be specified in the following two editable boxes.

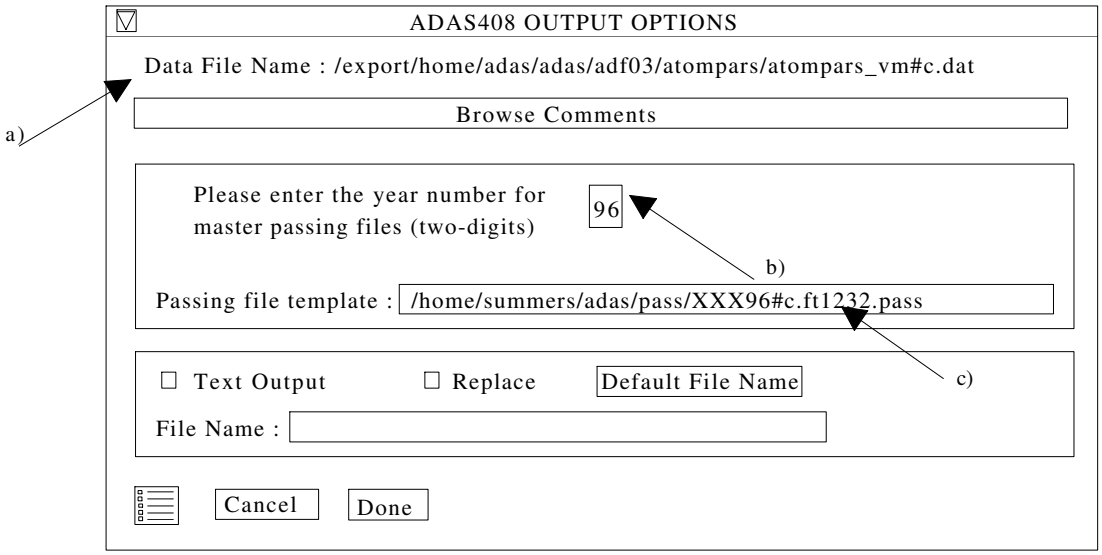
11. A suitable 'filter name' is created by ADAS408 which appears as part of the output radiated power file name. In the simple cut-off case, the filter name has the prefix 'ev' followed by the numerical value of the cut-off energy in eV. In the true filter case, the filter name has the prefix 'ft' followed by the first two significant figures of the beryllium and silicon thicknesses.

12. The lower sub-windows at e), f) and g) allow the plasma electron temperature and electron density for production of the output *adf11* standard master files to be specified. Click on the required temperature units at f). This choice relates to the units used in the adjacent temperature range selection window at e). Specify lower temperature limit, upper temperature limit and number of temperatures in the editable boxes. ADAS408 then creates the temperature grid equally spaced in the logarithm. Note that the output files in fact contain the temperatures in eV (see the ADAS User Manual, appxb-11).

13. Similarly specify the electron density limits and number of grid points at g).

14. The *Exit to Menu* icon is present in ADAS408. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **output options window** is of restricted form. It only offers the option of an output files.



15. The name of the source atompars file to be used in the bulk generation of *adf11* data is repeated at a) for information.

16. The standard line printer text output file summarising the options selected for ADAS408 is available. The *Replace* and *Default File Name* buttons are present for the text output file as usual.

17. The *adf11* iso-nuclear master file output comprises several files which are placed in your */pass* directory. Collections of *adf11* files are held by year number. Enter a two digit year number at b) for the output. Note that any two digits are acceptable and 'fictitious' years can be used for special collections if so desired. Using the year number and the filter name (see 3.2.4 above) a passing file template is created. The 'XXX' of the template is replaced by the three letter codes of the iso-nuclear master file classes ('acd', 'scd' etc.) to create the actual output files. The filter name part of the template only appears in radiated power classes of iso-nuclear master files. Note also the presence of the element chemical symbol in the template. Unfiltered radiated power master files are created as well as the filtered ones. The former do not include a filter name as part of the whole file name.

18. There is no graphical output option.

19. The *Exit to Menu* icon is present in ADAS408. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

Illustration:

Figure 3.8a

There is no graphical display from this code.

Table 3.8a

```
 ADAS RELEASE: ADAS91 V1.11  PROGRAM: ADAS408 V1.0   DATE: 14/07/94  TIME: 18:11

 ******************************    RUN SUMMARY FOR PROGRAM GENERATING STANDARD   ***********************************
 ******************************   ISONUCLEAR MASTER FILES FROM PARAMETRIC FORMS  ***********************************
 ***************************************** ADAS408 - DATE: 14/07/94 ************************************************


 INPUT PARAMETER FILE     : JETSHP.ATOMPARS.DATA(VM#C)

 OUTPUT PASSING FILES FORMS: JETSHP.XXX89#C.PASS
                             JETSHP.XXX89#C.FT0530.PASS
 ------------------- TEST                                        --------------------



 IMPURITY INFORMATION:
 ---------------------
  ELEMENT SYMBOL          =      C
  NUCLEAR CHARGE          =      6
  LOWEST ION CHARGE       =      0
  HIGHEST ION CHARGE      =      5
  ATOMIC MASS NUMBER      =  12.00

 NEUTRAL DONOR INFORMATION:
 --------------------------
  ELEMENT SYMBOL          =      H
  NUCLEAR CHARGE          =      1
  ATOMIC MASS NUMBER      =   2.00

 FILTER INFORMATION:
 -------------------
  FILTER TYPE             =  BE/SI FILTER
  BERYLLIUM LAYER (CM)    =  0.0050
  SILICON LAYER (CM)      =  0.3000

 ELECTRON TEMPERATURE/DENSITY INFORMATION:
 -----------------------------------------

                            TEMPERATURE (EV)      DENSITY (CM-3)
                            ----------------      --------------
  NUMBER OF VALUES        =        20                  10
  MINIMUM VALUE           =    1.0000D+00           1.0000D+10
  MAXIMUM VALUE           =    1.0000D+02           1.0000D+15

   (NOTE: EQUAL INTERVALS IN THE LOGARITHM ARE SET)
•
```

Notes: