

# Lecture 3 The ionisation state of ions in a plasma

## Preliminaries

### Generalised collisional-radiative theory

The basic model for obtaining effective ionisation and recombination rate coefficients in finite density plasmas was established by Bates et al. (1962). The ion in a plasma is viewed as composed of a complete set of levels indexed by  $\mathbf{i}$  and  $\mathbf{j}$  and a set of radiative and collisional couplings between them denoted by  $C_{ij}$  (an element of the 'collisional-radiative matrix' representing transition from  $\mathbf{j}$  to  $\mathbf{i}$ ) to which are added direct ionisations from each level of the ion to the next ionisation stage (coefficient  $q_i^{(i)}$ ) and direct recombinations to each level of the ion from the next ionisation stage (coefficient  $r_i$ ). There is no loss of generality in the present discussion in ignoring other ionisation stages provided couplings to and from them are only via ground states. For each level, there is a total loss rate coefficient for its population denoted by

$$-C_{ii} = \sum_{j \neq i} C_{ji} + N_e q_i^{(i)}$$

The population of any level is determined by the balance of processes populating and depopulating it. Suppose the dominant populations are a recombined ion ground state ( $i = 1$ ) and a recombining ion ground state denoted by  $+$ . These states alone are assumed significantly populated. Excited level populations (that is  $N_i$  for  $i > 1$ ) are small in comparison. Then the quasi-equilibrium statistical balance is

$$\begin{aligned} \frac{d}{dt} N_1 &= \sum_{j \neq 1} C_{1j} N_j + C_{11} N_1 + N_e N_+ r_1 \\ 0 &= \sum_{j \neq 1} C_{ij} N_j + C_{i1} N_1 + N_e N_+ r_i \quad , \quad i = 2, \dots \end{aligned}$$

In matrix form these become

$$\begin{bmatrix} \frac{d}{dt} N_1 \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{1j} \\ C_{i1} & C_{ij} \end{bmatrix} \begin{bmatrix} N_1 \\ \mathbf{N}_j \end{bmatrix} + N_e N_+ \begin{bmatrix} r_1 \\ \mathbf{r}_i \end{bmatrix}$$

The populations of the excited levels in quasi-equilibrium,  $N_j^{eq}$  are given by

$$N_j^{eq} = -N_e N_+ \sum_{i \neq 1} C_{ji}^{-1} r_i - \sum_{i \neq 1} C_{ji}^{-1} C_{i1} N_1$$

Substitution of equations 1.9 in equation 1.7 for  $N_1$ , allows identification of a collisional-dielectronic ionisation coefficient

$$S_{CD} = C_{11} - \sum_{j \neq 1} \sum_{i \neq 1} C_{1j} C_{ji}^{-1} C_{i1}$$

and collisional-dielectronic recombination coefficient

$$\alpha_{CD} = r_1 - \sum_{j \neq 1} \sum_{i \neq 1} C_{1j} C_{ji}^{-1} r_i$$

Physically, the collisional-dielectronic coefficients give the contributions to the effective growth rates for the ground state population due to recombination from and ionisation to the state  $+$ , so that the time dependent equation for  $N_1$  becomes

$$\frac{d}{dt} N_1 = -N_e S_{CD} N_1 + N_e \alpha_{CD} N_+$$

Some extension is required since populated metastable states can exist and there is no real distinction between them and ground states. We use the term 'metastables' to denote both ground and metastable states and index them by  $\rho$  for the recombined ion, and by  $\nu$  for the recombining ion. Therefore the ion of charge state  $z$  has metastable populations  $N_\rho^{(z)}$  and the recombining ion population,  $N^+$ , must

be subdivided into the set  $N_v^{(z+1)}$ . We sometimes call the recombining ion metastable states 'parent' states. Generalised collisional radiative theory provides effective coefficients which are the extension of those above as:

The ionisation coefficients

$$S_{CD,\sigma \rightarrow v} = (S_{v\sigma} - \sum_{j=1}^O S_{vj} \sum_{i=1}^O C_{ji}^{-1} C_{i\sigma})$$

the free electron recombination coefficients

$$\alpha_{CD,v' \rightarrow \rho} = (R_{\rho v'} + \sum_{j=1}^O C_{\rho j} \sum_{i=1}^O C_{ji}^{-1} R_{iv'})$$

the charge exchange recombination coefficients

$$C_{CD,v' \rightarrow \rho} = (Q_{\rho v'} + \sum_{j=1}^O C_{\rho j} \sum_{i=1}^O C_{ji}^{-1} Q_{iv'})$$

the metastable cross-coupling coefficients

$$X_{CD,\sigma \rightarrow \rho} = (C_{\rho\sigma} - \sum_{j=1}^O C_{\rho j} \sum_{i=1}^O C_{ji}^{-1} C_{i\sigma}) / N_e$$

and the parent metastable cross-coupling coefficients

$$Q_{CD,v' \rightarrow v} = \sum_{j=1}^O S_{vj} \sum_{i=1}^O C_{ji}^{-1} R_{iv'}$$

Note the latter coefficients distinguish the parts occurring via recombination from conventional metastable cross-coupling as they are determined in the course of the population structure calculation for the z-times ionised ion. The radiated power loss coefficients are obtained by summing over the population structure. The contribution due to excitation from the metastables of the recombined ion is

$$P_{LT,\sigma} = \sum_{k,j} \Delta E_{kj} A_{j \rightarrow k} F_{j\sigma}^{(exc)}$$

and there is a corresponding bremsstrahlung, recombination/cascade part

$$P_{RB,\sigma}$$

### The adf11 data format

The primary repositories of collisional-radiative recombination, ionisation etc. coefficients gathered together by element are *adf11* files sometimes called iso-nuclear master files. The various classes are

Mnemonic	Class	Data prefix
ACD	Coll.-diel. recom. coefft.	R & U (or none)
SCD	Coll.-diel. ionis. coefft.	R & U (or none)
CCD	Coll.-rad. charge exch. coefft.	R & U (or none)
PRB	Coll.-diel. recom./brems. power coefft.	R & U (or none)
PRC	Coll.-rad. charge exch. recom. power coefft.	R & U (or none)
QCD	Coll.-rad. metastable cross coupling coefft.	R
XCD	Coll.-diel. parent meta. cross-coupling coefft.	R
PLT	Coll.-rad. excit. line power coefft.	R & U (or none)
PLS	Coll.-rad. specific line excit. power coefft.	R & U (or none)

A file is associated with an element and a data class. There are separate files for ordinary and generalised data. The classes of data include 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 metastable cross-coupling

coefficient (QCD) and the collisional-dielectronic parent cross-coupling coefficient (XCD), the collisional-radiative excitation total line power coefficient (PLT) and the collisional-radiative excitation specific line power coefficient (PLS). Altogether there are nine classes. The internal organisation of the data is different depending on whether they are stage to stage (data prefix 'U' or no prefix) or metastable resolved (data prefix 'R'). The data classes QCD and XCD do not occur in the stage to stage case. ADF11 data based on different qualities of calculation and of standard and resolved types are assigned a two-digit year number. '89' is standard state-to stage, unresolved baseline data. '96' is high grade partial, metastable resolved data.

A typical organisation of unresolved (standard) organisation for helium ACD is

nuclear charge		Log Ne (cm-3)		Log(Te) (eV)					
2	13	51	1	2	/HELIUM	/ ARNAUD-ROTHEN (NE SCALED)	9/11/90		
4.00000	5.00000	6.00000	7.00000	8.00000	9.00000	10.00000	11.00000		
12.00000	13.00000	14.00000	15.00000	16.00000					
-0.06466	0.03533	0.13534	0.23535	0.33534	0.43534	0.53534	0.63534		
0.73534	0.83534	0.93534	1.03533	1.13534	1.23535	1.33534	1.43534		
1.53534	1.63534	1.73534	1.83534	1.93534	2.03533	2.13534	2.23535		
2.33534	2.43534	2.53534	2.63534	2.73534	2.83534	2.93534	3.03533		
3.13534	3.23535	3.33534	3.43534	3.53534	3.63534	3.73534	3.83534		
3.93534	4.03533	4.13534	4.23535	4.33534	4.43534	4.53534	4.63534		
4.73534	4.83534	4.93534							
----- / Z1= 1 / DATE= 09/11/90									
-21.02274	-21.02448	-21.01428	-20.98969	-20.97136	-20.98573	-21.03465	-21.02173		
-20.82594	-20.37585	-19.79799	-19.26837	-18.92128					
-8.26043	-8.26360	-8.25394	-8.22642	-8.19355	-8.17223	-8.17398	-8.18895		
-8.20194	-8.20187	-8.19411	-8.18816	-8.19132					
----- / Z1= 2 / DATE= 09/11/90									
-36.43890	-36.43925	-36.43584	-36.42578	-36.40593	-36.37265	-36.31938	-36.23863		
-36.10640	-35.80753	-35.19548	-34.17990	-32.98088					
-9.04721	-9.04720	-9.04707	-9.04648	-9.04495	-9.04234	-9.04021	-9.04073		
-9.04481	-9.04660	-9.03791	-9.01206	-8.97073					

A typical organisation of unresolved (standard) organisation for beryllium ACD is

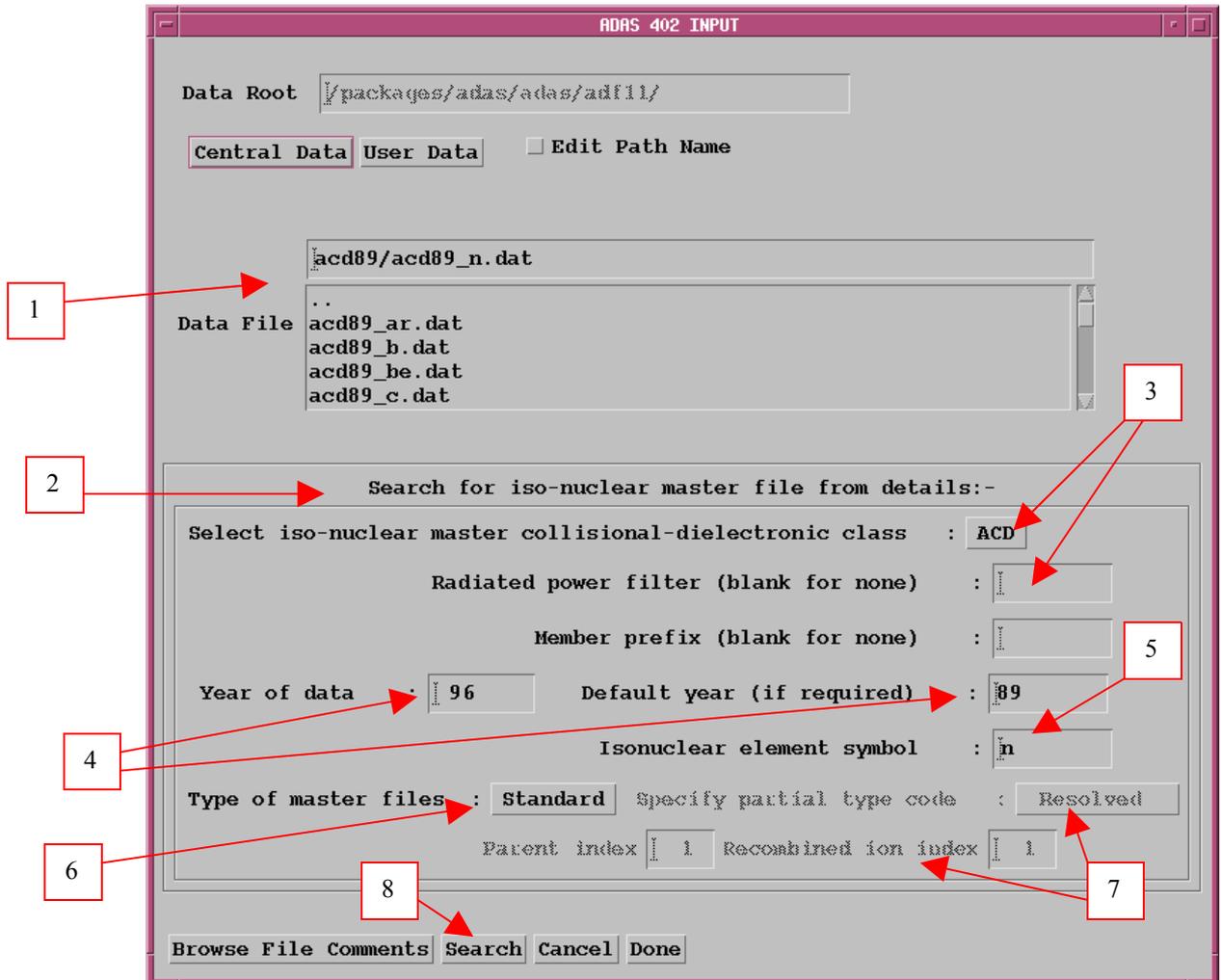
		Metastable partition							
4	26	35	1	4	/BERYLLIUM	/DICKSON ET AL 1992			
2	1	2	1	1					
10.00000	10.20003	10.40002	10.59999	10.80003	11.00000	11.20003	11.40002		
11.59999	11.80003	12.00000	12.20003	12.40002	12.59999	12.80003	13.00000		
13.20003	13.40002	13.59999	13.80003	14.00000	14.20003	14.40002	14.59999		
14.80003	15.00000								
0.00015	0.10016	0.20015	0.30015	0.40015	0.50015	0.60015	0.70015		
0.80015	0.90015	1.00015	1.10016	1.20015	1.30015	1.40015	1.50015		
1.60015	1.70015	1.80015	1.90015	2.00015	2.20015	2.40015	2.60015		
2.80015	3.00015	3.20015	3.40015	3.60015	3.80015	4.00015	4.20015		
4.40015	4.60015	4.70015							
----- / IPRT= 1 / IGRD= 1 / DATE= 16/11/93									
-11.57681	-11.55926	-11.53861	-11.51437	-11.48604	-11.45315	-11.41518	-11.37166		
-11.32210	-11.26598	-11.20285	-11.13244	-11.05561	-10.97341	-10.88689	-10.79719		
-10.70532	-10.61241	-10.51952	-10.42769	-10.33806	-10.25165	-10.16957	-10.09290		
-10.02268	-9.96003								
-7.20840	-7.21561	-7.22233	-7.22831	-7.23329	-7.23700	-7.23918	-7.23957		
-7.23791	-7.23394	-7.22740	-7.21811	-7.20627	-7.19216	-7.17605	-7.15822		
-7.13895	-7.11852	-7.09722	-7.07531	-7.05308	-7.03080	-7.00876	-6.98724		
-6.96650	-6.94684								
-6.85348	-6.85100								
----- / IPRT= 1 / IGRD= 1 / DATE= 16/11/93									
-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000		
-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000		
-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000		
-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000		

```
.  
.   
-9.42566 -9.42504 -9.42431 -9.42348 -9.42260 -9.42169 -9.42080 -9.41994  
-9.41916 -9.41849 -9.41796 -9.41761 -9.41747 -9.41757 -9.41794 -9.41862  
-9.41964 -9.42102 -9.42267 -9.42448 -9.42633 -9.42810 -9.42968 -9.43096  
-9.43182 -9.43215  
-----  
C  
C  
C RATE COEFFICIENTS IN UNITS OF CM**3 S-1  
C -----  
C  
C PREPARED USING CODE JETXLE.IONBAL.FORT(WJD404R)  
C  
C WILLIAM J. DICKSON 16/11/93  
C-----
```

## ADAS402

The code interrogates iso-nuclear master files of type ADF11. It extracts collisional radiative coefficients of various classes relevant to plasma modelling stored in iso-nuclear sequence sets. The data may be interpolated using cubic splines to provide the coefficients at a selected charge state of the chosen element and at selected electron temperature/electron density pairs. A minimax polynomial approximation is also made to the data. Interpolated data and some comparative source data are displayed and a tabulation printed. The printed output includes the minimax polynomial approximation.

The **file selection window** is illustrated below. Conventional file selection and selection via a directed search are possible.



1. Buttons are present to set the data root to that of the *Central data* or to your personal *User data* (provided it is in ADAS organisation). Alternatively the 'data root' may be edit explicitly. Available data sets are shown in the file display window. Selection is made by clicking on the appropriate name, whereupon it appears in the selection window above.
2. There are very many data sets of type *adf11* grouped by year, element and data class. A search strategy is available based on initial identification of an group of files of particular year and type and then conventional selection from the group list.
3. For dataset search, select the iso-nuclear master class first. A drop-down menu is offered. The radiated power data classes (PLT, PRB and PRC) can include the attenuation due to an energy filter. Enter the filter if required. At this stage only a very limited amount of filtered power data has been placed on the workstation database. The naming convention is defined in the *adf11* specification. To allow further distinction of data within the

same year, a prefix can be used within the dataset name structure (eg. *acd93r\_<prefix>.o.dat*). Enter this if required at *Member prefix*.

4. Enter the two-digit year number of the data required at *Year of data*. A *Default year* may be entered which will be used if there is no data of the required class in the *Year of data*.

5. Enter the *Iso-nuclear sequence symbol*.

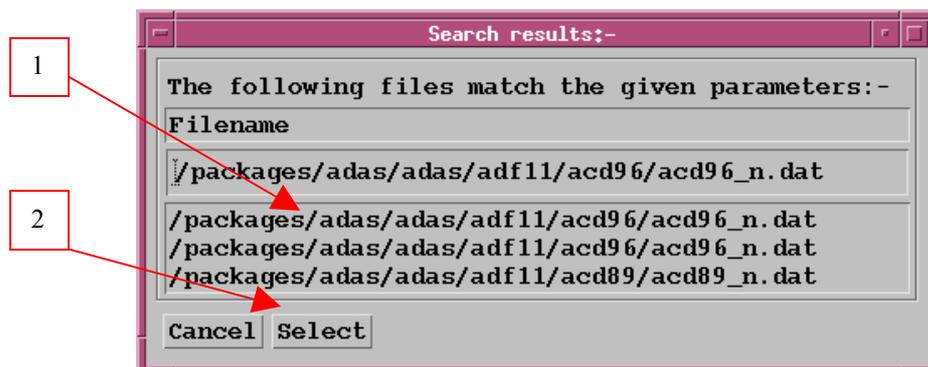
6. There are two primary organisations of adf11 data, Standard (ionisation stage to ionisation stage) and Partial (metastable to metastable). Select the type required in the drop-down menu at *Type of master file*.

7. If Partial is chosen, further selections may be made. Within the Partial type of organisation, true metastable to metastable subdivided data is called Resolved. Stage to stage data can be written into the Partial type of structure and is then called Unresolved. This un-necessary duplication is because of a historical precedent in IBM-ADAS at JET. Select as required in the drop-down menu at *Specify partial type code*. Finally within the Resolved type enter the particular metastable to metastable sought at *Parent index* and *Recombined ion index*. Note that the items selected here are only used when the dataset is opened at the Processing Options stage.

8. Initiate the search for the required dataset sub-list by clicking *Search*.

The **search result window** has the appearance shown above

1. If there is a choice of files, click on the one you wish.
2. Return to the input window by clicking *Select*.



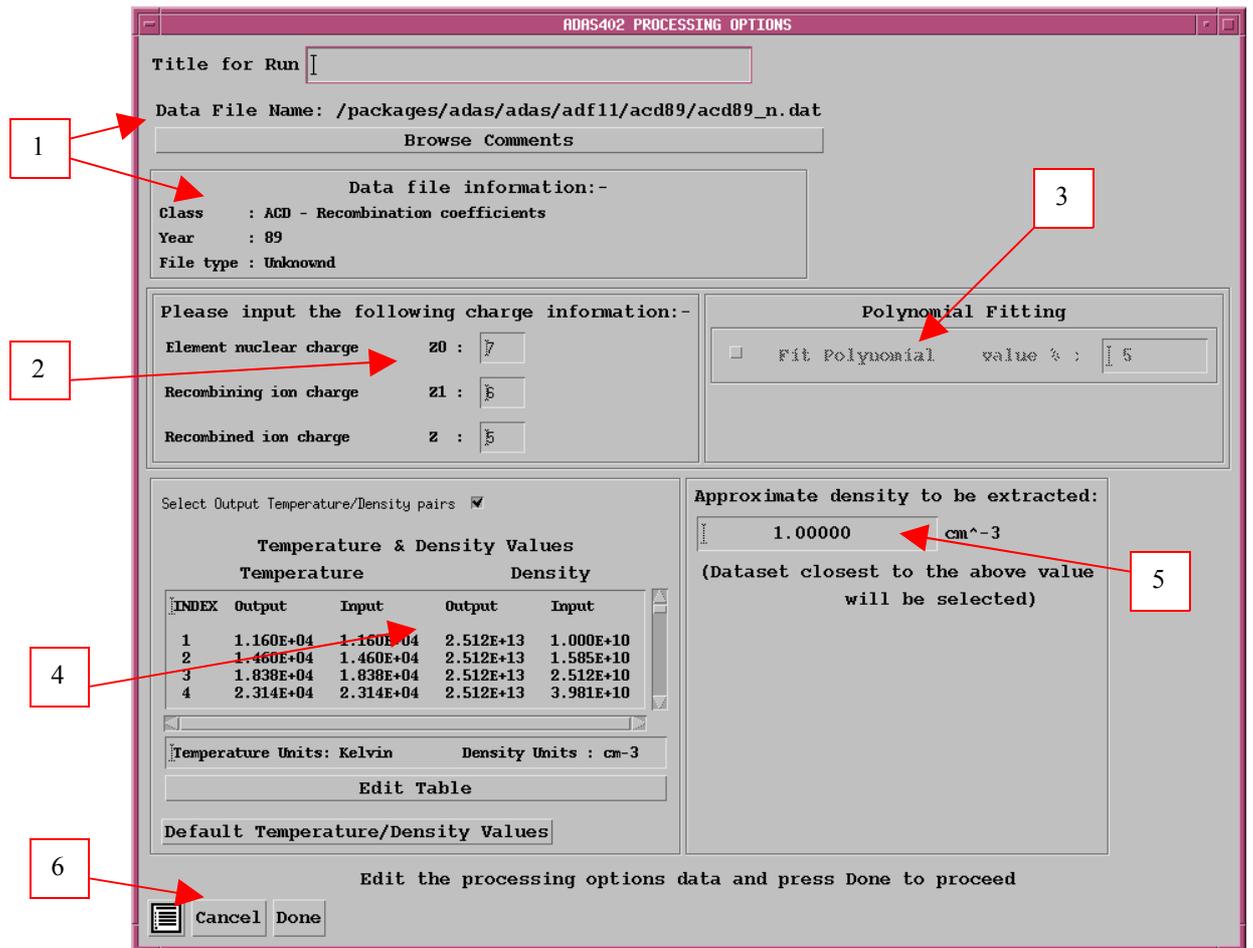
The **processing options window** has the appearance shown below

1. Data file and iso-nuclear sequence information is given.
2. A particular charge state of the iso-nuclear sequence should be selected. This is by entering any one of the three fields, namely, element nuclear charge (nuclear charge number or symbol), recombining ion charge or recombined ion charge
3. The extracted data is interpolated by a cubic spline to the selected ion and user temperature/density pairs for graphical display and tabular output. Additionally a polynomial approximation may be obtained by making the appropriate selections.
4. Select temperature and density pairs for data output (Output). The source data is held in two-dimensional arrays, that is as a function of electron temperature and electron density. The source (Input) values are also shown. The table may be edited by clicking on the *Edit Table* button..

The ADAS Table Editor window is then presented with usual set of editing operations available.

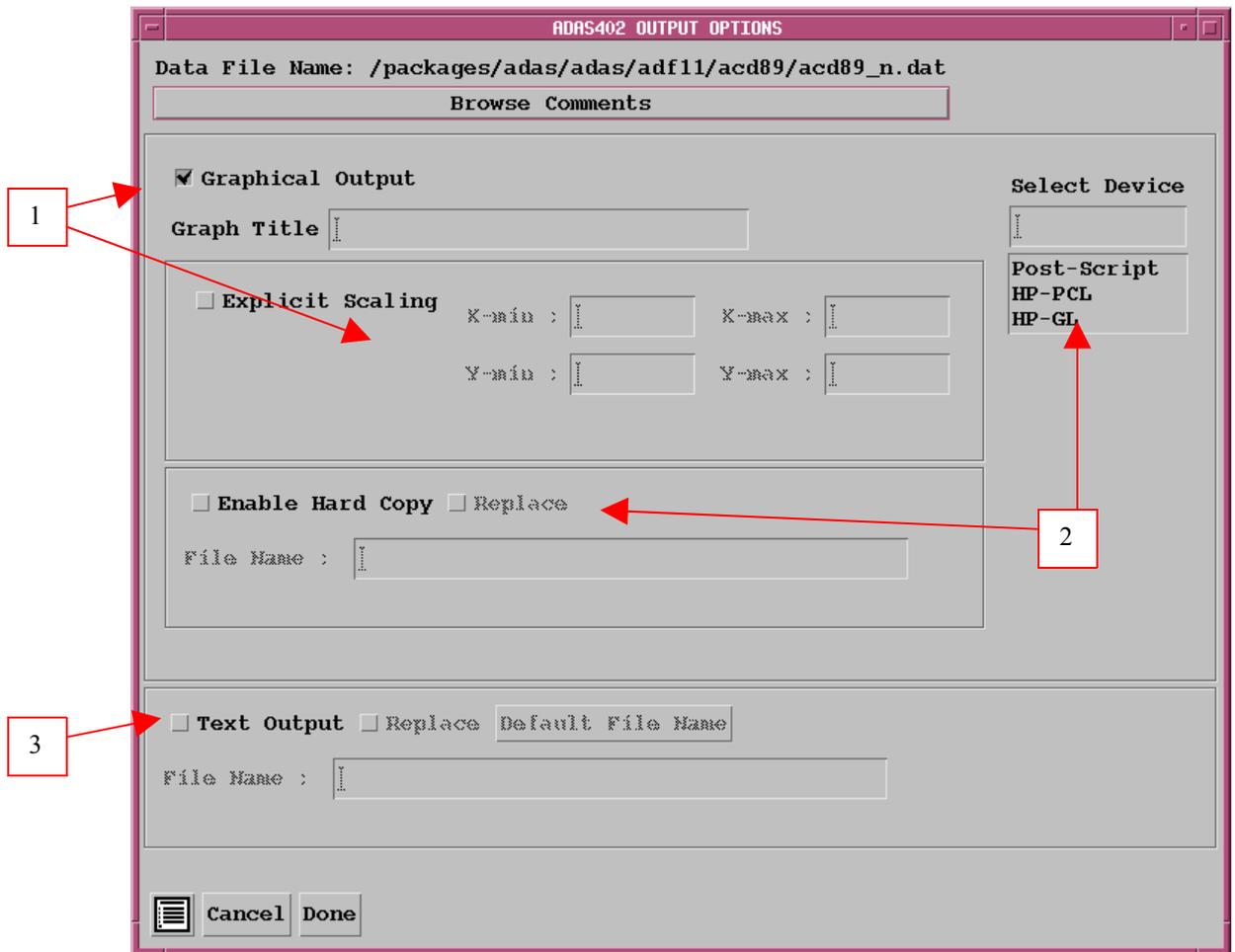
5. The displayed graph of the interpolated coefficient as a function of electron temperature also shows some additional curves from the dataset for comparison. These additional curves are drawn directly from the dataset and are not interpolated. Thus they must be at fixed electron density. Specify the *Approximate density to be extracted*. The nearest fixed density in the dataset will be used for the comparative curves.

6. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window. The *Escape to Menu* icon is also available for a quick exit at the bottom left hand corner.

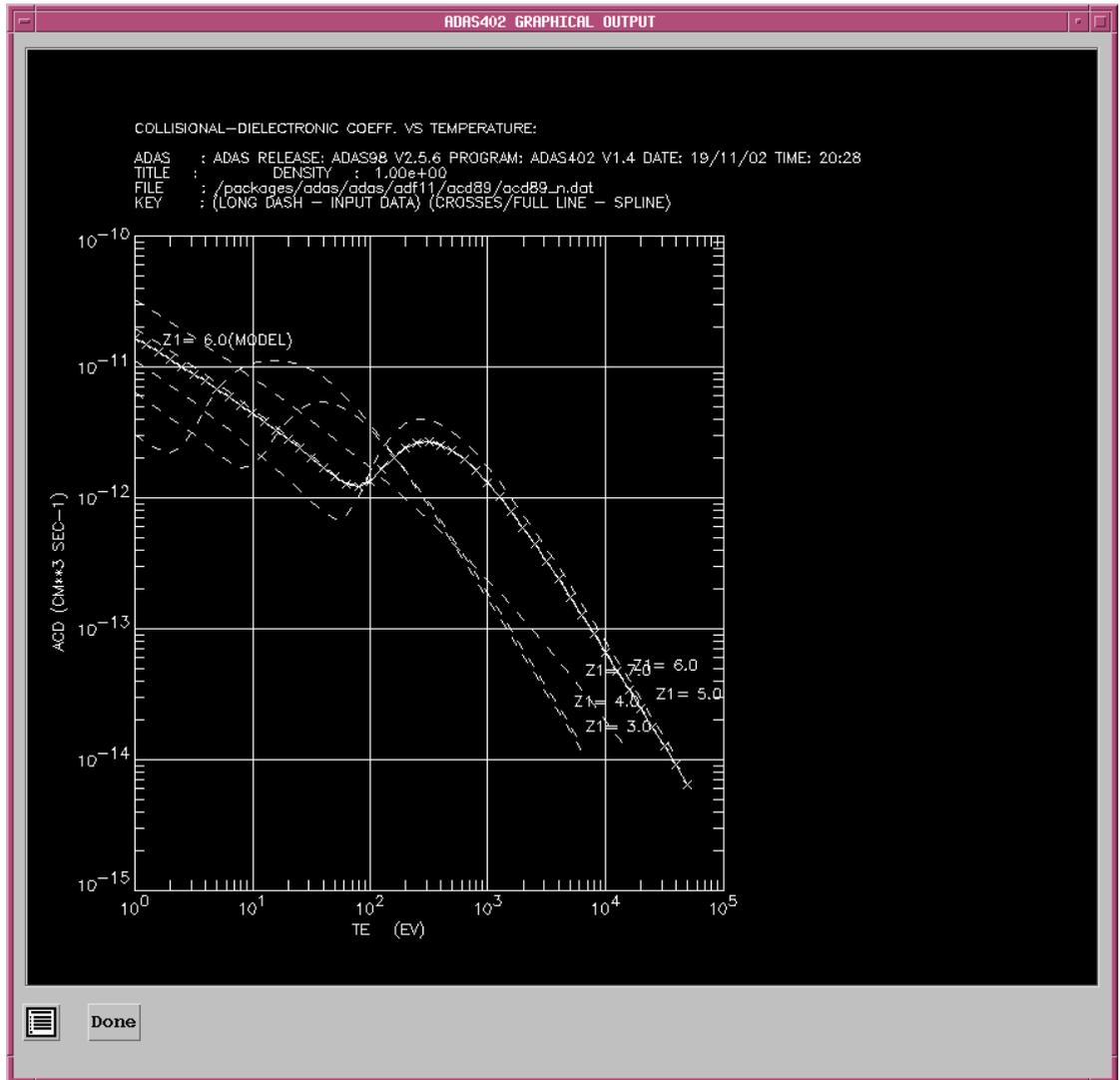


The **Output options window** is shown below. Broadly it follows the pattern of other ADAS interrogation codes.

1. Graphical output is enabled by clicking on the button. Default scaling of graphs may be over-riden by appropriate selections.
2. Hard copy may be enabled and the type of output device selected.
3. As usual a line printer text output file summarising the interrogation may be produced.



The graphical output is as shown below.



## ADAS405

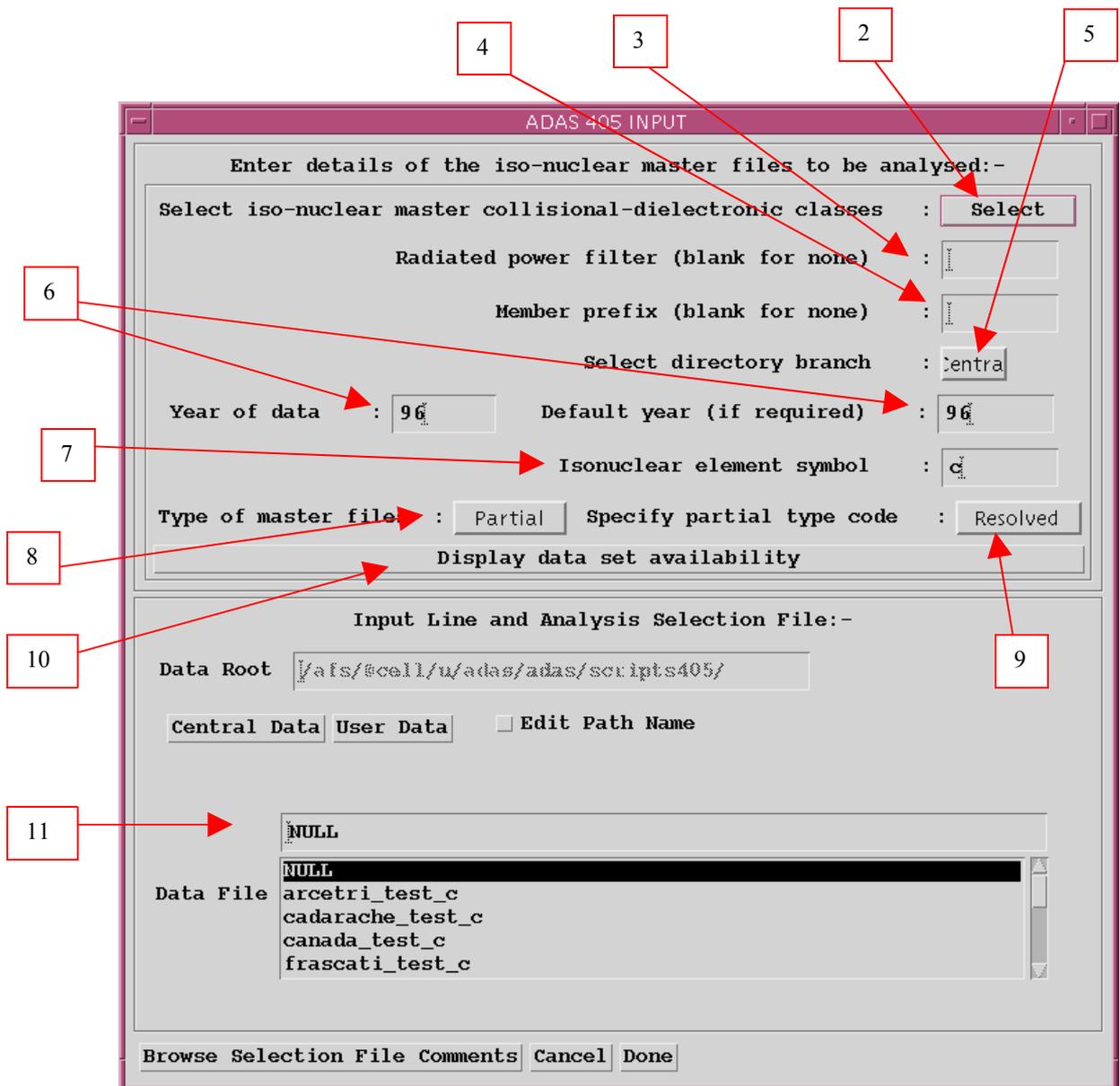
The program calculates the fractional abundances of resolved metastable or unresolved stage populations of the ions of an element in equilibrium in a thermal plasma. It also evaluates the radiated power function and line emission contribution functions. The evaluation of emission functions (and ratios of emission functions between lines of possibly different ions of the same element) is controlled by a 'script file'. This specifies the composition of the lines required.

The **file selection window** appears first as illustrated below

1. Two types of data file are identified in the file selection, namely, the iso-nuclear master files required for the ionisation balance and power calculations and the script file. The top part of the file selection window is concerned with identifying the master file data required and the lower part with identifying the script file.
2. Click on the *Select* button to drop down a selection list of master file data classes. Activate the buttons at the data classes required for your analysis. It is obligatory to select the 'acd' and 'scd' electron impact effective recombination and ionisation data classes since otherwise an ionisation balance cannot proceed. However the other data classes selected are at the

user's choice. This enables investigative studies of the importance of different contributions for example to radiated power.

3. Effective radiated power coefficients ('prb', 'plt' and 'prc') are often made available both as the whole emitted power and as the power which would pass through certain filters (such as Be/Si windows). The filter is specified either simply as an energy cut-off (eg. *ev2000*) or as filter specification (eg. *fl235*). These codes appear as an extension in the relevant master file names. Specify the filter choice.
4. Some flexibility for subdivision within a data year is provided by allowing a two character 'member prefix' (eg. 'pj') which may be present in the final part of a file name (eg. *./.../acd93r/acd93r\_pj#c.dat*).



5. Select the directory branch, that is the central ADAS or user data area.
6. Select the year of data. In general the two digit year number is used to provide the main groupings of data. Thus '89' is the standard, unresolved, JET base line data of low precision but fairly complete. '93' is metastable

resolved data, but available only for light elements of primary importance to fusion. Note that a default year must be specified. Often the complete set of data classes for a particular year and type are not available and the capability of filling in from a default (perhaps less accurate but more complete) year is allowed.

7. Specify the element.
8. Specify the type of master file. The distinctions between *standard* and *partial* master file types and *resolved* and *unresolved* types must be clarified. *Standard* data is stage to stage and has a specific layout. *Partial* data distinguishes metastables and has a different layout.
9. Within the partial data layout specify the partial type. It is possible simply to have each stage represented only by its ground state and therefore to be similar to standard data. However the layout is the partial one. We call such data *partial* but *unresolved*. The usual *partial* data with metastables present is called *resolved*. This distinction and added flexibility are helpful in iso-nuclear master file preparation and archiving.
10. Clicking the *Display data set availability* button at causes display of a file availability summary window as illustrated below. It is important to use this facility since it shows which master files classes sought by the user were not available, where default data files were substituted etc.

Class selection and file availability:-									
Class	Year	Element	Member		Type	USER DATA		DEFAULT DATA (96)	
			Prefix	Filter		Selected	Available	Used	Available
acd	96	c			RPartial	YES	YES	no	YES
scd	96	c			RPartial	YES	YES	no	YES
ccd	96	c			RPartial	no	YES	no	YES
prb	96	c			RPartial	YES	YES	no	YES
prc	96	c			RPartial	no	YES	no	YES
qcd	96	c			RPartial	YES	YES	no	YES
xcd	96	c			RPartial	YES	YES	no	YES
plt	96	c			RPartial	YES	YES	no	YES

All requested files available from user data sets.

OK

8. A script file selection may be made. The structure of script file is shown below. We have found it convenient to group script files in a personal ADAS database under a subdirectory classification */scripts405/*. Also, it is possible to bypass contribution function calculation and display by selecting the *'NULL'* script. You may find it helpful to copy the *'NULL'* script from the central ADAS database to your own space. Note that scripts apply to particular cases. Thus the references to emissivity coefficient data in a script applying to metastable resolved will not in general work for unresolved data, indeed will probably crash. We have not built much protection against faulty references into script files at the moment. More protection may be added if this proves a stumbling point for users. You may find it helpful to fetch the *test\_c* script from central ADAS for first trials.

A **script file** is illustrated below. Details of the species, number of (composite) lines and line ratios to be obtained are at the head of the file (SPECIES, NLINE, NRATIO). Note that you must follow the positional layout exactly. Emissivity coefficient data are obtained from *'pec'* files of ADAS format ADF15. The number of such files to be searched in the ADAS database are specified at NFILE and the full Unix paths to the files themselves in following lines at PHOTON EMISSIVITY FILE NAMES. The subsequent table identifies the index number of the *pecs* in these files required to build the particular line emission function. The lines are indexed at ILINE, the number of component parts of each line is at NCOMP, the charge of the ion to which the component attaches is at IZION and the components simply indexed at ICOMP. The metastable of the ion to which the component is attached is specified

by its ranked index number at IMET (the ground state is 1). INDPH gives the selection index of the component *pec* in the ADF15 file identified at IFILE from the list given earlier. Note the letter qualification on the INDPH index to distinguish electron collision driven *pecs* and charge exchange driven *pecs*. The composite lines may be ratioed as specified by IRATIO, an index number of the ratio; ILINE, the upper composite line of the ratio; JLINE, the lower composite line of the ratio. All other text is for information. Note that a 'c-----' line is used to separate comments which follow it. Each comment line begins with 'c' and we conventionally put in a 'c-----' terminator line for the comments section.

```

SPECIES = C
NLINE = 2
NRATIO = 1
NFILE = 4
PHOTON EMISSIVITY FILE NAMES = JETSHP.PEC93#C.DATA (PJR#C0)
                                JETSHP.PEC93#C.DATA (PJR#C1)
                                JETSHP.IONELEC.DATA (PEC#C3)
                                JETSHP.IONELEC.DATA (PEC#C4)

-----
ILINE  NCOMP  IZION  ICOMP  IMET   INDPH  IFILE  TITLE
-----
   1     4     0     1     1     1E     1     CI    1561A
           0     2     2     2     54E     1
           0     3     3     107E    1
           0     4     4     160E     1
-----
   2     2     1     1     1     3E     2     CII   904A
           1     2     2     25E     2
-----

IRATIO  ILINE  JLINE  TITLE
-----
   1     1     2     CI ( 1561A)/CII ( 904A)
-----

C-----
C ANALYSIS OF CARBON EMISSION.
C
C   LINES INCLUDED:
C           1.  CI,    1561A
C           2.  CII   904A
C
C
C-----
C CODES:
C   IMET - Trailing '+'      => IZION+1 metastable
C         <blank>           => IZION  metastable
C         trailing '-'      => IZION-1 metastable
C
C   INDPH - Trailing 'E'or <blank> => Electron coll. driven
C         Trailing 'H'       => Hydrogen CX  driven
C
C-----

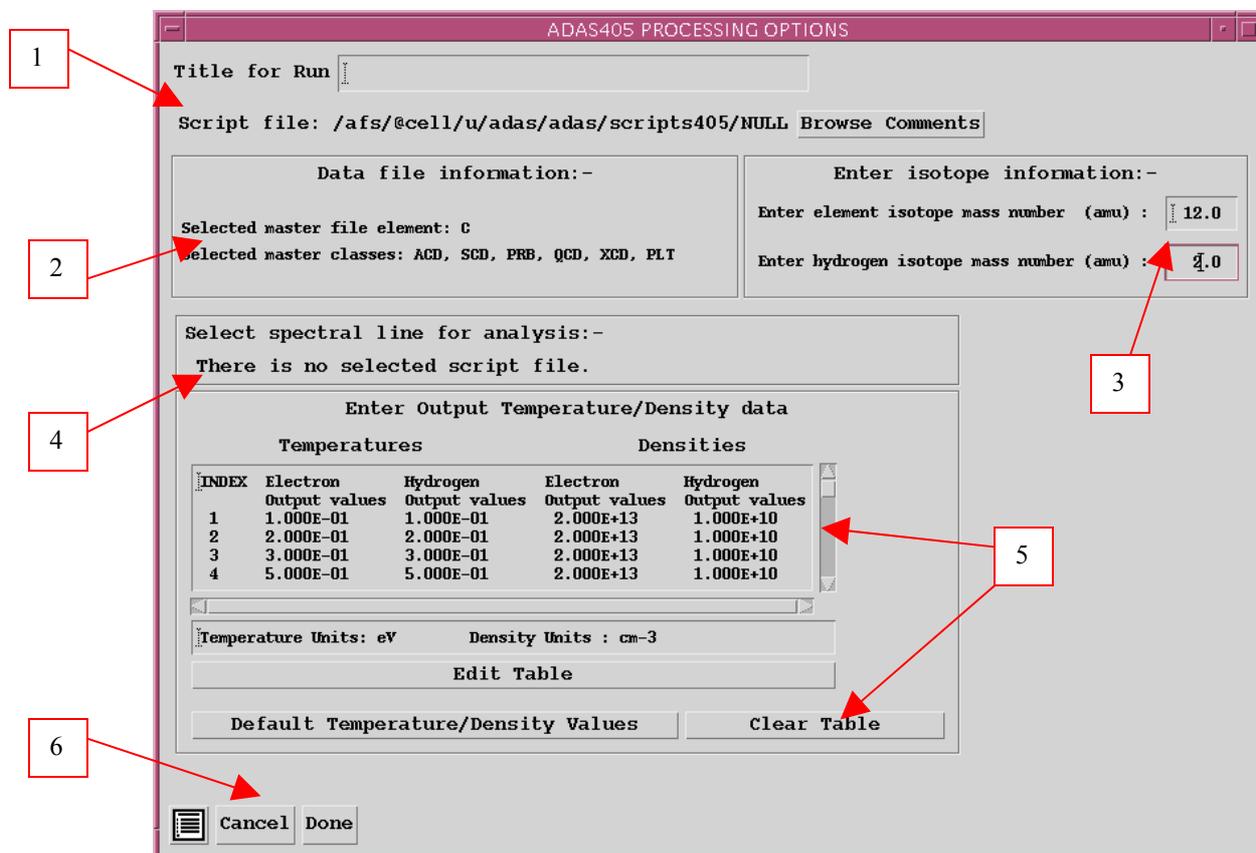
```

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

1. The script file selected by the user is identified at (a). The *Browse Comments* button displays the comments field at the foot of the script file.
2. Information is presented of the element and master files classes selected in the previous file selection option step.
3. Enter isotope mass numbers for the selected element and background neutral hydrogen in the plasma. This information is only used if charge exchange recombination master file data has been selected.
4. The spectrum lines set up in the script file are shown in the display window. This operates in the same manner as dataset display and selection windows in the input option window of a code such as ADAS205 (see chapter 2). Click on a line to select it. The selected line is shown in the selection window above the display window. Only one line is treated at a time for graphical display. However all lines and line ratios in the script file are computed and tabulated in the output text file.
5. Select temperature and density pairs for data output. The table may be edited by clicking on the *Edit Table* button.. The ADAS Table Editor

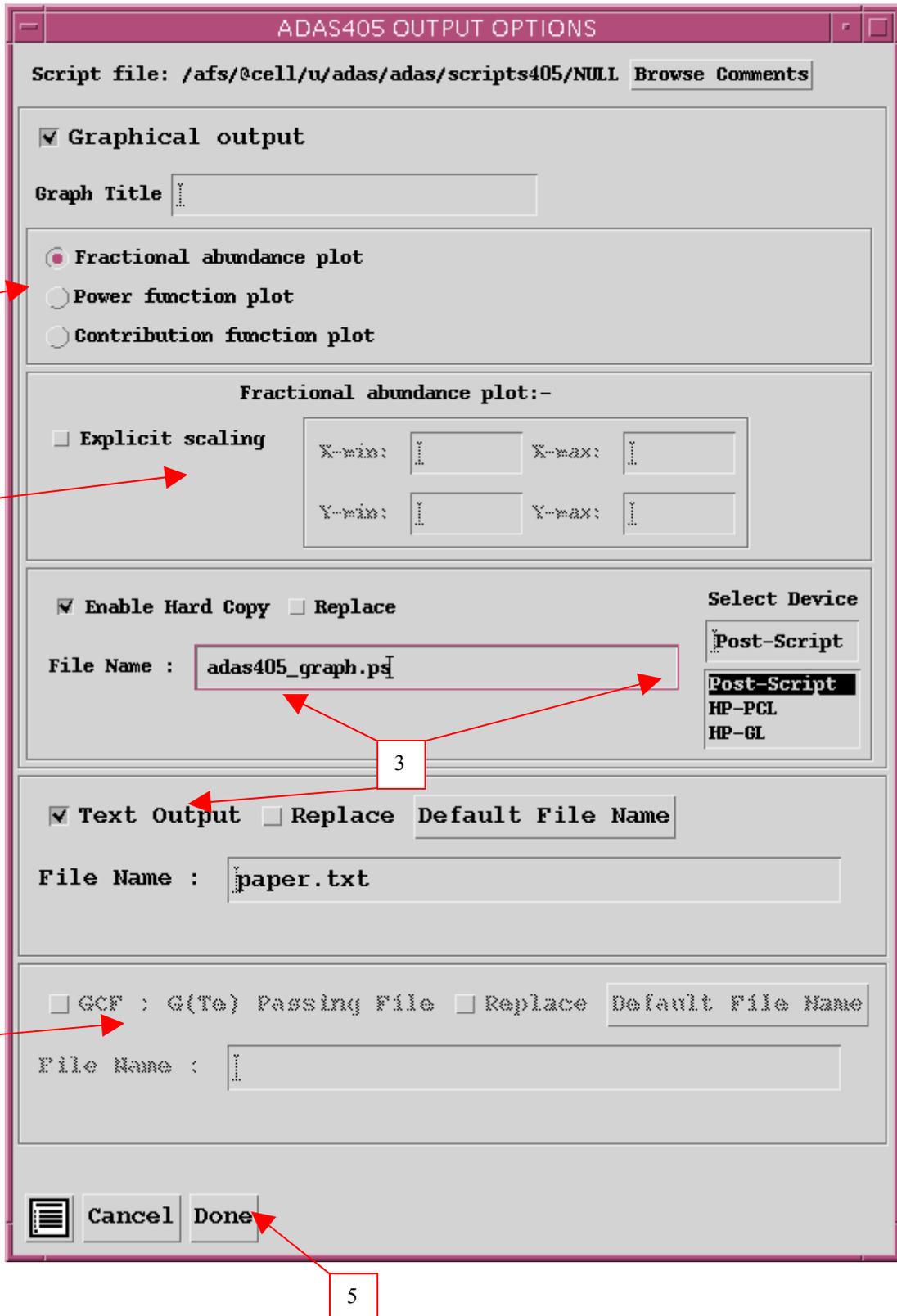
window is then presented with the same set of editing operations available as are described in the introductory chapter. Electron temperatures should be monotonic increasing. It has proved helpful to add a *Clear Table* button to remove all entries in the temperature and density output fields.

6. 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.

1. It follows the usual pattern except that there is a choice of graphs to display. Thus the fractional abundances, power functions and contribution functions are all of potential interest. Click on the appropriate button. Generally, we find that on the first one or two occasions we wish to see the fractional abundances and powers but then have a more sustained interest in the contribution function shapes and their location in temperature. All the graphs are provided as a function of electron temperature.
2. The sub-window presented depends on the graph choice above. The default scaling may be over-riden and explicit values for the graph limits entered.
3. Graphical output may enabled in the window together with hard copy device and output file name. This follows the pattern of other ADAS programs. Likewise text output selection is standard.
4. The '*Goft Passing File*' is the name used for the output dataset of calculated contribution functions. It is organised according to an ADAS data format ADF16. The widget is active only if a non NULL script file has been selected on input. Specify an output file name. Note that G(Te) functions of type ADF20 (*gft*) are organised differently and have a slightly different definition from the output here of generalised contribution functions of type ADF16 (*gcf*). The expected practice is that ADAS405 will be used either recursively or in distinct runs to examine contribution functions and then decide which to put into the Goft file.
5. An *Append* button has been provided to allow an existing output Goft file to be extended. The *Replace* and *Default file name* buttons have their usual meanings.



The **Graphical output window** is shown below

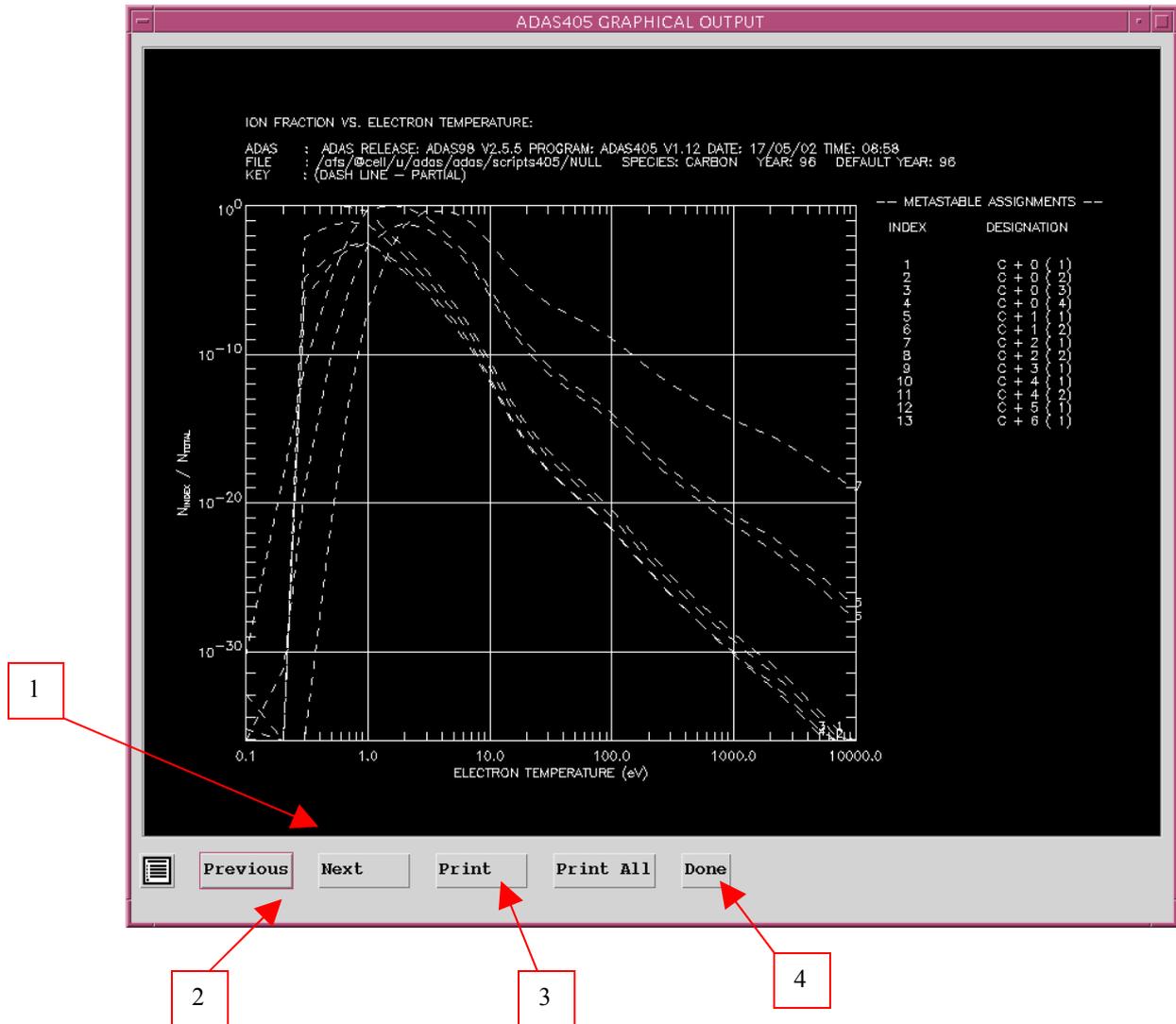
1. The graph has at its foot a *Done* button, and possibly *Next* and *Previous* buttons if there is a sequence of graphs to be displayed. A *Print*

and *Print all* button is also present if the *Enable Hard Copy* button on the previous window was activated.

2. Press the *Next* button to show the next graph in a sequence and the *Previous* button to show the previous graph.

3. Press the *Print* button to make a hard copy of the currently displayed picture. *Print all* makes a hard copy of all the pictures.

4. Pressing the *Done* button restores the previous Output Options window.



## Generating baseline ionisation, recombination and radiative power data

The main paths for moderate quality automatic ADF04 specific ion file creation available at present is:

COWAN STRUCTURE + BORN rate coefficients

giving files of group name

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

The specific ion files created by this method has 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

$$n_1 l_1^{s_1} n_2 l_2^{s_2} \dots n_m l_m^{s_m}$$

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

$$\{\epsilon_k : k = 1, \dots, m\}$$

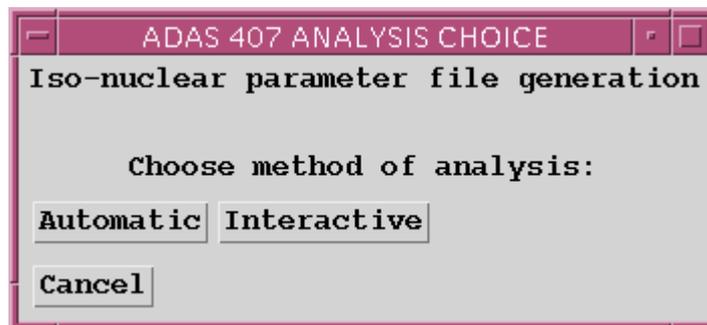
Apart from this enhanced rigidity in the use of the optional term naming character field, these files are of the standard ADF04 format.

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. ADAS407 is a semi-automatic generator of such parameter sets. ADAS408 uses these parameter sets to generate standard (unresolved, stage to stage) ADF11 files under the year number '89'. These baseline data are only of moderate quality but can be created rapidly for any element.

### ADAS407

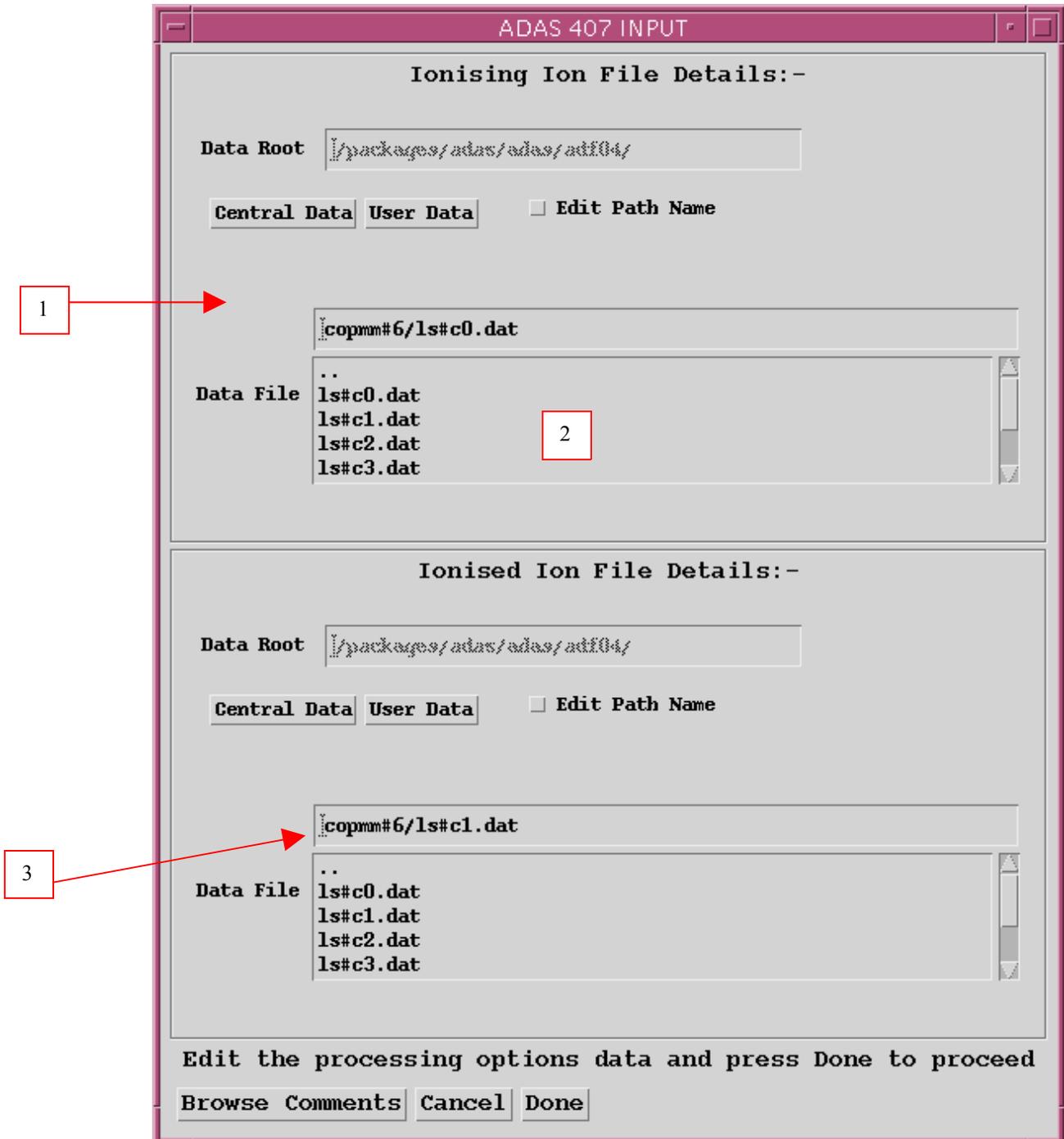
The code analyses specific ion files to obtain moderate accuracy numerical zero density recombination, ionisation and radiated power loss coefficient data. It deduces parameters of approximate forms for these coefficients which may be used to generate standard iso-nuclear master files.

The **analysis choice** window appears first as shown below.



The **file selection window** 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 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 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.



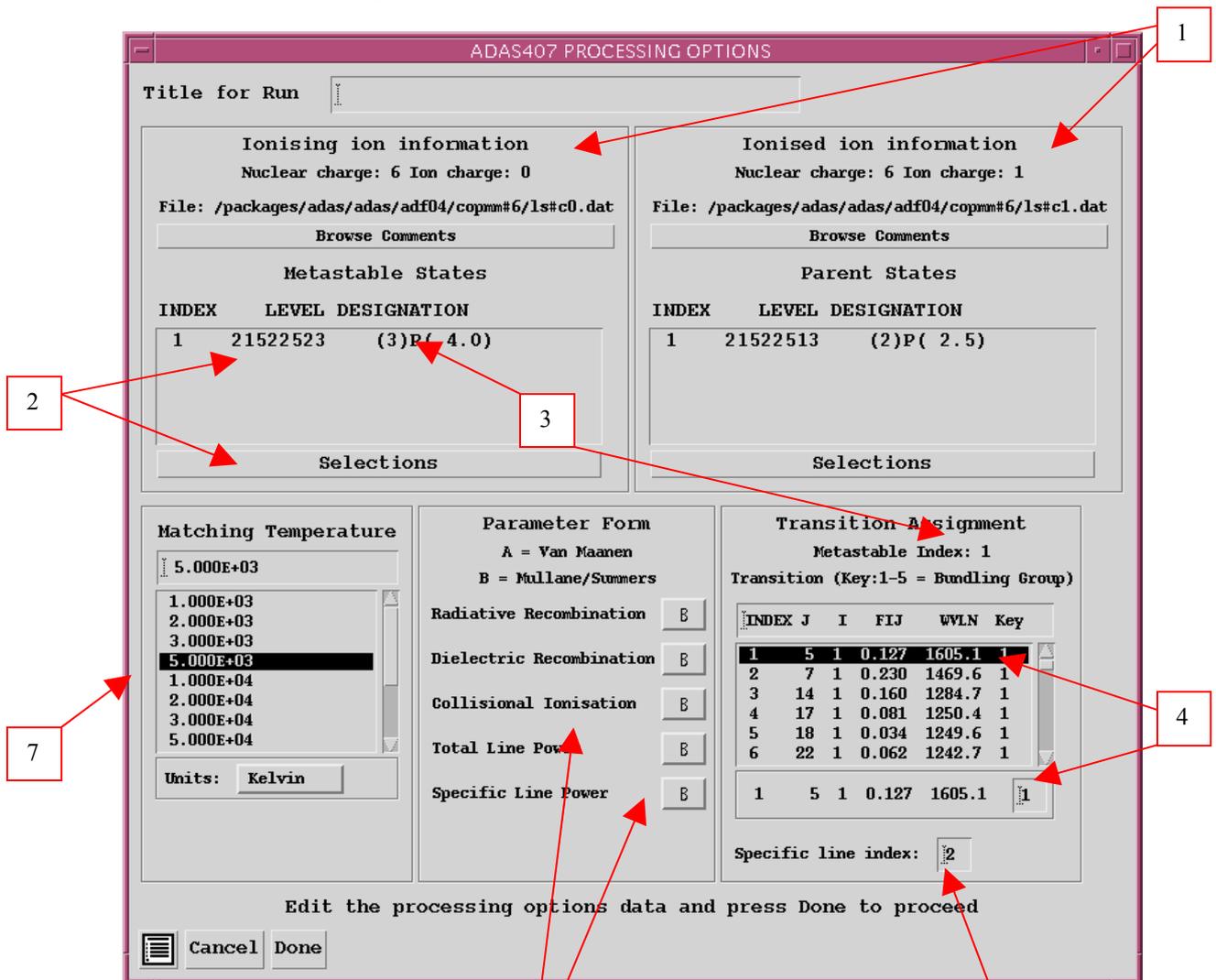
2. Available sub-directories are shown in the large file display window. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual data-files 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.

- 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-riden in the usual manner.

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

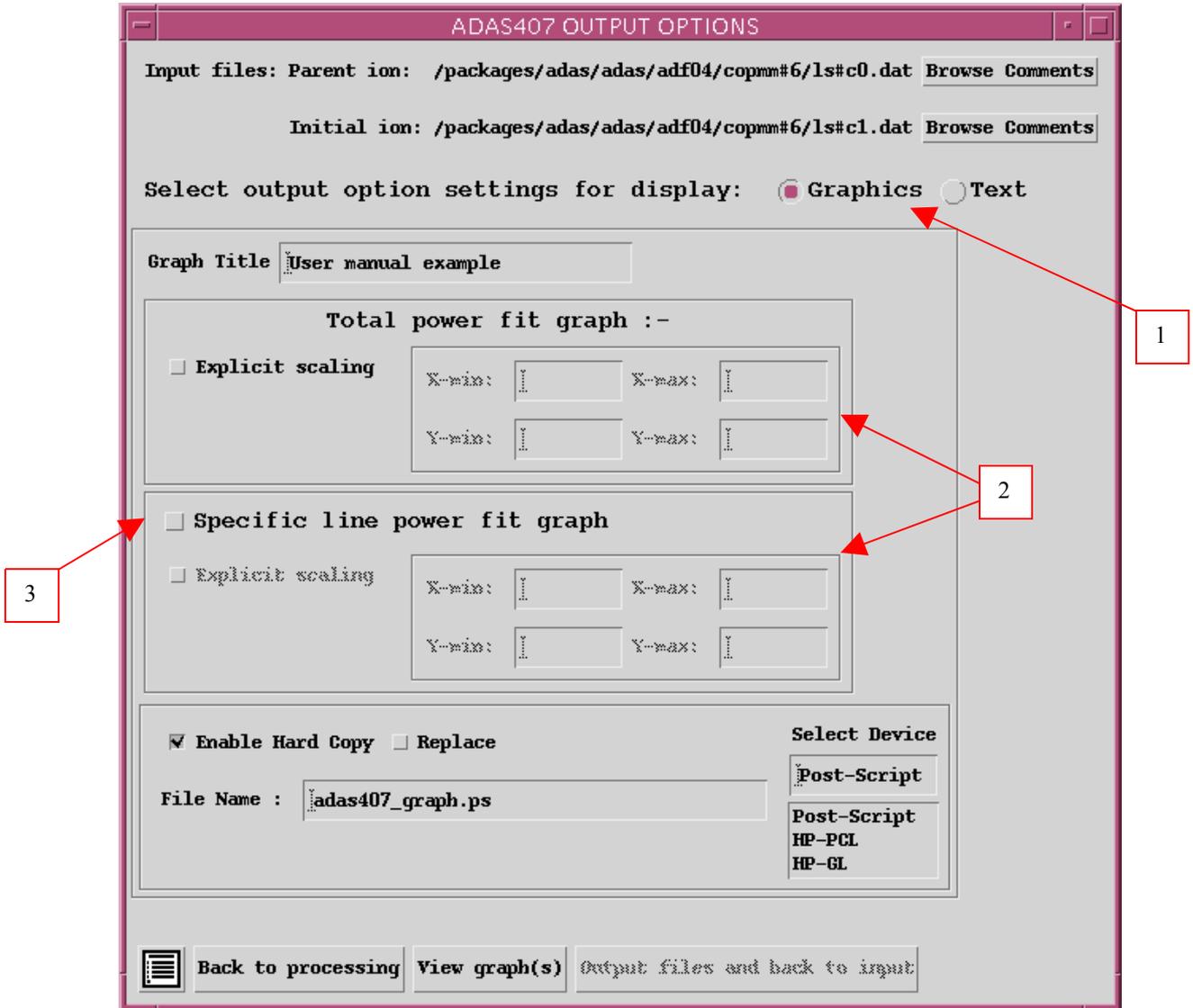
- At the top of the window, an arbitrary title may be given for the case being processed. Sub-windows for the ionising and ionised ions appear side by side below this. Summary data of the ions and the files opened are given first. The button *Browse Comments* in each sub-window again allows display of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



- The **6** of the ionising and ionised ions to be **5** at as metastable must then be decided. For the ionising ion, we choose 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. The '21522523' means  $1s^2s^2p^2$  in 'Eissner notation' (see the ADAS User Manual for more details).

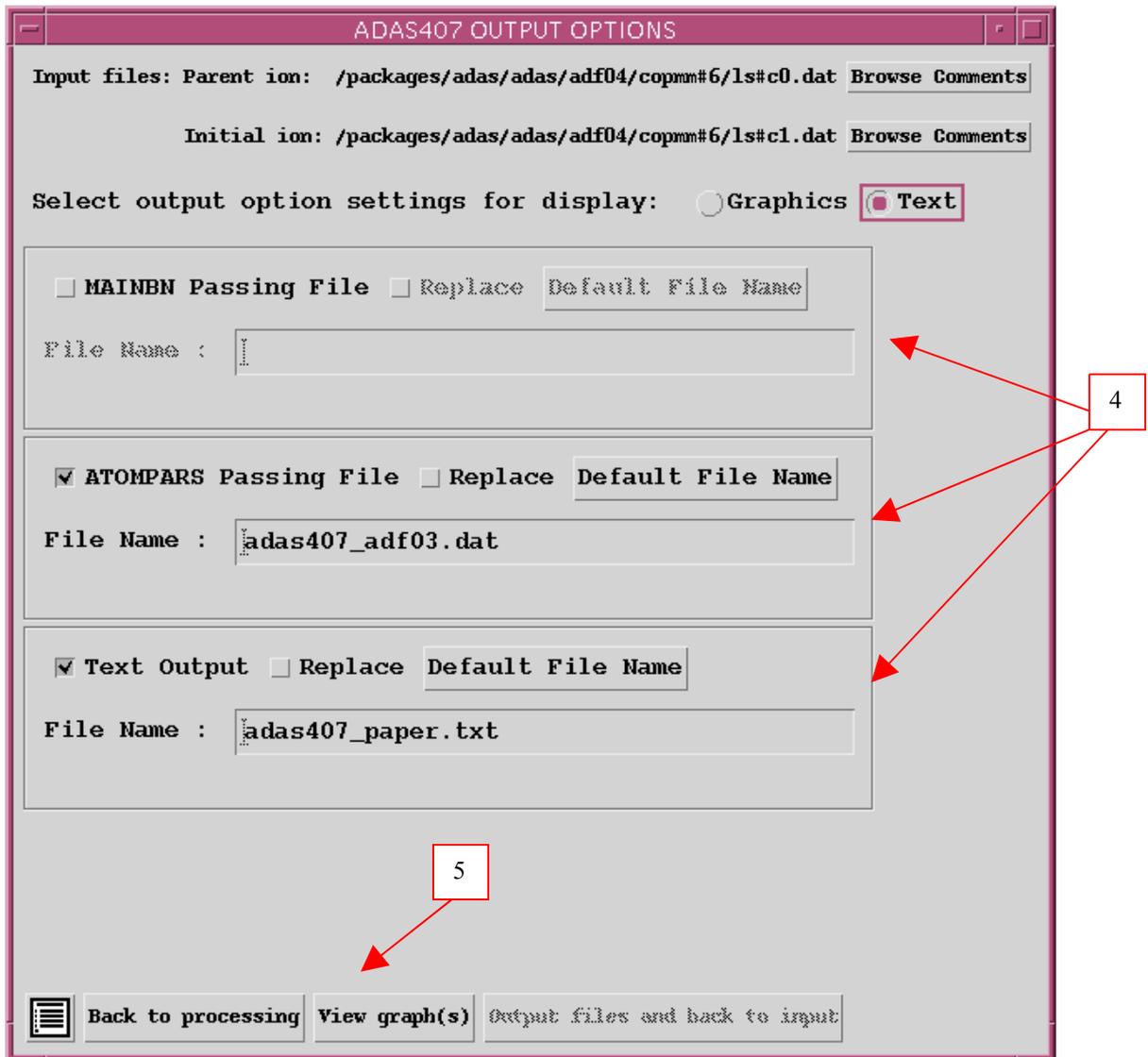
- Click on the particular driving metastable of the ionising ion whose associated radiated power loss is to be analysed and displayed. This choice

appears in the lower right sub-window,. In this 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.



4. 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.
5. 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.
1. 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. 5 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.

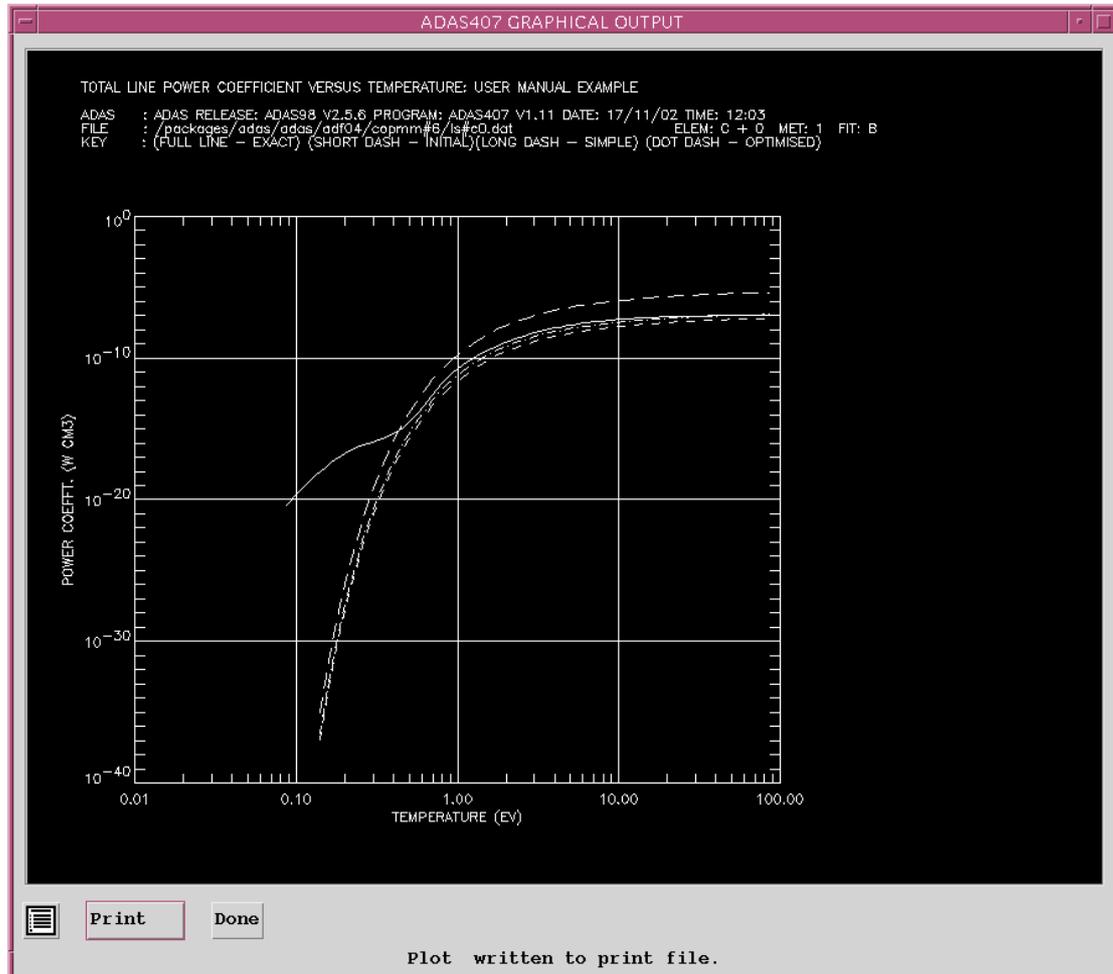


7. For the total zero density line radiated power, the specific ion files allow quite an accurate numerical estimate. Choose an electron temperature in the sub-window at which you wish the approximate form and accurate numerical values to agree.

The **output options window** is shown above. 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. As usual, the input specific ion files under analysis are shown and can be browsed. Two buttons have been added, 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.
- 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.
  - Click the appropriate box if you wish the specific line power fit graph. Default scaling of the chosen graph may be over-riden by appropriate selections. Below this the usual hard copy may be enabled and a choice of type of output device made.



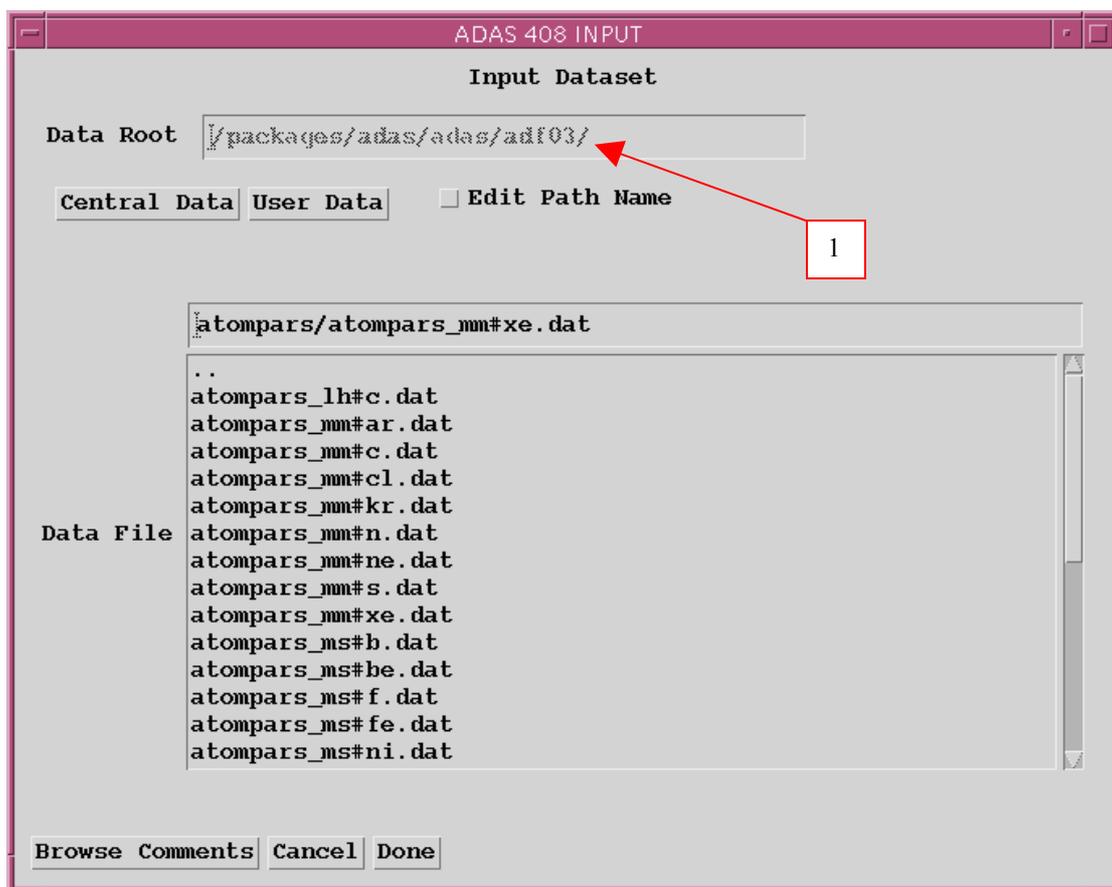
- In the Text case, three output files are permitted, namely, the standard line printer text output file summarising the interrogation, the 'MAINBN' file and the 'ATOMPARS' file. These are passing files which are placed by default in your /pass directory as *mainbn.pass* and *atompars.pass*. The MAINBN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

## ADAS408

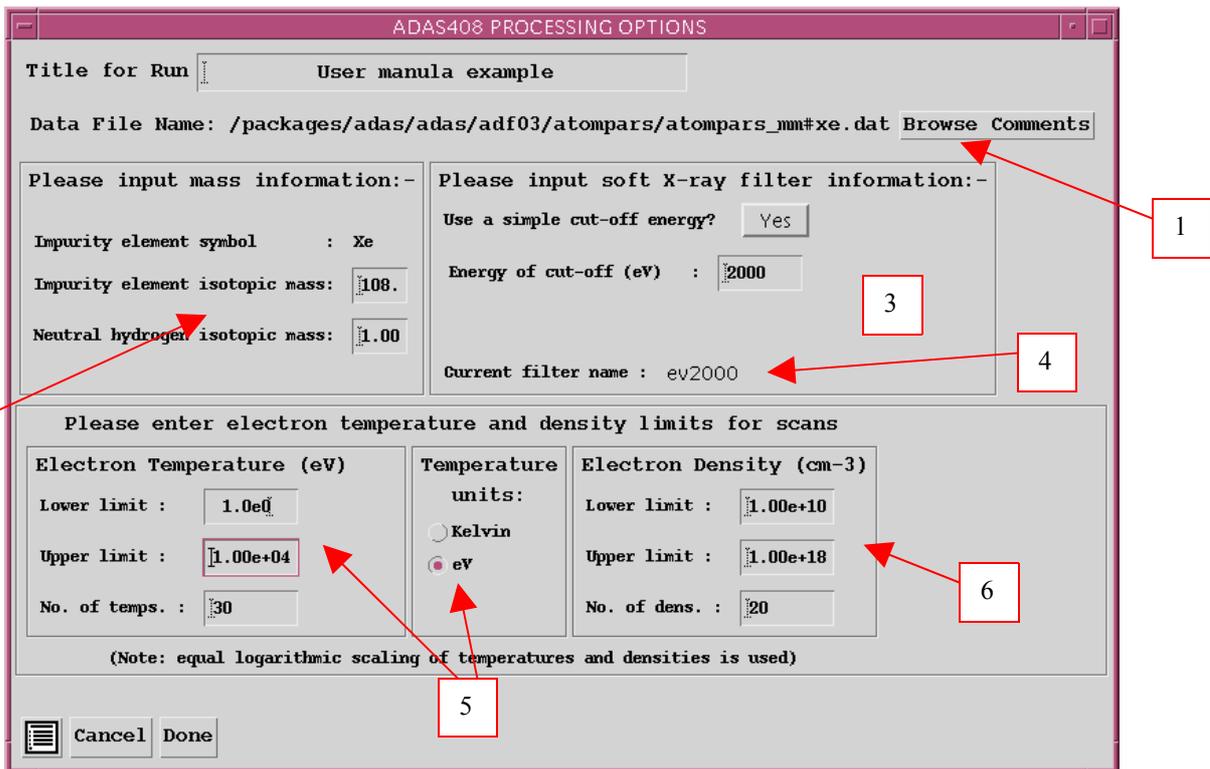
The program uses parametric forms for zero density recombination, ionisation and radiated power loss coefficients to prepare standard (unresolved, stage to stage) iso-nuclear master files for a particular element. The iso-nuclear master files may be prepared over arbitrary ranges of electron temperature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

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

1. Data root 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'). Operation of this file selection window follows the usual pattern.

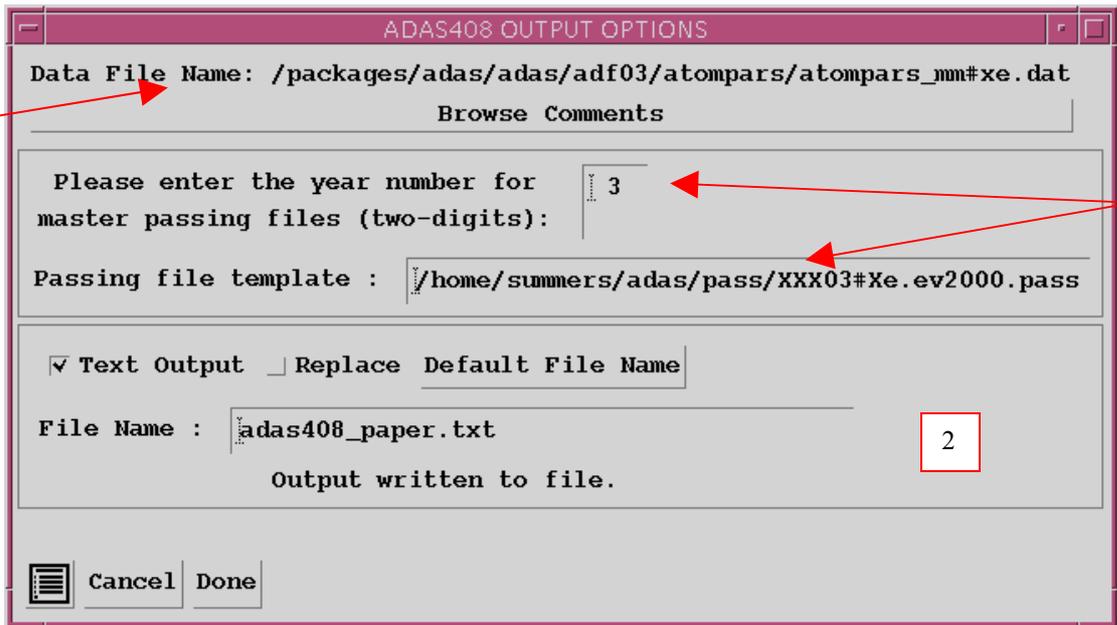


The **processing options window** has the appearance shown below



1. At the top of the window, an arbitrary title may be given for the case being processed. 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.
2. Enter the mass number for the actual isotope of the element of the atompars file present in the plasma. 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.
3. 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 to drop down a standard choice menu. In the beryllium/silica case thicknesses must be specified in the following two editable boxes.
4. 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.
5. The lower sub-windows allow the plasma electron temperature and electron density for production of the output *adf11* standard master files to be specified. For the temperatures, click on the required temperature units. This choice relates to the units used in the adjacent temperature range selection window. 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).
6. Similarly specify the electron density limits and number of grid points.

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



1. The name of the source atompars file to be used in the bulk generation of *adf11* data is repeated for information.
2. 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.
3. 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 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.

There is no graphical output option.

## Superstages and flexible partitioning

In the generalised-collisional-radiative picture, an element in a plasma is described by the abundances of all the metastables of every ionisation stage, by the effective recombination and ionisation coefficients which link them together and by the emission coefficients which are quasi-static with respect to and driven by these metastables. The complete set of populations, which are then in principle tracked in dynamic transport modelling, is large. However, not all populations are of equal importance and so grouping of populations may be appropriate. This is called a condensation and it reduces the problem to tracking the group populations with their equivalent effective recombination and ionisation coefficients and emission coefficients. The specification of a grouping is called a *partition*.

For example a parent partition with six members may be grouped into two child partition members with  $1_c = \{1,2\}$  and  $2_c = \{3,4,5,6\}$ . We can envisage a particular partition having parent and grandparent partitions and so on in *layers* back to a *root partition*. This is the basic idea, but it can be made more complete and consistent with earlier work in both the *CR* and *GCR* pictures.

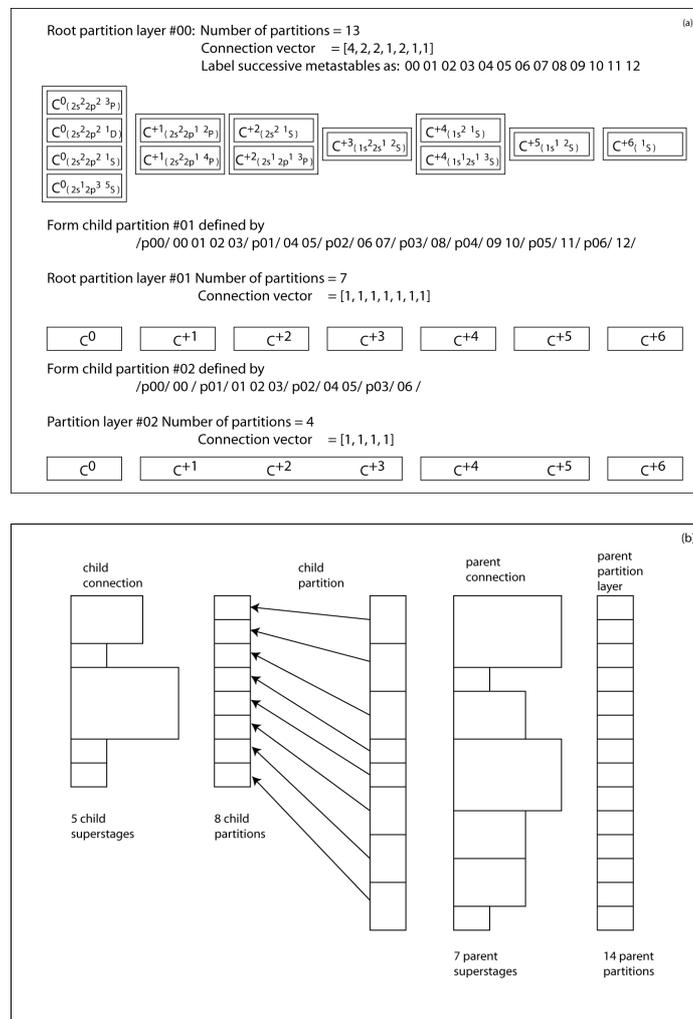


Fig: (a) Metastables of carbon in the resolved *GCR* picture. The child partition grouping to form the stage to stage picture is shown as the boxes enclosing the metastable sets. The connection vector specifies the metastables which are close-coupled. It corresponds in this particular illustration to the child partition grouping. (b) The general partitioning picture with independent child partition groupings and parent connection vector. Note that the child connection vector is determined from the child partition definition and the parent connection vector

Consider the metastables of carbon in the *GCR* picture, as shown schematically in figure-a. The complete set of thirteen metastables (including the bare nucleus) comprise the members of a partition. If the metastables of each ionisation stage are grouped together, then the child partition is composed of members which are the ionisation stages. Then further grandchild partitions can be formed as illustrated. There are really two starting points for partitioning, called the *#00* or *#01* root partition layers depending on whether we are in the *GCR* picture of resolved metastables or the unresolved *CR* picture. For computation, a partition is conveniently written as a string, so that the two root partitions layers for carbon appear respectively as

```
//#00//p00/00/p01/01/p02/02/p03/03/p04/04/
    p05/05/p06/06/p07/07/p08/08/p09/09/
    p10/10/p11/11/p12/12/p13/13/
```

and

```
//#01//p00/00/p01/01/p02/02/p03/03/p04/04/
    p05/05/p06/06/
```

The child *#01* stage-to-stage partition of carbon for computation from the *#00* root partition is

```
//#01//p00/00 01 02 03/p01/04 05/p02/06 07/
    p03/08/p04/09 10/p5/11/p6/12/
```

It should be noted that the metastables are not all on the same footing. Unlike ionisation stages which are each (usually) only coupled to the two adjacent stages up and down, the metastables are in groups which are close-coupled (for example the first four and the next two and so on). This close coupled grouping is specified by the *connection vector*, a name which will be familiar to those who have worked with ADAS *GCR* data. The connection vector for carbon in the *#00* root partition is (4,2,2,1,2,1,1). The connection vector is similar to a range vector and the range vector for grouping into the *#01* stage-to-stage partition from the *#00* root partition is the connection vector. Introduce a new name *superstage* for the members of a partition which are close coupled as specified by the connection vector. In the special case of the *#01* partition of carbon, the superstages are simply ordinary stages. The connection vector and range vector of a child partition are in the general case independent items. So a child partition can be formed from *#00* root partition which subdivides connected metastables into different child partition members and leaves a non-trivial connection vector for the child partition. This general case is illustrated in figure-b. With light elements, in usual plasma conditions, ionisation is a single electron loss process from ionisation stage. For heavy element ions, multiple electron loss through shake-down and shake-off is more likely. This would result in non-trivial connection vectors and superstages. The heavy element baseline has the root partition layer *#01* and in child partitions, the connection vector is trivially all 'ones'.

In practice, superstage condensation (bundling) is influenced by the shell structure of the element. There are two situations of interest at this time. Firstly there is aggressive condensation (bundling) aimed at enabling heavy elements to be handled with the same economy as light elements in sophisticated 2-d or 3-d transport codes. Secondly, there is condensation related to spectroscopy and the occurrence of quasi-continuum. It is in these contexts that the additional classes in the *adf11* data format and those in the *adf15* and *adf40* formats are determined for the child partition in the following two sub-sections.

### The natural partition and spectroscopy

Ions with closed shell configurations have an extended region of existence (in electron temperature) in a plasma. They and adjacent alkali-like ions are significant radiators of a resolvable line spectrum of diagnostic value. Sets of ions associated with a partially filled shell, particularly for heavy species, give a complex overlapped spectrum which is difficult to identify and resolve. They are usefully grouped. A map of the fractional variation of ionisation potential  $2(I_{z+1} - I_z)/(I_{z+1} + I_z)$  between successive ions of every element, as shown in the figure-a below, highlights the shell structure. We select ions corresponding to peaks and their immediate neighbours as individuals in a partition and group the others. Setting a fraction of the a running mean as a variance for stage individualising allows automatic partitioning. We call this the *natural partition*.

It is useful to be able to preview the natural partition and its approximate implications for the temperature distribution of superstages before executing the substantive generation of a complete ADAS data for a new child partition layer. An IDL procedure accomplishes this:

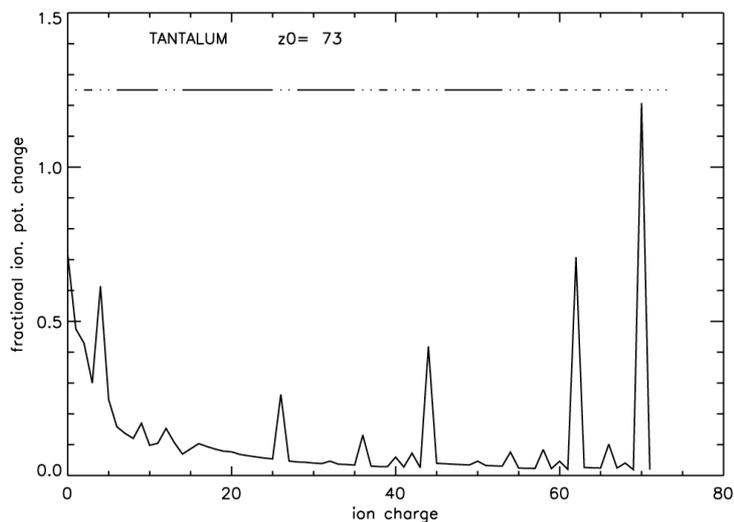
*preview\_natural\_partition.pro*

For example at the IDL command line type

```
IDL> preview_natural_partition,z0=73,plot_type=3,te_min=1,te_max=1e6,te_plot=1000
IDL> preview_natural_partition,z0=73,plot_type=4,partition=all
IDL> preview_natural_partition,z0=73,plot_type=1
IDL> preview_natural_partition,z0=73,plot_type=2
IDL> adas_writefile,file='partition.txt',all=all
```

The text lines of the parent and child partition layers, as required for driver scripts, are written to the screen and the figure is displayed. There are keywords to send the text lines and graphs to files. Plots available are 1: ionisation potential variation, 2: quasi-equilibrium fractions within a superstage, 3: stage-to-stage ionisation balance, 4: superstage ionisation balance. The output temperature used for fractional abundances within a superstage for the plot of type 2 is representative.

(a)



(b)

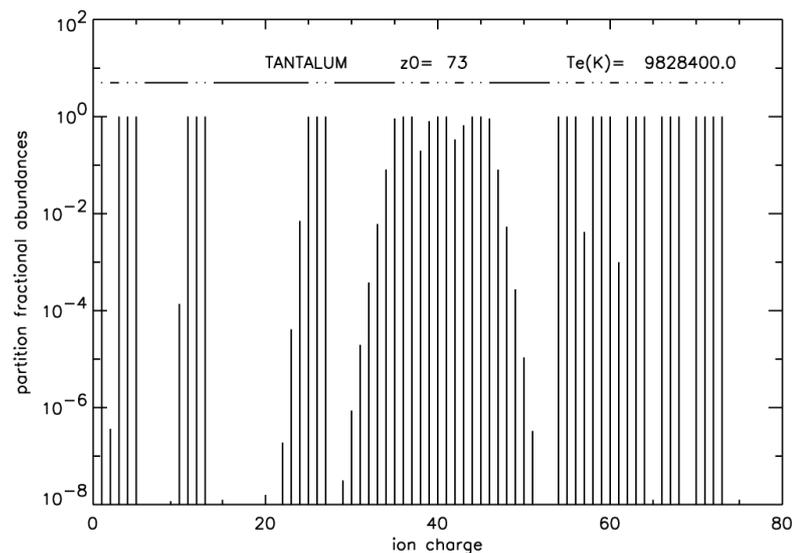


Figure (a) Fractional variation of ionisation potential for the ions of tantalum. The peaks indicate the quantum shell boundaries. The natural partition criterion is set at the  $3\sigma$  level and the individualised stages and bundles are indicated by dots and bars respectively above the graph. (b) Quasi-equilibrium fractions for each ionisation stage within a bundle with respect to the whole bundle.

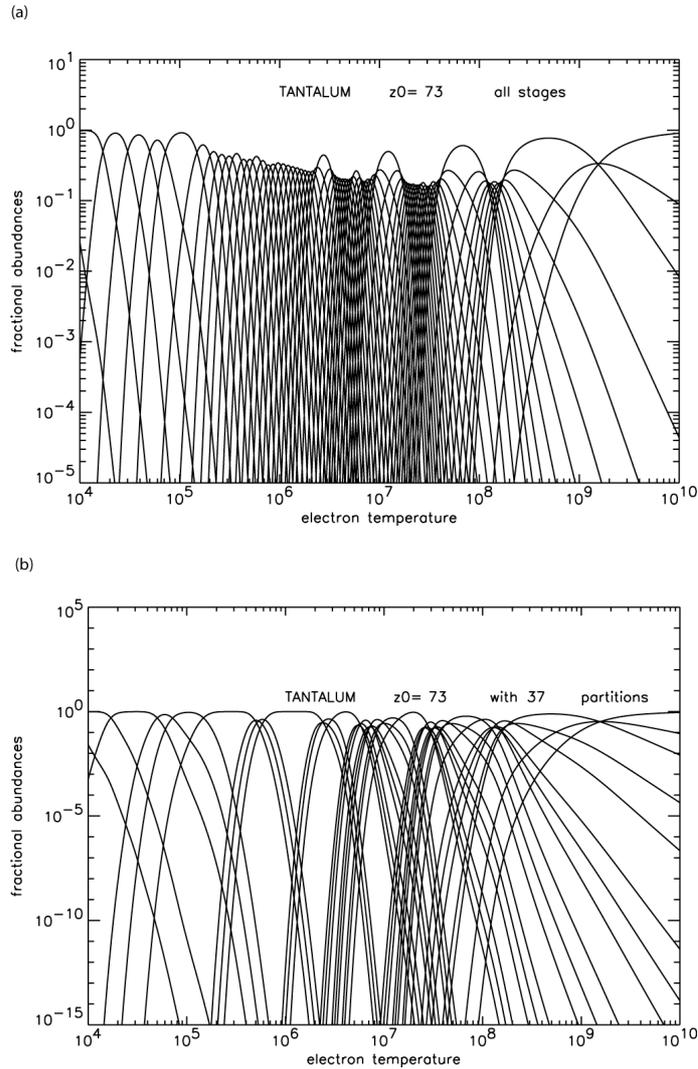


Figure: Ionisation balance for tantalum vs electron temperature. (a) Equilibrium fractional abundances with unresolved individualised stages corresponding to the #01 partition. (b) Equilibrium fractional abundances for ionisation stage bundles in the natural partition of the previous figure.

For superstages, photon emissivity coefficients still exist, but they are driven by the superstage. That is the actual emissivity of a line is obtained by multiplying the coefficient by the electron density and the population of the driving superstage. Since a child superstage has implicitly equilibrium ionisation fractional abundances imposed within the parent superstage contributors, the superstage emissivity coefficient is a bit like the astrophysicist's individual spectrum line *contribution functions* – see ADAS405, where they are called *GTNs*. The latter though include full ionisation equilibrium. In cases where superstages are useful there are often huge numbers of spectral lines in a typical observed wavelength range, so it is easiest to deal with the whole spectral interval and introduce so-called feature emissivity coefficients (*adf40*). The latter superpose all the lines in the interval with a broadening function. Feature emissivity coefficients work just the same with superstages. For a spectral interval  $\lambda_0 < \lambda < \lambda_1$ , written compactly as  $[0,1]$ , the envelope feature photon emissivity function vector (that is generally a pixellation vector over the spectral interval) is

$$FGTN^{[\#02][0,1](j)} = \sum_{i_0}^{i_1} FGTN^{[\#01][0,1](i)} \left( \frac{N^{[\#01](i)}}{N^{[\#02](j)}} \right)_{eq}$$

where the *FGTNs* are the generalisation of the astrophysicist's individual spectrum line *contribution functions* which we introduced with ADAS405 and called *GTNs*. Recall that a *GTN* is just a photon emissivity coefficient (*adf15*) multiplied by the equilibrium fractional abundance of the ionisation state in the *CR* picture. **The above superstage PEC and FGTN capabilities are just being finalised in central ADAS – some are missing in release v3.0.**

### Superstage condensation and plasma transport models

As discussed earlier, a main advantage of the condensation is in economising complex transport calculations without severe loss of accuracy. However there are some new issues which must be addressed first before superstages are compatible with transport models. A superstage, which is a composite of several ionisation stages has a superstage charge which depends on electron temperature and electron density. It is a collisional-radiative quantity. In fact fluid transport models make use of the ion charge, squared ion charge and ionisation potential in addition to familiar quantities such effective ionisation, recombination, radiated power and electron energy loss coefficients. The *adf11* classes must be extended with these extra quantities, which in superstages are all collisional-radiative quantities. In ADAS, these are given the mnemonics *zcd*, *yed* and *ecd*. ADAS codes and data structures have been adjusted accordingly and there is a revised specification of *adf11*. The definition and computation of *zcd* and *yed* are straightforward. *ecd* is more subtle. Consider a lowest superstage which is a condensation of low ionisation stages in addition to the first. Then from the point of view of energy conservation, the superstage has a birth energy associated with its appearance in the plasma. In the usual (simplified) ionisation stage picture, a neutral has zero birth energy, which is implicit in the computer codes. For consistency then, there is a 0<sup>th</sup> block in the *adf11/ecd* dataset which is the birth energy of the lowest superstage. The #01 root partition has all zeros in this block. In fact this problem is already present in the *GCR* picture, since the energy of metastables of the lowest ionisation stage are usually ignored. A properly formed *ecd* in the *GCR* picture should contain excitation energies from the lowest metastable (the ground state) to higher metastables of the same stage as well as ionisation potentials to the metastables of the next stage. These data are available for selected elements within ADAS under data format *adf00* in data sets of the form

```
<el.symb.>_ls.dat  
<el.symb.>_ic.dat
```

for *ls* and *ic* cases in addition to the usual unresolved form

```
<el.symb.>.dat
```

The FORTRAN subroutine *xxdata\_00.for* returns extra information on the metastables, including their configurations. The IDL procedure can also acquire these data if the keyword */ls* or */ic* is appended to the call.

As the historical ADAS *adf11* database does not contain *zcd*, *yed* and *ecd*, a PERL script can be supplied to create them as

```
/home/adas/offline_adas/adas4#1/scripts/generate_adf11_classes_10-12.pl
```

By default this scans the */home/<user>/adas/adf11* subdirectory for the various year numbers and creates matching *zcd*, *yed* and *ecd* classes for that year number back in */home/<user>/adas/adf11*. It will overwrite *zcd*, *yed* and *ecd* data already there. Both resolved and unresolved classes are handled and a running commentary is provided on progress and problems encountered. Two arguments may be given in the call to *generate\_adf11\_classes\_10-12.pl* to alter the input subdirectory and the output subdirectory respectively. It is unlikely that you will need this, since ADAS408 can also produce them. It is more a matter for central ADAS with a long history of *adf11* datasets

### ADAS416 - Generating the superstage} condensation

The creation of a data for a new child partition is largely automatic. It is in the province of ADAS416. The interactive code, selected from the series 4 menu, follows the usual pattern. It starts with an input screen, which seeks a script for the superstage compression. These are allocated to the */.../<uid>/adas/scripts416* directory. It is expected that the user will have his/her own scripts, the central ADAS ones only being samples, such as shown for argon below. The partition specification starts at the root

layer #01 in which each ionization is in its own partition. The layer #02 combines the stages in partitions at the user's wish. The choice of best partitioning is a subject of investigation in association with transport models, however the concept of 'natural partition' is helpful for the spectroscopist. The complete package for superstage compression includes a preview capability in IDL for the original and superstage ionization balance in natural partition, prior to the actual evaluation using ADAS416.

```

argon

89
unresolved

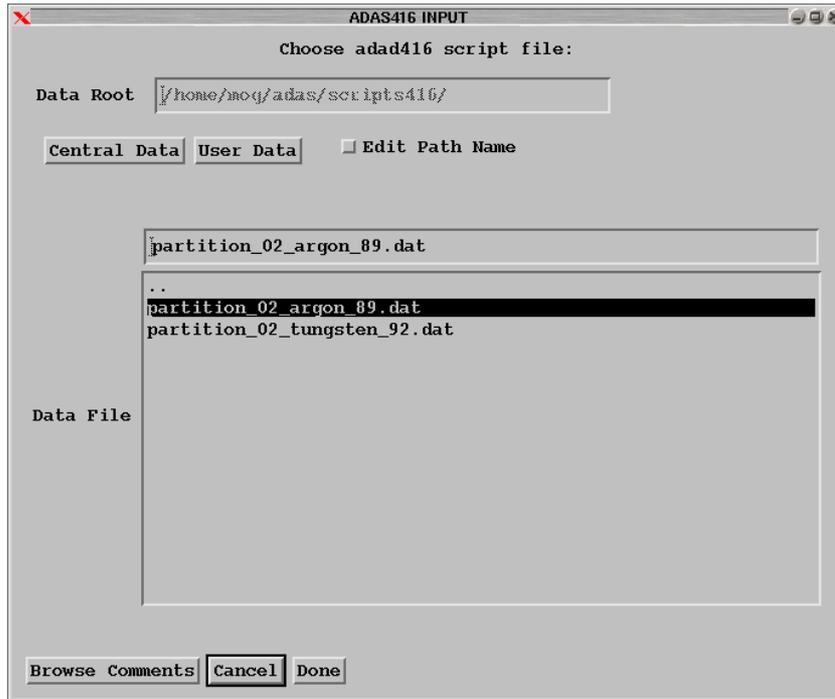
parent pathways
-----
gcr : /home/summers/adas/adf11/***89/***89_ar.dat
pec : /home/summers/adas/adf15/pec06#18/ar_01/ic#ar**.dat
f-pec: /home/summers/adas/adf40/fpec06#18/ar_01/ic#ar**.dat

partition specification
-----
//#02/p00/ 00/p01/ 01/p02/ 02 03 04 05 06/p03/ 07/p04/ 08/
      p05/ 09 10 11 12 13 14/p06/ 15/p07/ 16/p08/ 17/p09/ 18/
//#01/p00/ 00/p01/ 01/p02/ 02/p03/ 03/p04/ 04/p05/ 05/p06/ 06/p07/ 07/p08/ 08/
      p09/ 09/p10/ 10/p11/ 11/p12/ 12/p13/ 13/p14/ 14/p15/ 15/p16/ 16/p17/ 17/
      p18/ 18/
---

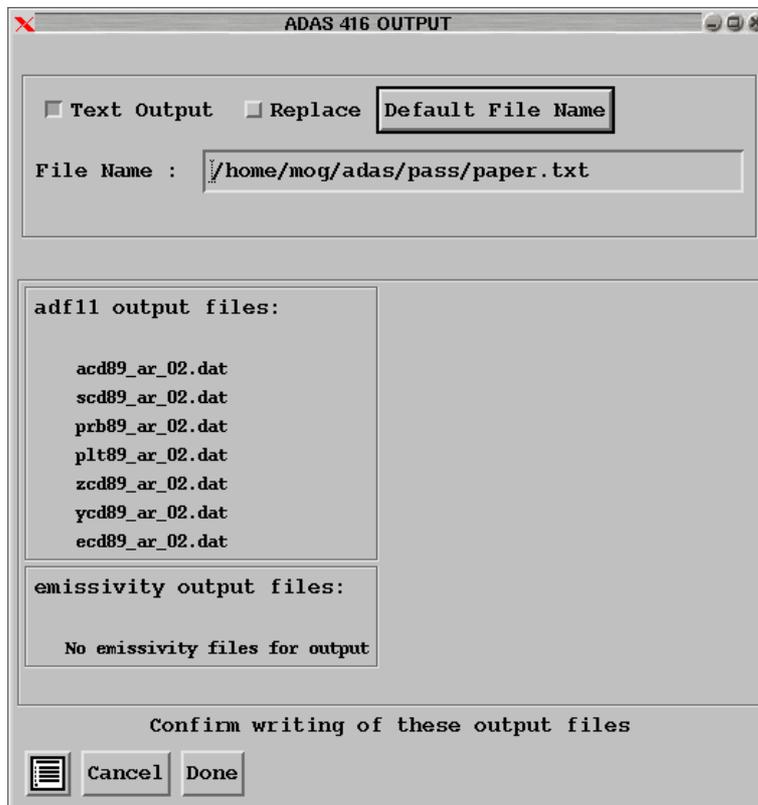
child pathways
-----
gcr : /home/summers/adas/adf11/***89/***89_ar_02.dat
pec : /home/summers/adas/adf15/pec06#18/ar_02/ic#ar**.dat
f-pec: /home/summers/adas/adf40/fpec06#18/ar_02/ic#ar**.dat

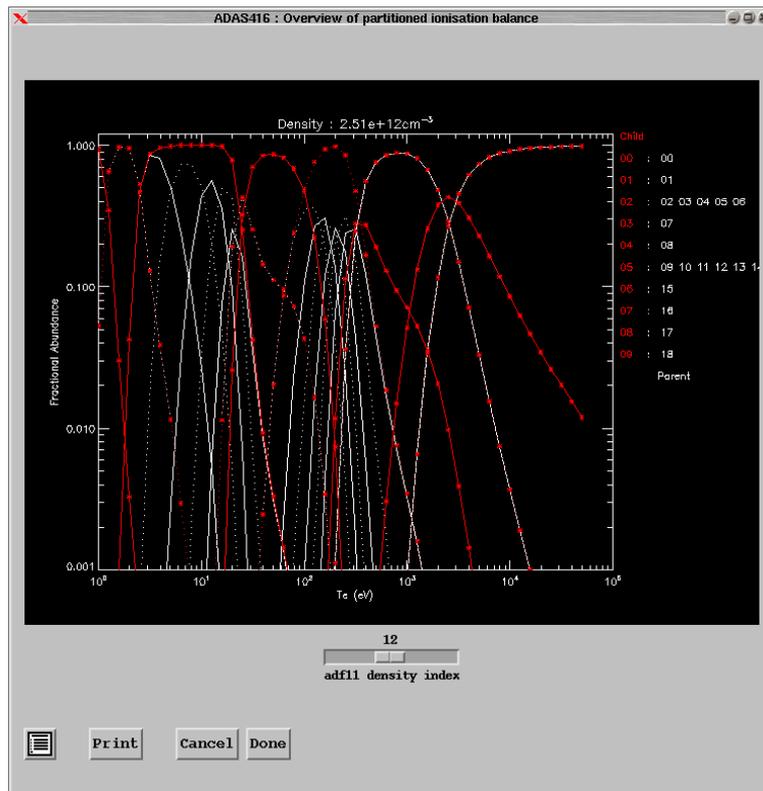
C-----
C sample scrip416 file
C
C Notes:
C (1) '***' in gcr pathway denotes 'acd', 'scd' etc
C (2) '***' in pec, gtn, f-pec and f-gtn pathways denote 'llr', 'pjr'
C      or 'pju'.
C (3) '***' in pec, gtn, f-pec and f-gtn pathways denote partition
C      member index. This is the ion charge for the #01 root
C      partition. The indexing begins at 00
C (4) Leave pathways which are not needed as blanks
C (5) Choices at line 4 are 'resolved' or 'unresolved'
C (6) Partitions are given in decreasing level order, that is
C      child before parent. This is the same rule as is used in
C      adf11 files with partition blocks and is required by the
C      partition block reader xxrptn.for.
C
C
C Author:  Hugh Summers
C Date :  18 august 2005
C
C-----

```



The input screen is shown below and, following *Done* leads directly to the output screen where the options of writing the new partition are given. This screen reacts to the available ADF11 files for the parent partition. Note the new classes *zcd*, *ycd* and *ecd*. The output ADF11 files uses an extended specification which includes partition and connection vector information at the head of the file. New ADF11 reading routines are in place in the ADAS libraries to which deal with the extended formatting as well as reading older versions of ADF11.





The main calculations are done by a FORTRAN code *adas416.for*, but as usual can be initiated from the IDL command line as \

```
IDL> z0 = 74
IDL> class_list = ['acd' 'scd' 'plt' ]
IDL> adas416_script = '$ADASHOME/adas/scripts416/partition_02_tungsten_1992.dat'
IDL> run_adas416, z0=z0, adas416_script=adas416_script
```

or

```
IDL> run_adas416, z0=z0, adas416_script=adas416_script, class_list=class_list
```

or

```
IDL> run_adas416, z0=z0, adas416_script=adas416_script, class_list=class_list,
/adf11_only
```

where the second form restricts the *adf11* classes handled and the third restricts to *adf11* data only, omitting *adf15* and *adf40* processing. This overrides the script driver. Note that the procedure will terminate if the *adf11* classes *acd* and *scd* are not present in the unresolved case (or *acd*, *scd*, *qcd*, *xcd* in the resolved case - that is when the connection vector is non-trivial. The parameter *z0* is merely a check if the script driver does name the element explicitly.

ADAS data format specifications, especially *adf11*, *adf15* and *adf40* have been modified to cope with heavy elements and superstage condensation. Updated access codes *xxdata\_11.for*, *xxdata\_15.for* and *xxdata\_40.for* read the new datasets and all older versions transparently to the user.