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* of format ADF04. 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:

> Autostructure (ADAS701) + impact parameter rate coefficients
> Cowan/O'Mullane (ADAS801) + plane wave Born rate coefficients

The output ADF04 files from these codes are assigned the group names

> *copss#<elem. nucl. charge>.dat(sm#<ion>)*
> *copmm#<elem. nucl. charge>.data(ls#<ion>)*

respectively.

The ADF04 specific ion files created by the 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

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

Also, the field for the energies of individual orbitals used in the configurations under study must be present (see appxa-04). These orbital energies are denoted by

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


```
Eissner ≡ 1s² 2s          ε_1s                    ε_3d

C + 3          6          4            520178.4
   1 21512              (2)0( 0.5)        0.0
   2 21513              (2)1( 2.5)     64555.4
   3 21514              (2)0( 0.5)    302849.0
   4 21515              (2)1( 2.5)    320071.2
   5 21516              (2)2( 4.5)    324886.1
  -1        28.35     4.77     4.18     1.99     1.83     1.79
 4.0     3         8.00+03 1.60+04 3.20+04 8.00+04 1.60+05 3.20+05 8.00+05 1.60+06 3.20+06 8.00+06
   3    1 1.00-30 5.68-01 5.49-01 5.16-01 4.46-01 3.96-01 3.84-01 3.87-01 3.83-01 3.83-01 3.85-01
   .        .        .
```

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

Using the above supplementary information, analysis by ADAS407 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. The parameters are returned in two

formats, namely, ADF03 and ADF25. ADF25 is format for drivers of the bundle-n population code ADAS204. ADF03 format is used as input to ADAS408 and parallels the original inputs for certain impurity transport modelling codes such as *Strahl*. The ADF03 parameters are allowed in two forms called cases A and B. A summary is given below with further details available in the description of ADAS408.

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

$$P_{i_m;LT}(T_e) = \sum_j \Delta E_{i_m,j} q_{i_m \to j}(T_e) \qquad 5.7.1$$

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

$$f_{i_m \to B} = \sum_{j \in B} f_{i_m \to j}$$

$$\Delta E_{i_m,B} = (\sum_{j \in B} \Delta E_{i_m,j} f_{i_m \to j}) / f_{i_m \to B} \qquad 5.7.2$$

$$\overline{g}_{i_m,B} = (\sum_{j \in B} \overline{g}_{i_m,j} f_{i_m \to j}) / f_{i_m \to B}$$

The approximate radiated power coefficient for the group is

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

$$5.7.3$$

in case A and

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

$$5.7.4$$

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

The whole approximate power coefficient is assembled as

$$P^{approx}_{i_m;LT}(T_e) = C \sum_B c_B P_{i_m,B;LT}(T_e) \qquad 5.7.5$$

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

$$\{\zeta_k, \varepsilon_k : k = 1,..,m_{i_{sys}}\} \qquad 5.7.6$$

The ionisation energy of the outer shell is improved to

$$\overline{\varepsilon}_{m_{i_{sys}}} = E_{i_{prt}}^{(z+1)} - E_{i_{sys}}^{(z)} + I^{(z)} \qquad 5.7.7$$

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

$$S_{i_{sys} \to i_{prt}}^{(z \to z+1)}(T)_e = C \sum_{k=k_0}^{m_{i_{sys}}} 1.42^{-6}(I_H / kT_e)^{3/2} a_k \zeta_k [E_1(\varepsilon_k / kT_e)/(\varepsilon_k / kT_e)$$

$$-b_k e^{c_k} E_1(\varepsilon_k / kT_e + c_k)/(\varepsilon_k / kT_e + c_k)] \quad cm^3 s^{-1}$$
$$5.7.8$$

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

$$S_{i_{sys} \to i_{prt}}^{(z \to z+1)}(T_e) = C \sum_{k=1}^{m_{i_{sys}}} 2.1715^{-8} \zeta_k (I_H / \varepsilon_k)^{3/2} (\varepsilon_k / kT_e)^{1/2} E_1(\varepsilon_k / kT_e) w \quad cm^3 s^{-1}$$
$$5.7.9$$

with

$$w = \{\ln(1.0 + kT_e / \varepsilon_k)\}^{\beta/(1.0+kT_e/\varepsilon_k)} \qquad 5.7.10$$

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

$$\{n_k, I_{k,i_{prt}}^{(z)}, w_k : k = 1,.., K_{sys,i_{prt}}\} \qquad 5.7.11$$

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

$$Ph_{n,sys,i_{prt}} = 1 - (\sum_{k:n_k=n} w_k) / w_{i_{prt}} n^2 \qquad 5.7.12$$

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

$$v_{n,sys,i_{prt}} = \sqrt{(\sum_{k:n_k=n} w_k)z_1^2 I_H / (\sum_{k:n_k=n} w_k I_{k,i_{prt}})} \qquad 5.7.13$$

The recombination coefficient is then evaluated from the expression

$$\alpha_{i_{prt}}^{(z+1\to z)}(T_e) = scale(z_1^2 I_H / kT_e v_0^2)^{edisp} \alpha^H(v_0) + \sum_{n>n_0+1} \alpha^H(n_n)$$

$$= [2.6^{-14}]z_1(z_1^2 I_H / kT_e)^{\frac{1}{2}} \{\frac{2 phfrac}{v_0}(z_1^2 I_H / kT_e v_0^2) EEI(z_1^2 I_H / kT_e v_0^2)$$

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

$$5.7.14$$

where v_0 denotes $v_{n,sys,i_{prt}}$, 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

$$\alpha_{i_{prt}\to sys}^{(z+1\to z)}(T_e) = [(2S_{sys}+1)/2(2S_{i_{prt}}+1)]\alpha_{i_{prt}}^{(z+1\to z)}(T_e) \quad 5.7.15$$

For case A parameters, expression 5.7.14 is simplified with *scale*=1, *edisp*=0 and n_0 replacing v_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

$$n_{cut,i_{prt}} = INT\{\sqrt{z_1^2 I_H / (E_{i_{prt}}^{(z+1)} - E_1^{(z+1)})}\} + 1 \qquad 5.7.16$$

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. Dielectronic recombination coefficient is evaluated using an adjusted Burgess general formula in case B as

$$\alpha^{approx}(p_\rho; p_\rho) = scale_1 \exp(-edisp_1/akT_e) \sum_{i_1 \in grp_1} \alpha^{GF}(p_\rho; p_{i_1}; p_\rho)$$

$$+ \quad scale_2 \exp(-edisp_2/akT_e) \sum_{i_2 \in grp_2} \alpha^{GF}(p_\rho; p_{i_2}; p_\rho)$$

$$5.7.17$$

with $\alpha^{GF}(p_\rho; p_i; p_\rho)$ is the basic general formula for initial recombining parent ion p_ρ and final parent ion $p_\sigma = p_\rho$. p_i is the intermediate excited parent ion. In optimising, adjustment is made for each group as a whole. There are at most two groups allowed. $scale_1$ and $scale_2$ are the adjustable parameters, $edisp_1$ and $edisp_2$ being preset. In Case A, the unadjusted form is used.

Program steps:

These are summarised in figure 5.7.

Figure 5.7
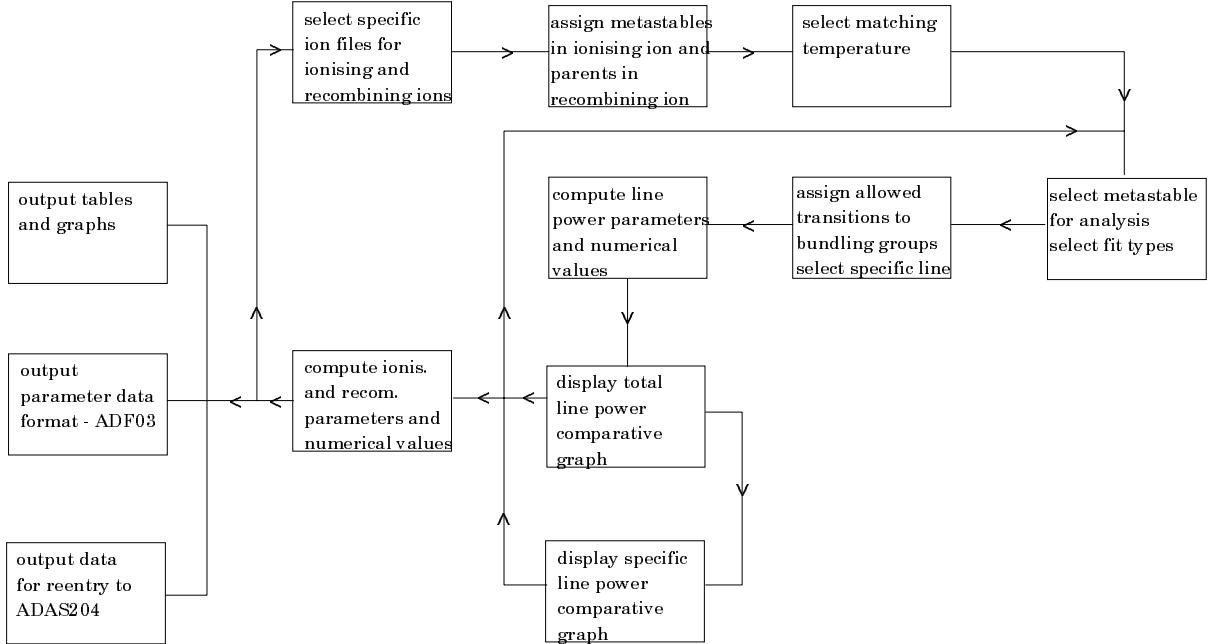
Interactive parameter comments:

The **analysis choice** window appears first as shown below.
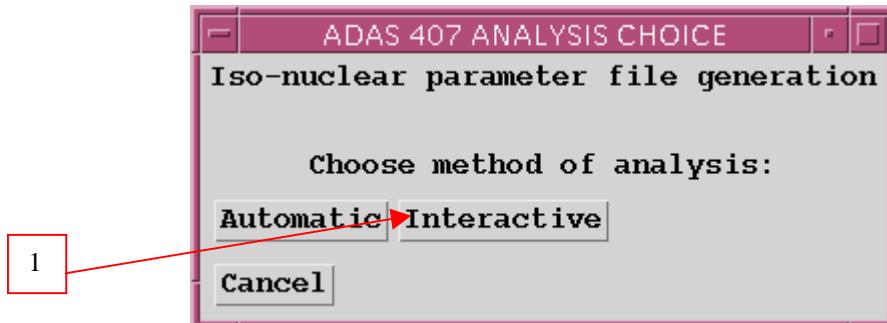
The **file selection window** in interactive operation is shown below. *adf04* is the appropriate format for use by the program ADAS407.   ADAS407 requires two such files, namely, for the 'Ionising Ion' and the 'Ionised Ion'. If you wish to use personal data of this type, then as it should be held in a similar file structure to central ADAS with your identifier replacing the first *adas*.   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 is upper one. A Data root path to the correct data type *adf04* appears automatically. 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. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
2.   Available sub-directories are shown in the large file display window. Click on a name to select it. The selected name appears in the smaller selection window 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.

3. When an ionising ion has been chosen, then the corresponding ionised ion has to be chosen . ADAS407 creates the expected file name and displays it if it exists. This name can be over-ridden in the usual manner.
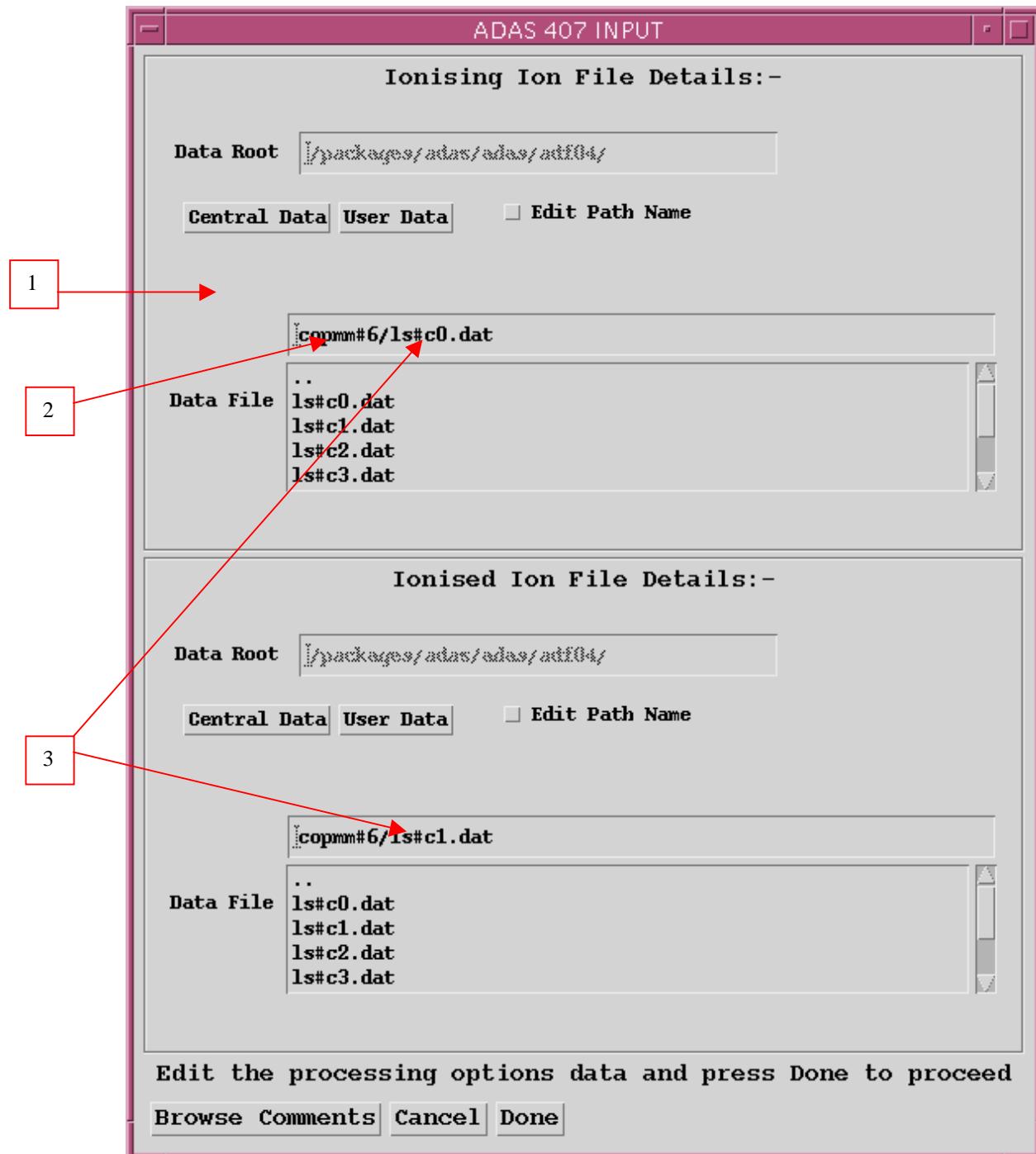
The **processing options window** has the appearance shown below

1. 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. 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.

2. 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.

3. Notice the appearance of the configuration specification part of the level designation. The '21522523' means $1s^2 2s^2 2p^2$ in 'Eissner notation' (see the ADAS User Manual for more details).

4. Click on the particular driving metastable whose associated radiated power loss is to be analysed and displayed.
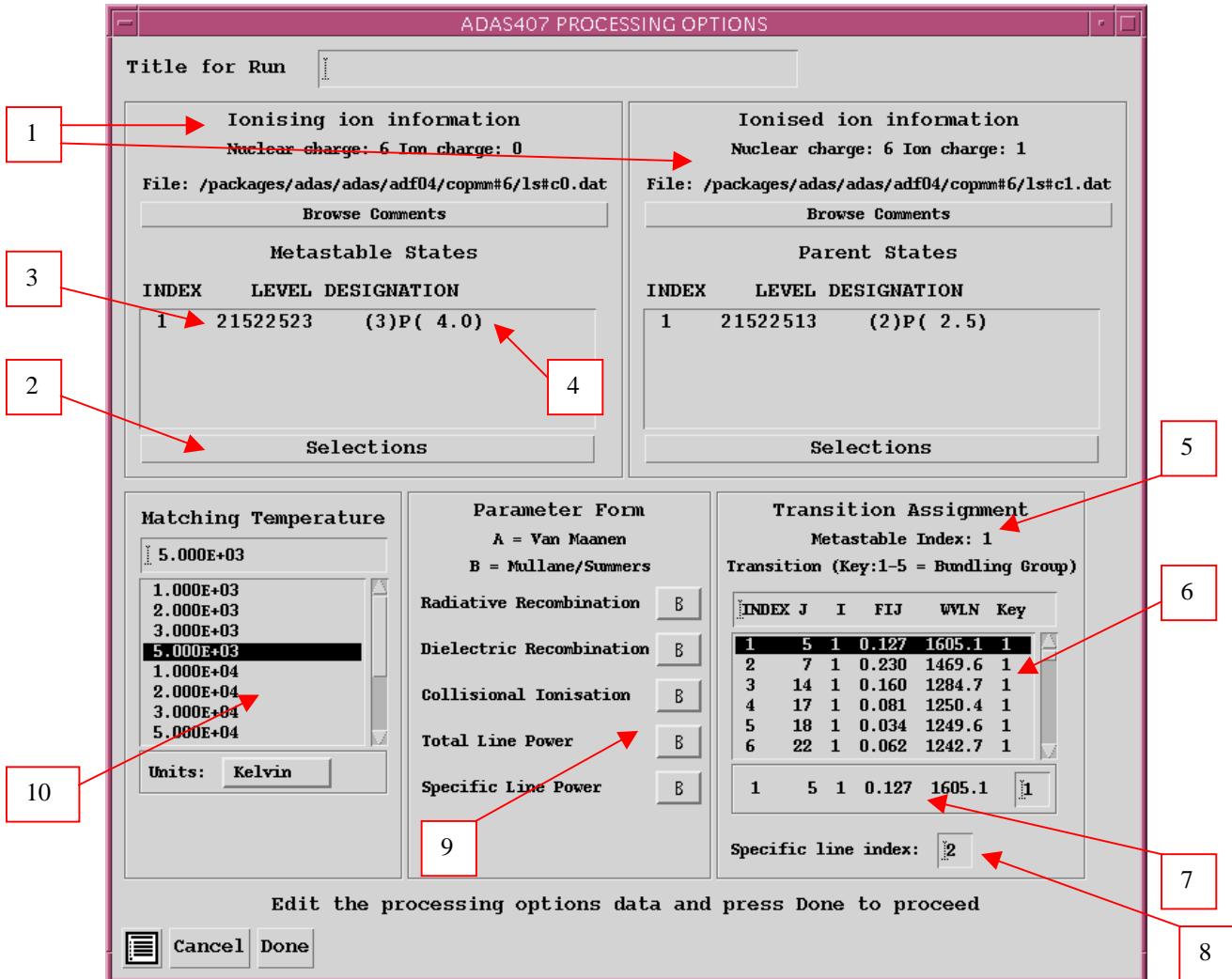
5. This choice appears in the lower group of sub-windows.

6. In the sub-window, below the metastable index information a display window and associated selection window is present. The display window 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. 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.

7. 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.

8. 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.

9. 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. 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 to drop down the A or B choice menu.

10. 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 at which you wish the approximate form and accurate numerical values to agree.

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.

1. The input specific ion files under analysis are shown and can be browsed. Two buttons have been added to switch between *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.

2. In the Graphics case, there are two types of graph, namely, the total radiated power fit graph and the specific line power graph. The former is mandatory and the latter optional. Default scaling of the chosen graph may be over-ridden by appropriate selections.

3. Below this the usual hard copy may be enabled and a choice of type of output device made.

4. In the Text case, three output files are permitted, namely, the standard line printer text output file summarising the interrogation, the '*mainbn*' file and the '*atompars*' file. These are passing files which are placed by default in your */pass* directory as *mainbn.pass* and *atompars.pass*. The *mainbn* file of format ADF25 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.

5. Note the various completion buttons. 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.
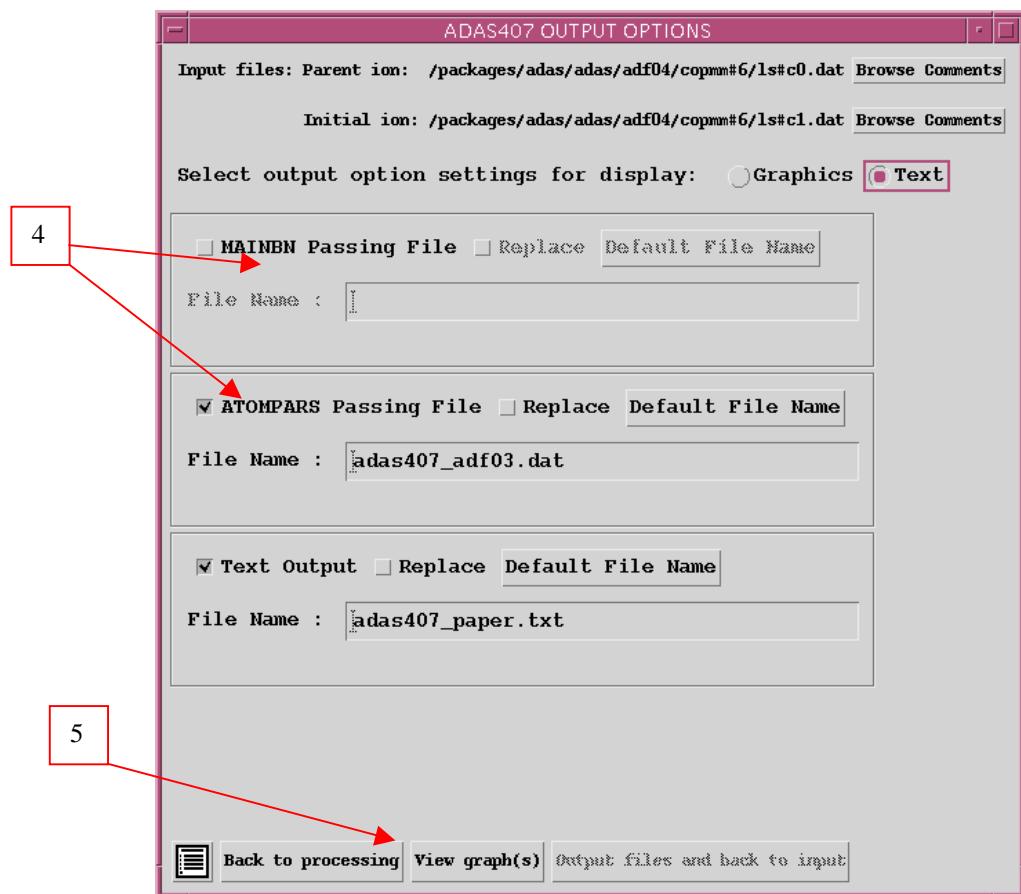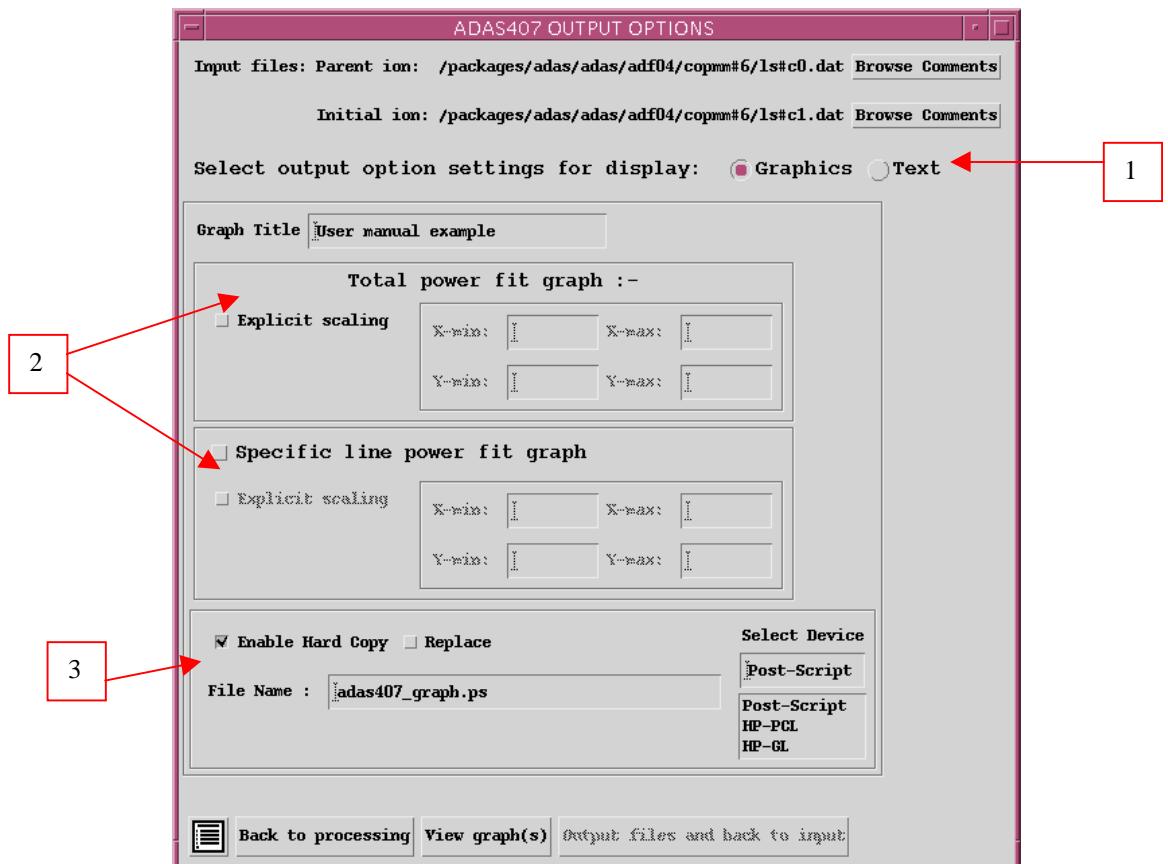
Illustration:

Figure 5.7a

TOTAL LINE POWER COEFFICIENT VERSUS TEMPERATURE: TEST

ADAS   : ADAS RELEASE: ADAS98 V2.0 PROGRAM: ADAS407 V1.7 DATE: 28/07/98 TIME: 21:06

FILE   : /u/adas/adas/adf04/copmm#7/ls#n3.dat   ELEM: N + 3 MET: 1 FIT: A

KEY   : (FULL LINE – EXACT) (SHORT DASH – INITIAL)(LONG DASH – SIMPLE) (DOT DASH – OPTIMISED)
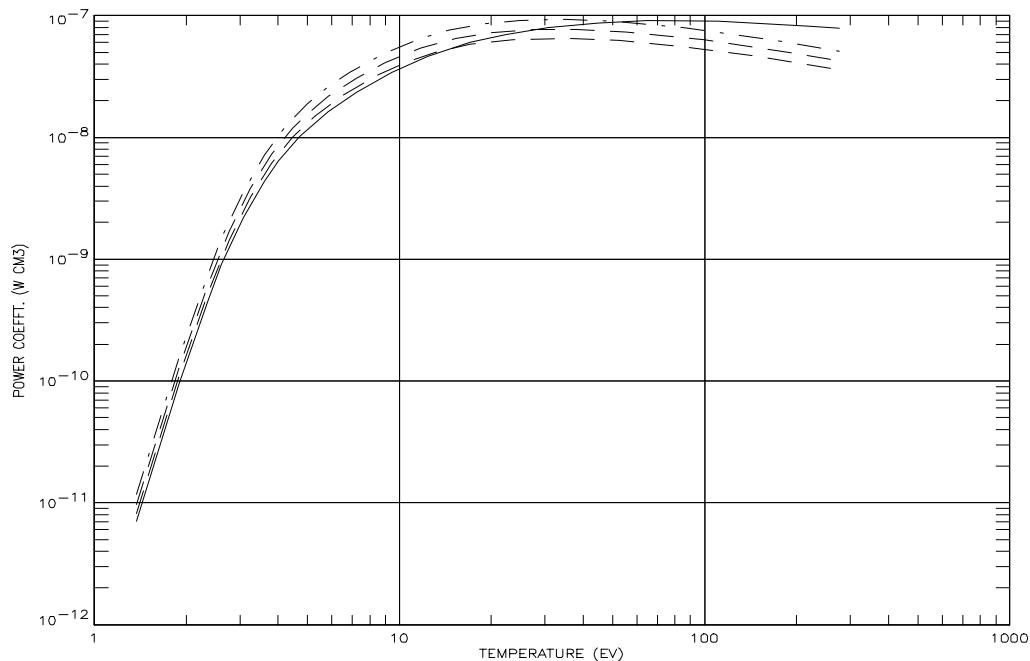
Figure 5.7b

SPEC. LINE POWER COEFFICIENT VERSUS TEMPERATURE: TEST

ADAS   : ADAS RELEASE: ADAS98 V2.0 PROGRAM: ADAS407 V1.7 DATE: 28/07/98 TIME: 21:06
FILE   : /u/adas/adas/adf04/copmm#7/ls#n3.dat   ELEM: N + 3 MET: 1 FIT: A WVLN: 817.8A
KEY   : (FULL LINE — EXACT) (SHORT DASH — INITIAL)(LONG DASH — SIMPLE)
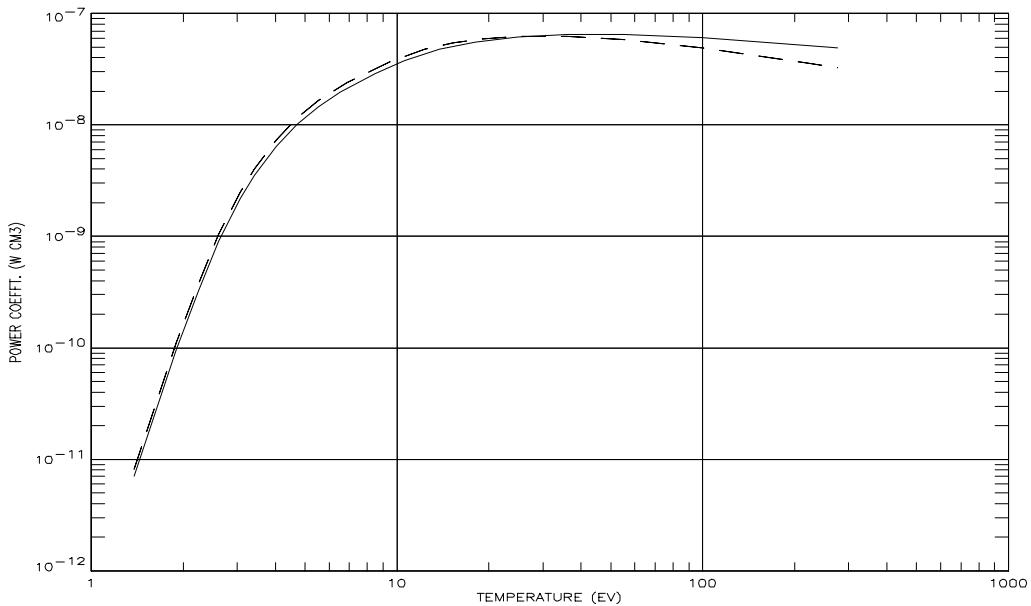
Table 5.7a

```
******************* 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   LEVEL    PARENT      PARENT            SYSTEM     SYSTEM     SPIN WT.
 INDEX    INDEX    TERM    MULTIPLICITY          INDEX   MULTIPLICITY 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  EISSNER    N      L      EFFECTIVE
  INDEX   SYMBOL                 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    WVLN   BNDL  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
           STREN    (A)    INDX  -------------------------------------- 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 5.76D-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     DE-POW    F-POW    G-POW      SCALE     SCALE     SCALE     G-SCLD
        INDX     (eV)                         INITIAL   SIMPLE    OPTIM.
 -----------------------------------------------------------------------------------------------------------------------
---------
          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  SYSTEM  IONIS. GRP.  ORBITAL  ION. ENER.   EQUIV.
  INDEX   INDEX   MULTIPLIER   INDEX    (RYD)     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  SYSTEM                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                    ------------------------- 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 5.74D-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 5.75D-12 2.75D-12 2.19D-12 1.58D-12 1.03D-12 7.66D-13 5.54D-
13 5.78D-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 5.78D-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 5.71D-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 5.71D-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 5.7b

```
&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   5.77000    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
  5.74D-13  6.54D-12  6.71D-11  2.27D-10  8.06D-10  2.34D-09  5.77D-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   5.77000    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   5.77000    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  5.79D-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 5.7c

```
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: