

apr18-96

ADAS Bulletin

Seven new programs are ready. The first is ADAS203 from series 2. This code is designed to assist in quick preparation of a specific ion file (*adf04*) for an unknown ion when an interpolable data collection for the associated isoelectronic sequence (*adf05*) is available. Then there are two more programs from series 4, namely ADAS407 and ADAS408. These programs are part of ADAS' capability for generating low to moderate accuracy recombination, ionisation and radiated power data when more refined material is not available. The programs work together with ADAS407 generating parameter sets (*adf03*) and then ADAS408 using these parameter sets to generate the derived data (*adf11*) over ranges of plasma parameters. In ADAS series 5, two new interrogation routines have been added. These are ADAS505, which interrogates thermal charge exchange rate coefficient data (*adf14*) and ADAS509, which interrogates the corresponding state selective charge exchange cross-sections (*adf24*).

As promised, Alessandro's differential emission measure analysis code, ADAS601, is included in this release. It now incorporates the refinements discussed in the last bulletin and is designed to work on a standard 'intensity file' formatted in a manner agreed with SOHO-CDS project scientists.

Finally, the most sophisticated code in ADAS for modelling excited level populations and generating derived collisional-radiative data, ADAS208, is made available. This is quite a complex code and to work fully requires advanced format specific ion files (*adf04*), expansion cross-reference files (*adf18*), projection files (*ad17*) and encourages you to access interactively high quality ionisation rate coefficient data (*adf07*).

This is rather a large release and I anticipate that we shall have some teething troubles. Please let us know if you encounter difficulties and we shall endeavour to remedy them quickly. **Remember to delete your defaults file for a revised program and let ADAS recreate it if you have problems. Many programs may be affected this time since Table Editor has been modified.**

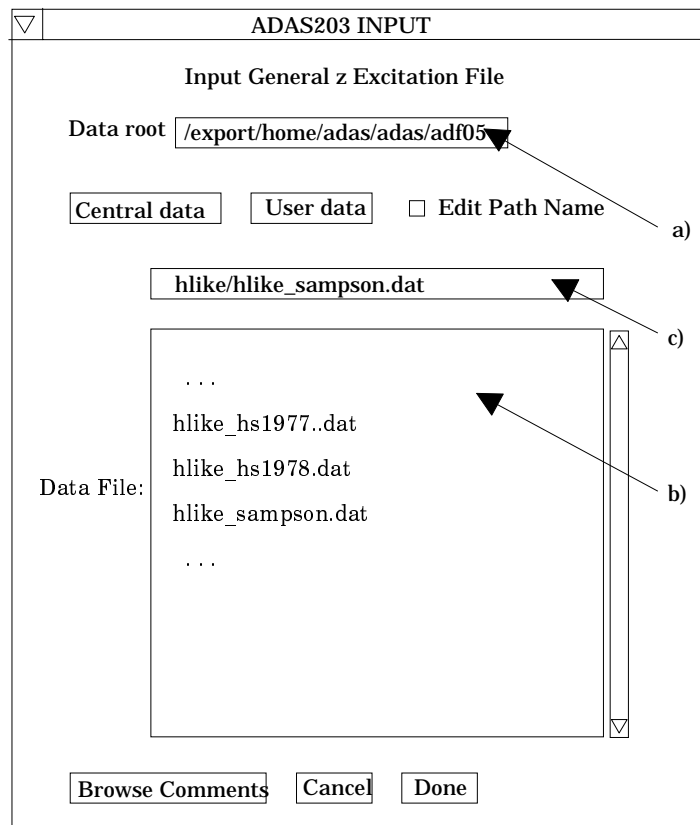
It is now also time to plan the next ADAS Workshop for the Autumn. I shall be sending out a circular to try to reach a consensus on date shortly.

1. ADAS203

The program prepares a fully specified specific ion file of type *adf04* for an unknown ion of an isoelectronic sequence from a general z excitation file of type *adf05* for the sequence. The general z excitation file contains ionisation potentials, energy levels and transition probabilities in addition to rate parameter (Upsilon) data for a set of members of the isoelectronic sequence. Since the primary starting point of population calculation in ADAS series 2 is the specific ion file, ADAS203 allows us to make a start on population and emissivity studies of an ion even though an individually prepared specific ion file for the ion in question is not available. It does of course depend on the existence of a general z excitation file for the associated iso-electronic sequence and the procedure is subject to rather uncertain error. As we build up specific ion files for members of a sequence, if they are compatible, we try also to create from them such general z excitation files. As part of its operation ADAS203, which is essentially a z-interpolation code, also allows display of individual reaction rates for the selected ion and improvement 'visually' of the fitting parameters beyond those present in the general z excitation file.

- 1.1. Move to the directory in which you wish any ADAS created files to appear. These include the output text file produced after executing any ADAS program (*paper.txt* is the default) and the graphic file if saved (e.g. *graph.ps* if a postscript file). Initiate ADAS and move to the series 2 menu. Select ADAS203.
- 1.2. The **file selection window** appears first and is illustrated below. Its operation follows the usual pattern.
 - 1.2.1. *adf05* is the appropriate format for use by the program ADAS203 (ADAS User Manual, *appxb-05*). Your personal data of this type should be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*.

- 1.2.2. A Data root path to the correct data type *adf05* appears automatically a). Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
- 1.2.3. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
- 1.2.4. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.
- 1.2.5. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
- 1.2.6. Clicking on the *Browse Comments* button displays any information stored in the selected charge exchange datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
- 1.2.7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window



- 1.3. The **processing options window** has the appearance shown below
 - 1.3.1. An arbitrary title may be given for the case being processed a). For information the full pathway to the general z dataset being analysed is also shown. The button *Browse Comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
 - 1.3.2. Enter at b) your selection of the ion for analysis and for which a specific ion file is sought. For guidance, some details of the content of the source general z file are displayed. The isoelectronic sequence is shown first.

We call this the 'recombined ion' isoelectronic sequence. Then the nuclear charge, recombined ion charge and element symbol is shown for each member of the isoelectronic sequence, explicitly present in the general z file, is shown in the scrollable display window. The object of the code is to interpolate to an intermediate ion of the sequence within the span of the members. Enter the nuclear charge of the ion for which you wish output.

- 1.3.3. At c) a summary of the number of energy levels and number of electron impact transitions present in the general z file is given and then an actual list of these transitions in the display window. You can choose to examine (or modify) the z-interpolation for a particular transition by clicking on that transition In the list. The selected transition is shown in the transition selection window above.

▼
a)
ADAS203 PROCESSING OPTIONS

Title for Run
 General-z file : /export/home/adas/adas/adf05/hlike/hlike_sampson.dat

Select Ion For Analysis
 Recombined ion iso-electronic sequence = H
 ----- members -----

Index	Nuclear Charge	Recombined Ion Charge	Element Symbol
1	14	13	Si
2	18	17	Ar
3	26	25	Fe
4	42	41	Mo

Specify nuclear charge of member required

Select Specific Electron Impact Transition :-
 No. of electron impact transitions = 11
 No. of index energy levels = 6
 ----- Transitions -----

Transition Index	Upper Level Index	Upper Level Designation	Lower Level Index	Lower Level Designation
1	2	2s (2)S(0.5)	1	1s (2)S(0.5)
2	3	2p (2)P(2.5)	1	1s (2)S(0.5)
3	4	3s (2)S(0.5)	1	1s (2)S(0.5)

Select option for display :

Settings/scalings (I)

Settings/scalings (II)

Transition energy - z-zpline independent variable

Einstein coefficient - z-spline independent variable

Einstein coefficient - Transition type

Einstein coefficeint - z1 power for scaling factor

Output Electron Temperatures

INDEX	Output values	Input values
1		
2		
3		
4		

Temperature Units : Kelvin

Edit the processing options data and press Done to proceed

☰

- 1.3.4. The general z file has predefined settings and scaling parameters for each transition within it, designed as far as possible to give acceptable interpolation. The settings are divided into two classes namely those for obtaining the transition energy and transition probability (I) and those for obtaining the upsilons (II). Activate the appropriate button at d) and the corresponding settings and scalings are shown in the sub-window. These choices may be changed by the user. The usual practise is to choose values which make the graphs of the transition energy, transition probability and upsilon look as flat as possible (in fact reduced quantities

- are displayed on the graphs). This is done by visual inspection of the displayed graphs and iteration back to this window.
- 1.3.5. Your settings of electron temperatures for the output specific ion file are shown in the temperature display window f). The temperature values present in the source general z file are also shown for reference. Note that the general z file has the upsilon data for all the member ions at the same set of z-scaled temperatures. Thus the actual input temperatures change as you select different ions for output.
 - 1.3.6. The program recovers the output temperatures you used when last executing the program. The output temperatures may be edited in the usual manner. Click on the *Edit Table* button if you wish to change the values. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures. For convenience a *Clear Table* button has been added.
 - 1.3.7. The *Exit to Menu* icon is present in ADAS203. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.
- 1.4. 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.
- 1.4.1. As usual, the input general z file under analysis is shown at a) and can be browsed. Two buttons have been added at a), namely, *Graphics* and *Text*. Activate *Graphics* and the standard graphical output sub-window appears. Activate *Text* and the standard text file output sub-windows appears instead.
 - 1.4.2. In the Graphics case, on screen graphical display is enabled by clicking on the *Graphical output* button. There are three choices of graph, namely, transition wave number, A-value and rate parameter. Click the appropriate button at b). Default scaling of the chosen graph may be over-ridden by appropriate selections. Labelling of the separate curves on the rate parameter plot may switched on by the choices at c). Below this the usual hard copy may be enabled and a choice of type of output device made.
 - 1.4.3. In the Text case, two output files are permitted (arrowed at e)), namely, the standard line printer text output file summarising the interrogation and the output specific ion file of type *adf04*. For historic and nostalgic reasons we call this the COPASE passing file. It is put in your */pass* directory as *copase.pass* by default. The usual *Replace* and *Default File Name* buttons are present for both output files.
 - 1.4.4. 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 and Exit* to write the COPASE passing file and then exit. Note that the COPASE file contains all the transitions in the general z file with the default settings for the transition interpolations except where you have conducted an analysis. In these latter cases, your adjusted settings are used and suitably documented in the comments section at the foot of the COPASE passing file. There is an alternative button, *Output and Return Here* which similarly creates the COPASE file but instead of exiting returns you to this window. The option is helpful for producing comparative specific ion files. The *Exit to Menu* icon takes you directly to the ADAS2 series menu.

ADAS203 OUTPUT OPTIONS

Script file : /export/home/adas/adas/adf05/hlike/hlike_sampson.dat

Select output option settings for display : Graphics Text

Graphical output

Graph Title

Scaled transition wave number vs. ion charge
 Scaled A-value vs. ion charge
 Scaled rate parameter vs. z-scaled electron temperature

Scaled A-value plot :-

Explicit scaling

X-min : X-max :
Y-min : Y-max :

Label Lines with indices on rate parameter plot : No Yes

Enable Hard Copy Replace

File Name :

Select Device

COPASE Passing File Replace

File Name :

Text Output Replace

File Name :

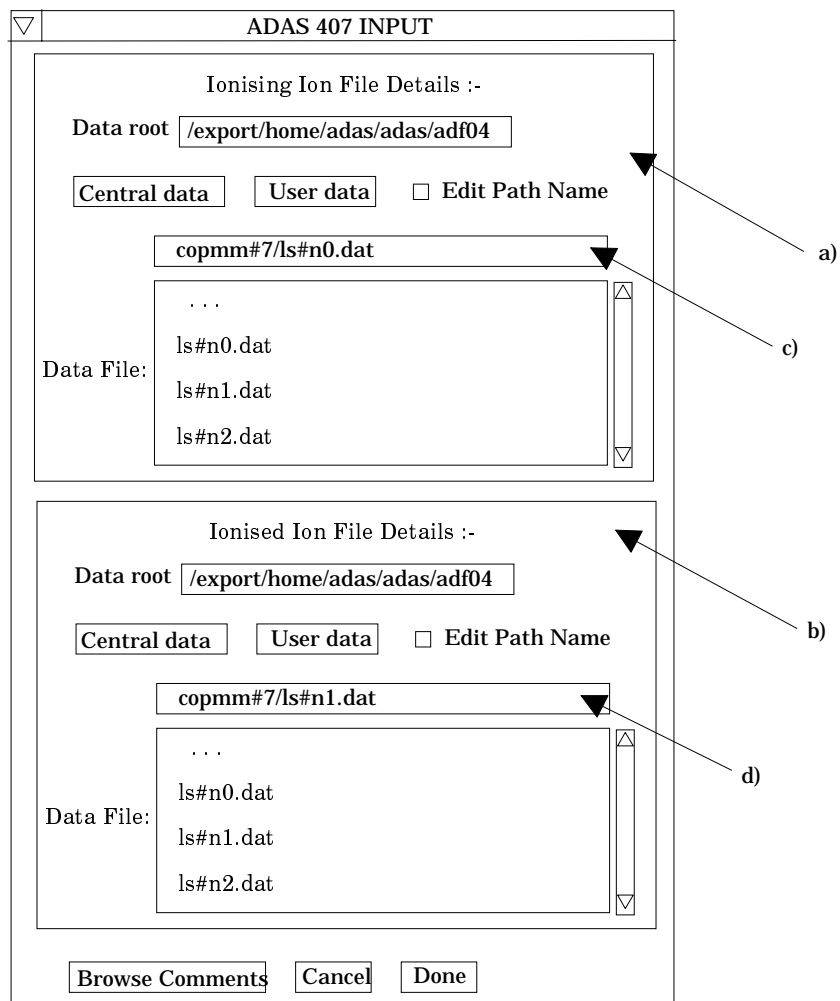
2. ADAS407

The code analyses certain specific ion files, type *adf04*, 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 are grouped as an ADAS data type *adf03*. The latter may be used by the code ADAS408 to generate standard isonuclear master files, type *adf11*, for ionisation balance and radiated power loss calculations. ADAS407 can also create a driver file for the ADAS204 program which we shall come to probably in the next release.

Specific ion files provide the fundamental collections of energy levels, transition probabilities and collisional rate coefficients which allow detailed excited population calculations and then production of collisional radiative coefficients. The ADAS database contains many such files however complete coverage of all possible species at the highest accuracy levels is not possible. 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 mass produce specific ion files. These automatically generated files are less accurate than individually prepared and assessed files. However they are highly structured with special alphanumeric conventions for configurations etc. recognisable by ADAS407. ADAS407 can glean extra information from such specific ion files to obtain the data mentioned in the first paragraph. Incidentally, these automatically generated specific ion

files can be recognised in the central ADAS database since they have directory names like `../adas/adf04/copmm#.` and `../adas/adf04/copss#.`

- 2.1. Move to the directory in which you wish the ADAS created files to appear. These include the output text file produced after executing any ADAS program (*paper.txt* is the default), and up to four further output data files. There is no graphical output from this program. Initiate ADAS407 from the program selection menus in the usual manner.
- 2.2. The **file selection window** appears first as illustrated below. *adf04* is the appropriate format for use by the program ADAS407 (ADAS User Manual, *appxb-04*). ADAS407 requires two such files, namely, for the 'Ionising Ion' and the 'Ionised Ion'. If you wish to use personal data of this type, then as usual it should be held in a similar file structure to central ADAS with your identifier replacing the first *adas*, but in addition it must have the configuration fields in 'Eissner' notation and the orbital binding energy fields not empty.



- 2.2.1. The upper sub-window a) is for the ionising ion. A Data root path to the correct data type *adf04* appears automatically a). Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data.
- 2.2.2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

- 2.2.3. Available sub-directories are shown in the large file display window. Scroll bars appear if the number of entries exceed the file display window size.
 - 2.2.4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*. Note that datasets in subdirectories of the form */copss* and */copmm* are the only ones guaranteed to work.
 - 2.2.5. When an ionising ion has been chosen, then the corresponding ionised ion has to be chosen in sub-window b). ADAS407 creates the expected file name and displays it at d) if it exists. This name can be over-ridden in the usual manner.
- 2.3. The **processing options window** has the appearance shown below
- 2.3.1. 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 at b) and c). Summary data of the ions and the files opened are given first. The button *Browse Comments* in each sub-window again allows display of the information field section at the foot of the named ion file, if it exists.
 - 2.3.2. 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. Notice the appearance of the configuration specification part of the level designation at b) and c). The '21522533' at b) means $1s^2 2s^2 2p^3$ in 'Eissner notation' (see the ADAS User Manual for more details).
 - 2.3.3. At b) click on the particular driving metastable whose associated radiated power loss is to be analysed and displayed. In the lower group of sub-windows, this choice appears at d). In this sub-window, below the metastable index information a display window and associated selection window is present. The display window e) shows all the dipole collisional transitions in the ionising ion *adf04* file linked to selected metastable. The oscillator strength and wavelength of each transition is given.
 - 2.3.4. 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.
 - 2.3.5. 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 to view.
 - 2.3.6. 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. 2.3.5 above). These are listed in the sub-window at f). Simple approximate forms are used to obtain these coefficients. For most of the coefficients an 'A' and 'B' choice of approximate forms are available. The 'A' forms have been used quite widely in fusion historically. The 'B' forms are better but may sometimes be unstable in

fitting. We are in the process of tightening these up. Click on the selection button to the right of the type of coefficient at f) to drop down the A or B choice menu.

- 2.3.7. 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 g) at which you wish the approximate form and accurate numerical values to agree.

ADAS407 PROCESSING OPTIONS

Title for Run ← a)

Ionising ion information
Nuclear charge : 7 Ion charge : 0
File:/export/home/adas/adas/adf04/copmm#7/ls#n0.dat

Metastable States

INDEX	LEVEL	DESIGNATION
1	21522533	(4)S(1.5)

b) →

Ionised ion information
Nuclear charge : 7 Ion charge : 1
File:/export/home/adas/adas/adf04/copmm#7/ls#n1.dat

Parent States

INDEX	LEVEL	DESIGNATION
1	21522523	(3)P(4.0)

c) →

Matching Temperature

1.000E+03
2.000E+03
5.000E+03
1.000E+04
...

Units :

g) →

Parameter Form
A = Van Maanen
B = Mullane/Summers

Radiative Recombination

Dielectronic Recombination

Collisional Ionisation

Total Line Power

Specific Line Power

f) →

Transition Assignment
Metastable Index : 1 ← d)

Transition (Key : 1-5 = Bundling Group)

INDEX	J	I	FIJ	WVLN	Key
1	4	1	0.230	1198.9	1
2	6	1	0.375	1123.0	1
3	16	1	0.116	958.2	1
4	17	1	0.014	957.9	2
...					

e) →

Specific line index :

Edit the processing options data and press Done to proceed

g) →

f)

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

2.4. 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.

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

ADAS407 OUTPUT OPTIONS

Input files: Parent ion: /export/home/adas/adas/adf04/copmm#7/ls#n0.dat [Browse Comments](#)
Initial ion: /export/home/adas/adas/adf04/copmm#7/ls#n1.dat [Browse Comments](#)

Select output option settings for display : Graphics Text

a) Graph Title

b) Total power fit graph :-
 Explicit scaling X-min : X-max :
Y-min : Y-max :

Specific line power fit graph
 Explicit scaling X-min : X-max :
Y-min : Y-max :

c) Enable Hard Copy Replace
File Name : Select Device

d)

MAINBN Passing File Replace
File Name :

ATOMPARS Passing File Replace
File Name :

Text Output Replace
File Name :

e) f)

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

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

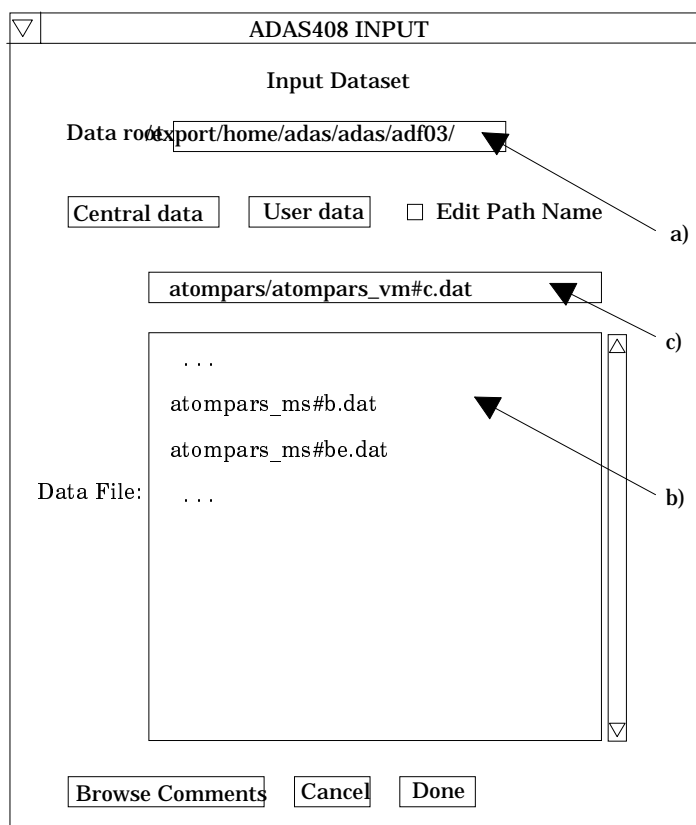
2.4.4. Various completion buttons are available at d). Click the *View Graph* button to show the graph. *Back to Processing* returns you to the previous window for choice of another transition for analysis. **Note that the settings from analyses carried out by you are accumulated.** Click the

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.

3. ADAS408

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

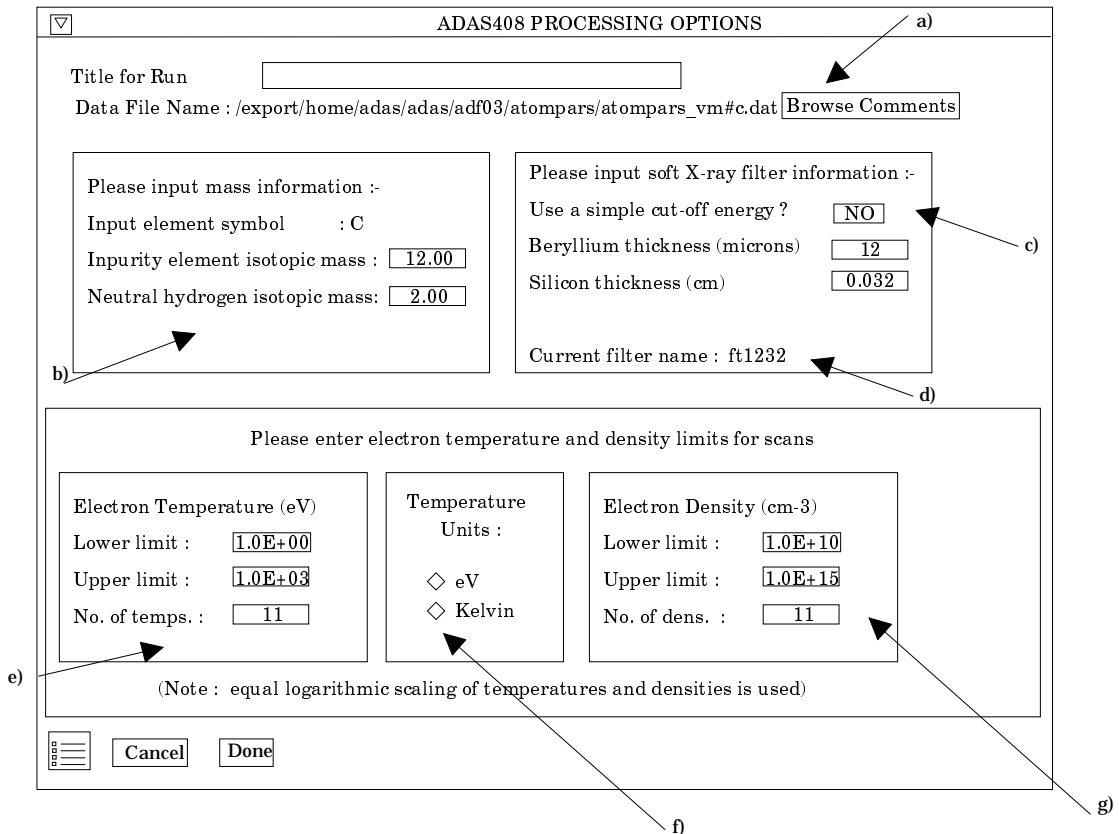
3.1. The **file selection window** has the appearance shown below



- 3.1.1. Data root a) shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. The appropriate ADAS data format for input to this program is *adf03* ('atompars files'). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
- 3.1.2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
- 3.1.3. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.
- 3.1.4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.

- 3.1.5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
- 3.1.6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
- 3.1.7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

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



- 3.2.1. 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.
- 3.2.2. At b), the mass number for the actual isotope of the element of the atompars file present in the plasma is entered. For information the element chemical symbol is displayed. Likewise, the mass number of hydrogen isotope constituting the primary plasma species is sought. Type the values in the editable boxes and press return.
- 3.2.3. 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 at c) to drop down a standard choice menu. In the beryllium/silica case thicknesses must be specified in the following two editable boxes.
- 3.2.4. 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.

- 3.2.5. The lower sub-windows at e), f) and g) allow the plasma electron temperature and electron density for production of the output *adf11* standard master files to be specified. Click on the required temperature units at f). This choice relates to the units used in the adjacent temperature range selection window at e). Specify lower temperature limit, upper temperature limit and number of temperatures in the editable boxes. ADAS408 then creates the temperature grid equally spaced in the logarithm. Note that the output files in fact contain the temperatures in eV (see the ADAS User Manual, appxb-11).
- 3.2.6. Similarly specify the electron density limits and number of grid points at g).
- 3.2.7. The *Exit to Menu* icon is present in ADAS408. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

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

The screenshot shows the 'ADAS408 OUTPUT OPTIONS' dialog box. It has a title bar with a checkmark icon. The main content area includes:

- 'Data File Name : /export/home/adas/adas/adf03/atompars/atompars_vm#c.dat'
- 'Browse Comments' button
- A prompt: 'Please enter the year number for master passing files (two-digits)' with a text input field containing '96'.
- 'Passing file template : /home/summers/adas/pass/XXX96#c.ft1232.pass'
- Options: Text Output, Replace, and a 'Default File Name' button.
- 'File Name :' followed by an empty text input field.
- Bottom controls: a small icon, 'Cancel' button, and 'Done' button.

 Arrows labeled 'a)', 'b)', and 'c)' point to the Data File Name, the year number input, and the Default File Name button respectively.

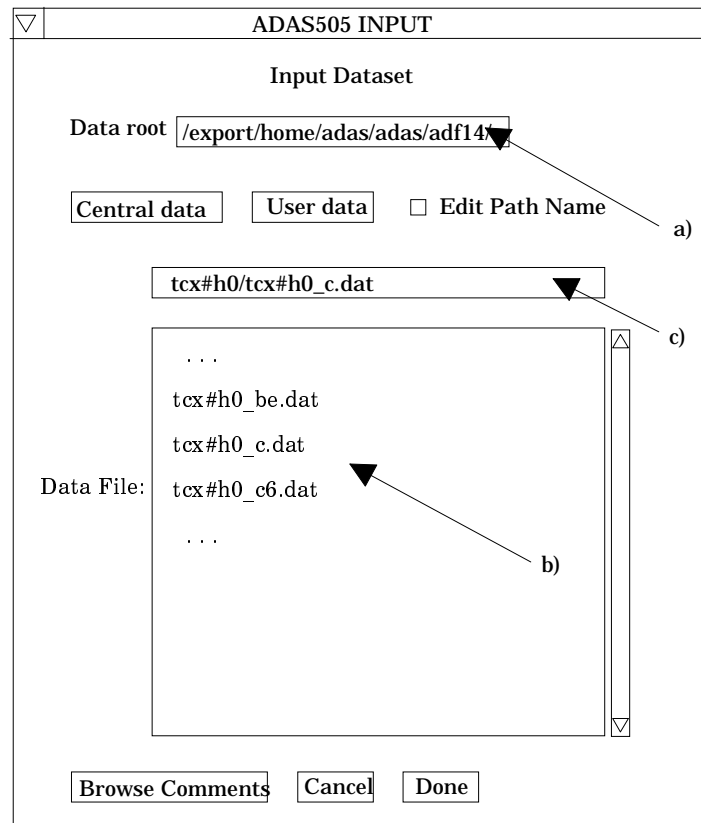
- 3.3.1. The name of the source atompars file to be used in the bulk generation of *adf11* data is repeated at a) for information.
- 3.3.2. The standard line printer text output file summarising the options selected for ADAS408 is available. The *Replace* and *Default File Name* buttons are present for the text output file as usual.
- 3.3.3. 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 at b) for the output. Note that any two digits are acceptable and 'fictitious' years can be used for special collections if so desired. Using the year number and the filter name (see 3.2.4 above) a passing file template is created. The 'XXX' of the template is replaced by the three letter codes of the iso-nuclear master file classes ('acd', 'scd' etc.) to create the actual output files. The filter name part of the template only appears in radiated power classes of iso-nuclear master files. Note also the presence of the element chemical symbol in the template. Unfiltered radiated power master files are created as well as the filtered ones. The former do not include a filter name as part of the whole file name.
- 3.3.4. There is no graphical output option.

- 3.3.5. The *Exit to Menu* icon is present in ADAS408. Clicking the *Done* button causes the requested files to be created and written to. Remember that *Cancel* takes you back to the previous window.

4. ADAS505

This code interrogates thermal charge transfer rate coefficients ('tcx') files of type *adf14*. The coefficient is extracted for capture by a thermal receiving ion from a neutral thermal donor. The data is interpolated at selected donor/receiver temperature pairs. The usual minimax polynomial fit, graph and tabular outputs are available.

- 4.1. The **file selection window** has the appearance shown below



- 4.1.1. Data root a) shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
- 4.1.2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
- 4.1.3. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
- 4.1.4. Once a data file is selected, the set of buttons at the bottom of the main window become active.
- 4.1.5. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out

what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.

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

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

ADAS505 PROCESSING OPTIONS

Title for Run

Data File Name : /export/home/adas/adas/adf14/tcx#h0/tcx#h0_c.dat

Polynomial Fitting

Fit Polynomial Value % :

Select Data Block

INDEX	Receiver Identity	Donor Identity	Final State Spec.
1	C+1 (1)	H+0 (1)	TOTAL
2	C+2 (1)	H+0 (1)	TOTAL
3	C+3 (1)	H+0 (1)	TOTAL

Receiver and Donor Temperature Values

INDEX	Receiver		Donor	
	Output	Input	Output	Input
1	1.16e+04	1.16E+04	1.16E+04	1.16E+04
2	...			

Temperature Units : Kelvin

Select Isotopic A.M.

	Receiver	Donor
Atomic Mass	<input type="text" value="12.00"/>	<input type="text" value="1.00"/>
Isotopic Atomic Mass	<input type="text" value="12.00"/>	<input type="text" value="2.00"/>

Edit the processing options data and press Done to continue

4.2.1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* a) again allows display of the information field section at the foot of the selected dataset, if it exists.

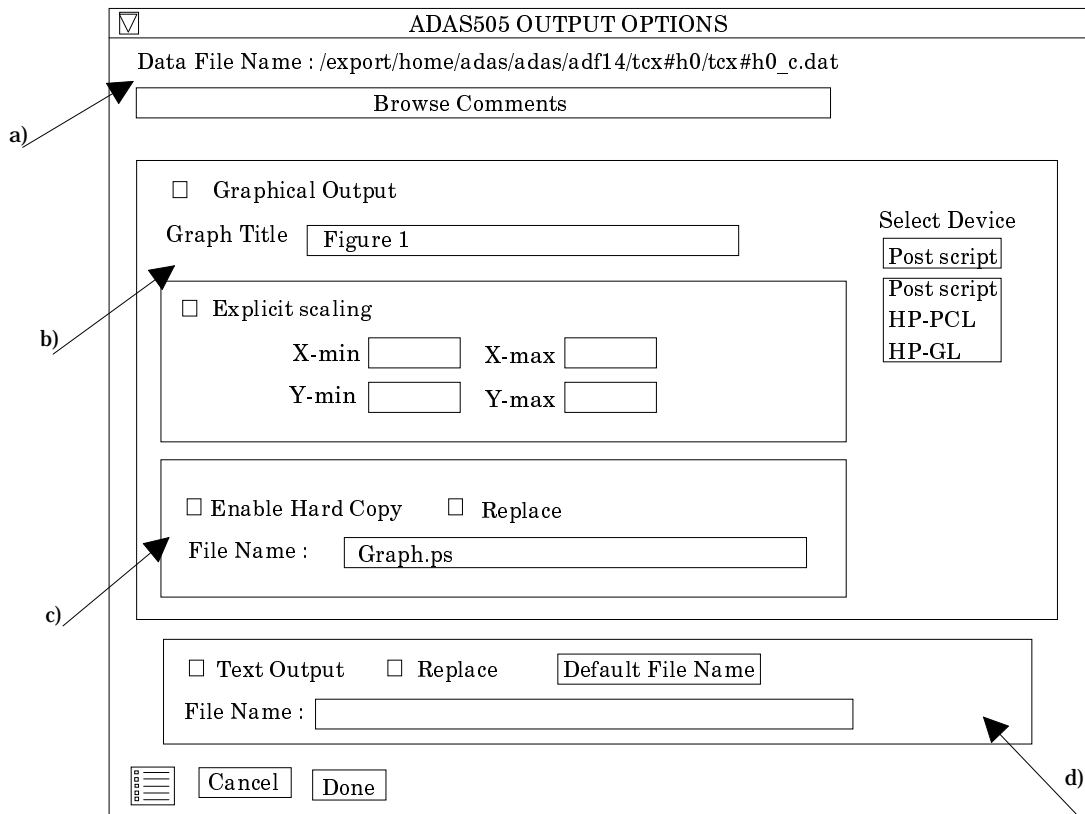
4.2.2. The output data extracted from the datafile, in the case of ADAS505, a double Maxwell averaged charge transfer rate coefficient, may be fitted with a polynomial. This is as a function of temperature. Clicking the *Fit polynomial* button f) activates this. The accuracy of the fitting required may be specified in the editable box. The value in the box is editable only if the *Fit Polynomial* button is active

4.2.3. Available rate coefficients in the data set are displayed in the coefficient list display window at b). This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a coefficient to select it. The selected rate appears in the selection window just above the coefficient list display window.

4.2.4. Your settings of temperatures (output) for donor and receiver are shown in the temperature display window c). The donor and receiver temperature values at which the rate coefficients are stored in the datafile (input) are also shown for information.

4.2.5. The program recovers the output temperatures you used when last executing the program. The Temperature Values are editable. Click on

- the *Edit Table* button if you wish to change the values. A 'drop-down' window, the ADAS Table Editor window, appears.
- 4.2.6. Pressing the *Default Temperature values* button inserts a default set of temperatures. This depends on the switch settings at d). For plot as a function of receiver temperature, the source receiver temperatures are used and a pop-up window allows choice of a single donor temperature from the source set. Conversely, for plot as a function of donor temperature, the source donor temperatures are used and the pop-up allows choice of a single receiver temperature.
 - 4.2.7. At e) choice of donor and receiver atomic mass numbers is available. For information, the isotope mass numbers in the source dataset are given. Note that these masses are simply used to locate the effective donor and receiver temperatures in the source dataset.
 - 4.2.8. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 5 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.
- 4.3. The **output options window** is shown below. It is of standard form with the same layout as codes previously described.
- 4.3.1. As in the previous window, the full pathway to the file being analysed is shown for information at a). Also the *Browse comments* button is available.
 - 4.3.2. Graphical display is activated by the *Graphical Output* button b). This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.
 - 4.3.3. Hard copy is activated by the *Enable Hard Copy* button c). The File name box then becomes editable. If the output graphic file already exists and the *Replace* button has not been activated, a 'pop-up' window issues a warning.
 - 4.3.4. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
 - 4.3.5. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.
 - 4.3.6. The graph is displayed in a following Graphical Output window.



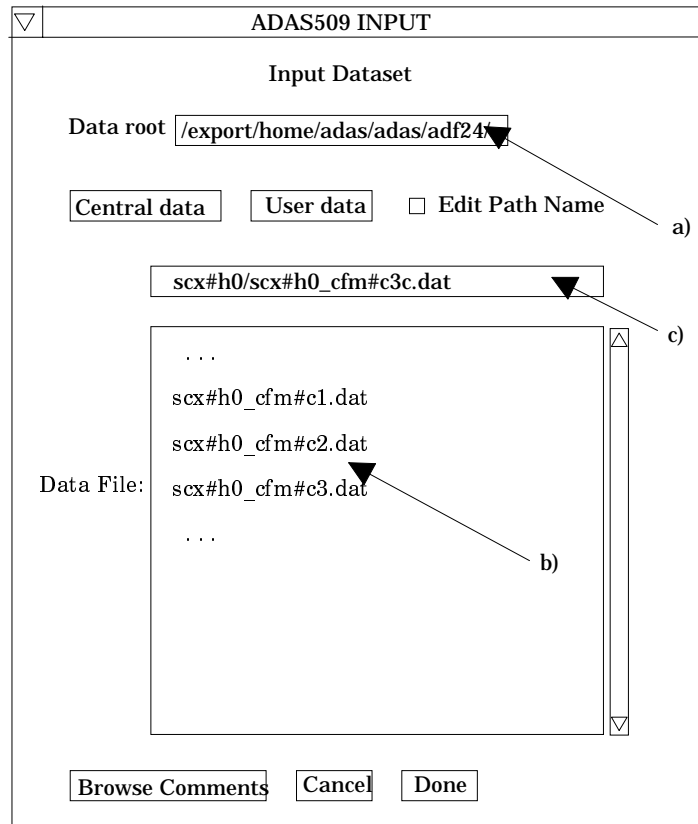
5. ADAS509

This code interrogates state selective charge exchange cross-sections ('scx') files of type *adf24*. The cross-section is extracted for capture by a receiver ion from a neutral donor. The data is interpolated at selected donor/receiver energies. The usual minimax polynomial fit, graph and tabular outputs are available. Additionally Maxwell averaged rate coefficients (over donor and receiver temperature ranges) may be obtained and a 'tcx' file of type *adf14* output.

5.1. The file selection window has the appearance shown below

- 5.1.1. Data root a) shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
- 5.1.2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
- 5.1.3. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.
- 5.1.4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
- 5.1.5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
- 5.1.6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.

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



- 5.2. The **processing options window** has the appearance shown below
- 5.2.1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* a) again allows display of the information field section at the foot of the selected dataset, if it exists.
- 5.2.2. The output data extracted from the datafile, in the case of ADAS509, a state selective charge transfer cross-section, may be fitted with a polynomial. This is as a function of energy. Clicking the *Fit polynomial* button g) activates this. The accuracy of the fitting required may be specified in the editable box. The value in the box is editable only if the *Fit Polynomial* button is active
- 5.2.3. Available cross-sections in the data set are displayed in the cross-section list display window at b). This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a cross-section to select it. The selected cross-section appears in the selection window just above the cross-section list display window.
- 5.2.4. For production of rate coefficients, the donor and receiver isotopic mass numbers are required. Enter these at c)
- 5.2.5. To obtain an output text file of the interpolated cross-section at chosen energies click the button at d). Your settings of collision energy (output) are shown in the energy display window c). The energy values at which the cross-sections are stored in the datafile (input) are also shown for information.
- 5.2.6. The program recovers the output energies you used when last executing the program. Pressing the *Default Energy Values* button inserts a default set of energies equal to the input energies.

ADAS509 PROCESSING OPTIONS

Title for Run

Data File Name : /export/home/adas/adas/adf24/scx#h0/scx#h0_cf m#c3.dat a)

Browse Comments

Polynomial Fitting

Fit Polynomial Value % :

Select Data Block

INDEX	Donor Ion	Receiver Ion	Final State	Type
1	H+0 (1)	C+3 (1)	Tot. Singl.	1
1	H+0 (1)	C+3 (1)	Total	1
2	H+0 (1)	C+3 (1)	Tot. Singl.	1
3	H+0 (1)	C+3 (1)	Tot. Tripl.	1

Please enter the reactant mass numbers Donor : Receiver : c)

Select Energies for Output File

Output Collision Energies

INDEX	Output	Input
1	1.16e+04	1.16E+04
2	...	

Energy Units : eV/amu

Edit Table

Default Energy Values

Select Temperatures for TCX File

Output Temperatures

INDEX	Output	Input
1	1.16e+04	1.16E+04
2	...	

Energy Units : eV Don.

Edit Table

Default Temperature Values

Edit the processing options data and press Done to continue

- 5.2.7. The Energy Values are editable. Click on the *Edit Table* button if you wish to change the values.
- 5.2.8. Note that you can work in a choice of energy units, namely eV/amu, atomic velocity units or cm s^{-1} .
- 5.2.9. To obtain an output 'tcx' file Maxwell averaged charge exchange rate click the button at e). Your settings of temperature (output) are shown in the temperature display window. The energy values at which the cross-sections are stored in the datafile (input) are also shown for information.
- 5.2.10. The program recovers the output temperatures you used when last executing the program. Pressing the *Default Temperatures Values* button f) inserts a default set of temperatures equal to the input energies.
- 5.2.11. The Temperature Values are editable. Click on the *Edit Table* button if you wish to change the values.
- 5.2.12. Note that you can work in a choice of temperature units. ADAS509 creates a two-dimensional array of thermal charge exchange rate coefficients from the selected cross-section. The same set of temperatures is used for both donor and receiver.
- 5.2.13. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 5 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

5.3. The **output options window** appearance is shown below

- 5.3.1. As in the previous window, the full pathway to the file being analysed is shown for information at a). Also the *Browse comments* button is available.
- 5.3.2. Graphical display is activated by the *Graphical Output* button b). This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.

ADAS509 OUTPUT OPTIONS

Data File Name : /export/home/adas/adas/adf24/scx#h0/scx#h0_cfm#c3.dat

Graphical Output

Graph Title

Select Device

Explicit scaling

X-min X-max

Y-min Y-max

Enable Hard Copy Replace

File Name :

Text Output Replace

File Name :

TCX Coefft. File Replace

File Name :

NB. Only when you exit ADAS 509 will TCX output be sent to this file

- 5.3.3. Hard copy is activated by the *Enable Hard Copy* button c). The File name box then becomes editable. If the output graphic file already exists and the *Replace* button has not been activated, a 'pop-up' window issues a warning.
- 5.3.4. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
- 5.3.5. At d) the *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.
- 5.3.6. At e) output of the 'tcx' file may be enabled. The *Default file name* and *Replace* options are set up at the first pass through this window. Note that the actual output is deferred. This is to allow processing of further cross-

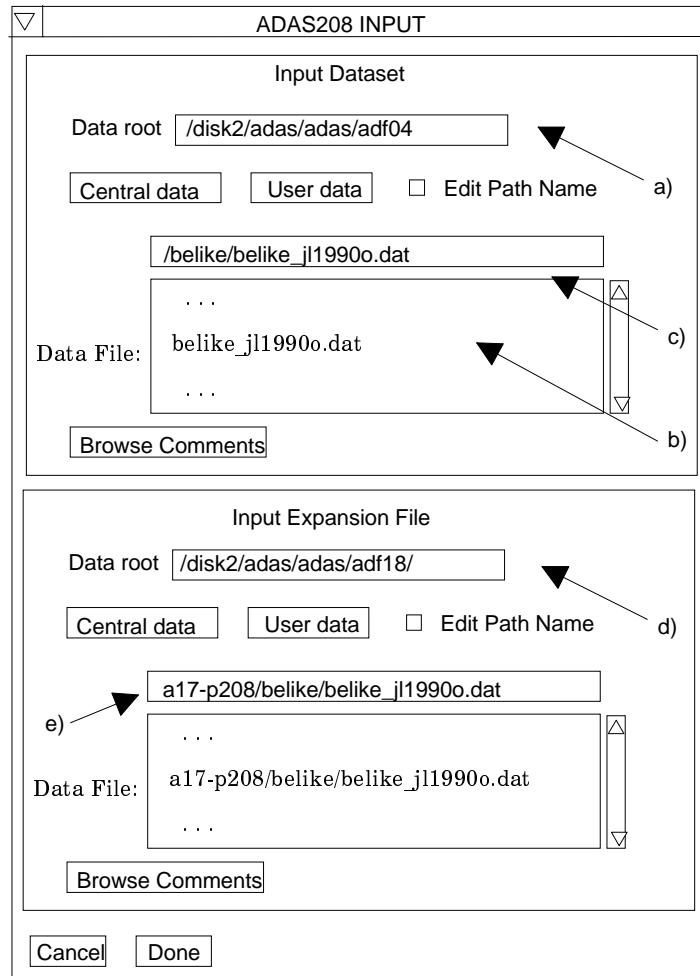
sections so that a complete 'tcx' file for applications may be built up in one session. The TCX file is written on exiting ADAS509 and is placed by default in your */pass* directory

- 5.3.7. The graph is displayed in a following Graphical Output window.
- 5.3.8. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 5 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

6. ADAS208

The program allows calculation of excited state populations of ions in a plasma of specified temperatures and densities by drawing on fundamental energy level and rate coefficient data from a specific ion file. It extends ADAS205 by inclusion of metastable parents, the condensed influence of very highly excited level populations and inner shell ionisation forming excited states. It allows consistent inclusion of three-body recombination and selective improvement of metastable ionisation rates. Datafiles of derived generalised collisional-radiative coefficients may be generated.

- 6.1. The **file selection window** has the appearance shown below
 - 6.1.1. Data root a) shows the full pathway to the appropriate data subdirectories. 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 *adf04* ('specific ion files'). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
 - 6.1.2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
 - 6.1.3. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.
 - 6.1.4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
 - 6.1.5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
 - 6.1.6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
 - 6.1.7. A second file selection is given. This is the choice of expansion file of type *adf18* (subdirectory */a17-p208*) which cross-references projection matrices (*adf17*) into the specific ion file under examination. The expansion file must be consistent with the specific ion file with which it is linked and in fact contains the specific ion file name.
 - 6.1.8. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window



- 6.2. The **processing options window** has the appearance shown below
- 6.2.1. There are three 'pop-up' windows for setting temperatures, densities and for designating metastable levels. For the temperature window a), click on the *Edit Table* button to open up the table editor. The editing operations are as described in the introductory chapter. Note that there is a set of input electron temperatures from the selected file. These indicate the safe range of temperatures if extrapolation is to be avoided. Note that altering units (which must be done with the table edit window activated) converts the input values and interprets the output values in the selected units. It **does not convert** output values already typed in. *Default Temperatures* are inserted in the selected units on clicking the appropriate button. Note that the ion and neutral hydrogen temperatures are **only used if** such collisional data is present in the input *adf04* file.
 - 6.2.2. There are three choices of densities tables. Click the choice at b) to enter the table in the display window. Thereafter it is handled in like manner to the temperature table. Note that in this case there are no input density values. Thus unit changing only affects the interpretation of the output values created by the user. The N_H/N_e , etc.) **are only used if** the corresponding data are present in input *adf04* file. The values of the densities on the same row as the electron density are used together in the calculation, so the vectors and electron density vector are of the same length. By contrast the output electron temperatures are independent so that final calculated populations are obtained at points of a two-dimensional electron temperature/electron density grid.
 - 6.2.3. The Metastable State *Selections* button c) pops up a window indexing all the energy levels. Activate the buttons opposite levels which you wish

treated as metastables. See the main ADAS USER Manual for a detailed explanation of the handling of metastables in the collisional-radiative picture.

- 6.2.4. Various processes, supplementary to the primary electron excitation collisions and bound-bound radiative transitions, are activated as desired by clicking on the appropriate buttons d). Note again these only have an effect if such data is present in the *adf04* file except for *Ionisation rates*. This activates ionisation out of excited states and is obtained by an internal calculation of these rates in the ECIP approximation. **Warning**-ionisation should **not** be switched on if you have included autoionising levels in your *adf04* dataset but have omitted the details of alternative thresholds etc present in advanced *adf04* files.
- 6.2.5. Proton collisions may be present in the *adf04* file. If so, these rate coefficients may be scaled to represent a mixture of other charged projectiles with a mean Z-effective e).
- 6.2.6. The *ionisation coefficient search* button activates a new process equivalent to ADAS502.

ADAS208 PROCESSING OPTIONS

Title for Run

Data File Name : /disk2/adas/adas/adf04/belike/belike_wjd92#c.dat

Browse comments

Nuclear Charge : 6 Ion Charge : 2

a) **Temperatures**

Index	Electron	Ion	Neutral Hydrogen	Input Value
1	5.000E+04	5.000E+04	5.000E+04	2.000E+04
2	7.000E+04	7.000E+04	7.000E+04	3.000E+04
3	1.000E+05	1.000E+05	1.000E+05	5.000E+04
4	1.500E+05	1.500E+05	1.500E+05	1.000E+05
5	2.000E+05	2.000E+05	2.000E+05	2.000E+05

Temperature Units : Kelvin

Edit Table

Default Temperatures

b) **Densities**

Input densities : NE & NH N(z-1) N(z+1)

Index	Electron Densities	Ion Densities	NH/NE Ratio	N(z1)/N(z) Ratio
1	1.000E+10	0.0	0.0	0.0
2	1.000E+11	0.0	0.0	0.0
3	1.000E+12	0.0	0.0	0.0
4	1.000E+13	0.0	0.0	0.0
5	1.000E+14	0.0	0.0	0.0

Density Units : cm-3

Edit Table

Default Densities

Metastable States

2s2 (1)S(0.0)

Selections

c)

Reaction Selection

Proton Impact Collisions

Scale Proton Impact for Zeff

Enter Z-effective for Collisions

d)

Ionisation Rates

Neutral H Charge Exchange

Free Electron Recombination

Inner shell ionisation

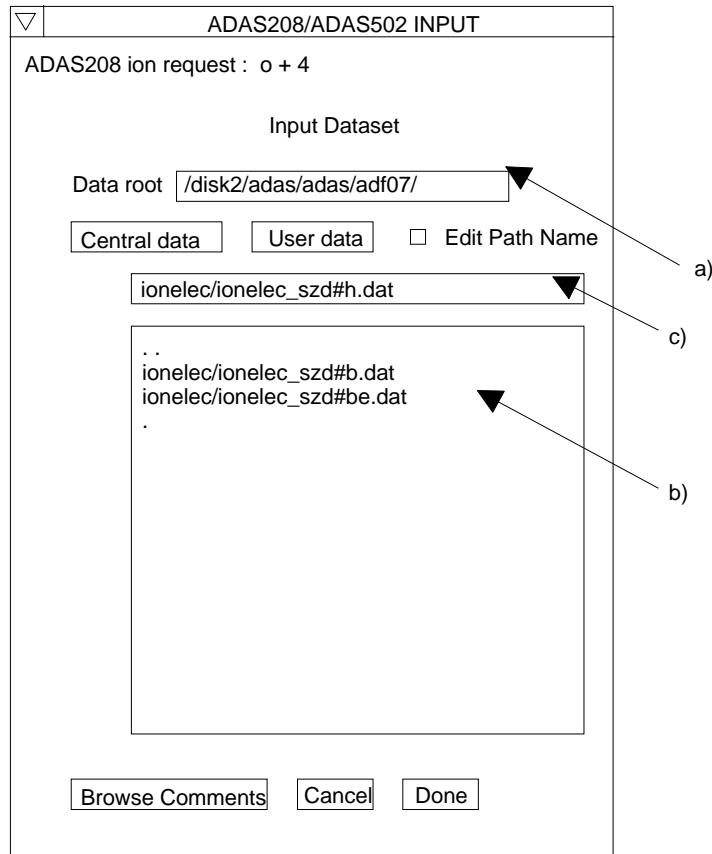
Include projection data

e)

Spawn Ionisation coefficient search f)

Edit the processing options data and press Done to proceed

- 6.2.7. The **ionisation rate coefficient acquisition windows** are as follow:
- 6.2.8. The usual file selection window is presented, in this case for an *adf07* file containing ionisation rate coefficients. The ion for which data is required is given for information.



- 6.2.9. The processing options window is similar to the usual ADAS502 one but with an extra sub-window a) for matching the selected coefficients to the initial state/ final state metastable pairs in the ADAS208 program. The ADAS208 code notifies the initial state/final state metastable pairs it needs and these appear in the lower transition list window b). If a requested transition from ADAS208 is not satisfied then a default ionisation rate coefficient is used for that transition.
- 6.2.10. Note that the output temperatures c) are not editable but transmitted from ADAS208. The 'Exit to menu' icon at d) in this case in fact restores the spawning ADAS208 window.
- 6.2.11. Press the *Done* button to progress to the output options window as for ADAS502. The ionisation coefficient graph may be displayed in the usual manner. When it is displayed, pressing the *Record* button below the graph causes the selected ionisation coefficient to be recorded and made available to the main ADAS208 processing.
- 6.2.12. It is possible to fill the ionisation coefficient requirements by opening other *adf07* files. Simply move back to the file selection window for ADAS208/ADAS502 above.
- 6.2.13. Return to the spawning ADAS208 window by clicking the *Cancel* button on the ADAS208/ADAS502 file selection window above or the 'Exit to menu' icon.

▽
ADAS208/ADAS502 PROCESSING OPTIONS

Title for run

Data file name : /disk2/adas/adas/adf07/ionelec/ionelec_szd#h.dat

Browse comments

Polynomial fitting

Fit Polynomial value %

Select data block

Index	Initial ion	Metastable index	Final ion	Metastable index
2	H + 0	1	H + 1	1
1	H + 0	1	H + 1	1
2	H + 0	1	H + 1	1

Initial ion: o + 4 Final ion : o + 5

Select matching states

Initial metastable	Final metastable
1(1)S(0.0)	1(2S)
1 (1)S(0.0)	1(2S)
2(3)P(4.0)	1(2S)

Output Electron Temperature

Index	Output	Input
1	1.000E+00	1.000E+00
2	2.000E+00	2.000E+00
3	5.000E+00	5.000E+00
4	1.000E+01	1.000E+01
5	2.000E+01	2.000E+01
6	5.000E+01	5.000E+01
7	1.000E+02	1.000E+02
8	2.000E+02	2.000E+02

Temperature units : eV

Edit the processing options data and press Done to proceed

☰

- 6.3. The ADAS208 **output options window** has the appearance shown below
- 6.3.1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
 - 6.3.2. Graphical display is activated by the *Graphical Output* button a). This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.
 - 6.3.3. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exists and the *Replace* button has not been activated, a 'pop-up' window issues a warning.
 - 6.3.4. The temperature choice for the graphs is made at b). A choice of output graph plotting devices is given in the Device list window c). Clicking on the required device selects it. It appears in the selection window above the Device list window.

6.3.5. The *Text Output* button at d) activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.

6.3.6. A number of output files are created by ADAS208 if requested at e). These are the PEC, photon emissivity file, the SXB, ionisation per photon file and the GCR, generalised collisional-radiative files. These are of *adf15*, *adf13* and *adf10* structure respectively. The GCR files in fact refer to a group of files (ACD, SCD etc). They go by defaults into

$...../<uid>/adas/pass/pec.pass$
 $...../<uid>/adas/pass/sxb.pass$
 $...../<uid>/adas/pass/<...>.pass$

respectively.

6.3.7. The graph is displayed in a following **Graphical Output** when the *Done* button is pressed.

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

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

6.3.10. Press the *Print* button to make a hard copy of the currently displayed picture.

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

7. **ADAS601**

Given a set of observed spectral intensities, $G(T_e)$ functions and elemental abundances, the program evaluates an estimate for the emission measure differential in temperature, using the integral inversion algorithm of A. M. Thompson. Selection of the input data files for elemental abundances, $G(T_e)$ functions, and observed spectral intensities can be made at any time during the analysis. The output consists of displays of the differential emission measure vs. electron temperature and the reconstructed observed spectral intensity ratios. A tabulation of these quantities is also produced. The input set of $G(T_e)$ functions can be displayed and examined at any time.

7.1. The organisation of the interactive windows differs in ADAS601 from the ADAS norm. Initiate ADAS601 from the ADAS6 series menu. The 'control window' is displayed first.

7.2. The **Control window** has the appearance shown below:

ADAS601						
File	Temperature	Weight	Smoothing	Noise	Plot	Run
Abundance file : /disk2/adas/adas/arch601/abundance/abund.alan						
Intensity file : /disk2/adas/adas/arch601/intensity/A.dat						
Kernel file : /disk2/adas/adas/arch601/kernel/goft.pmwa						
No. of temperature points		100	Tmin :	1.00e+04	Tmax :	1.00e+07
Step in Log(T)		3.0303e-02	Log(T-min)	4.00e+00	Log(T-max)	7.00e+00
Smoothing :			automatic	Noise :	4.00e-04	
Weight:		from intensity data file				
Status:		ready				

7.2.1. There are various actions activated by clicking on the names at a). Each yield a drop down menu for further sub-selection. Information on the actions taken is shown in the various display sub-windows at b), c) and d). There are three input data file name information windows, the temperature information window at c), the smoothing information window and then at the bottom of the control window, shorter information windows for the weighting strategy and the current activity. One can jump freely between actions, but on the first use of this program, the 'File' action must be taken first and files loaded sequentially (see below).

7.3. The **File** action drops down the menu shown at a) below:

7.3.1. Clicking on the file type opens the usual form of ADAS file selection window.

7.3.2. The data type sought is shown at a)

7.3.3. The central ADAS database has no formal data collections of the three types required here, but only sample data. It is suggested that you use the same organisation and main sub-directory naming as the ADAS example. Clicking the *Central data* or *User data* buttons sets up a Data root of the ADAS pattern automatically. Personal data for the program ADAS601 should be held in the subdirectory

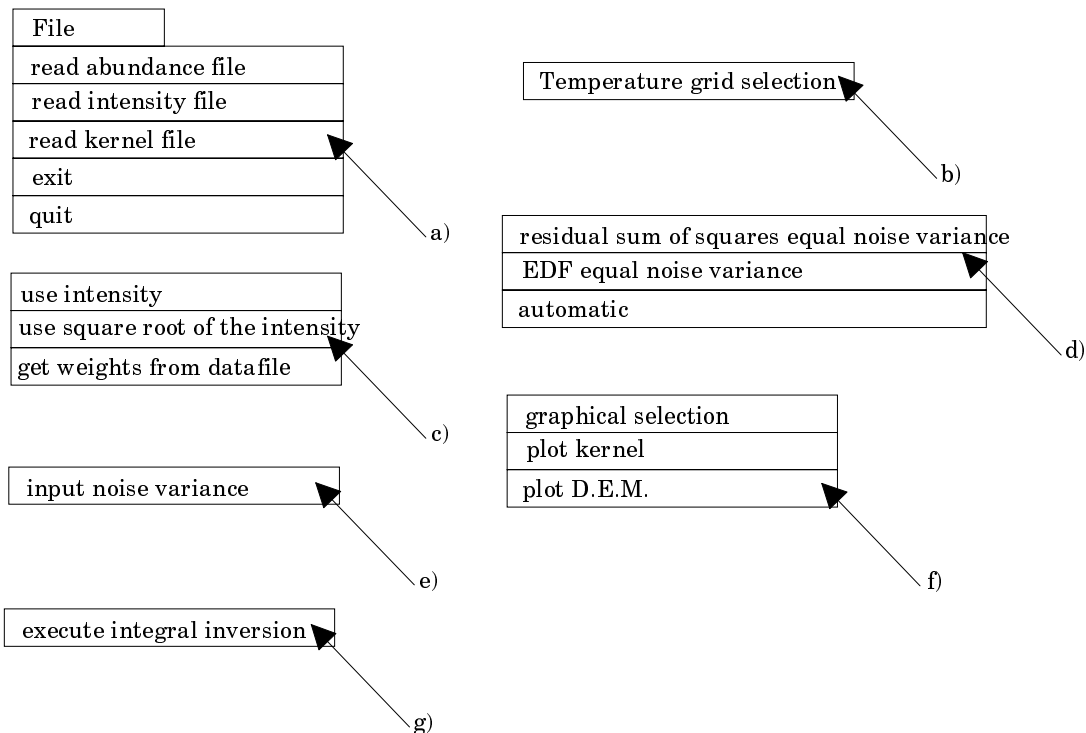
./.../<user>/adas/arch601

corresponding to the ADAS central subdirectory

`./.../adas/adas/arch601.`

Further subdirectories of `/arch601` should be assigned, namely, `/abundance`, `/intensity` and `/kernel`. Thus your abundance files should be held in the subdirectory

`./.../<user>/adas/arch601/abundance/...`



7.3.4. It is convenient to set up an additional subdirectory `/run` to hold output data from the program. Move to this subdirectory before initiating ADAS if you wish to ensure output files are placed directly into this subdirectory.

7.3.5. All three files must be identified before executing the integral inversion.

7.3.6. The intensity file has the standard format shown below:

=====					
	Spectr. wavelength	configuration	configurqtion	blnd G-in	
----- ----- ----- ----- -----					
C + 3	312.429	2s1(2)0(0.5) -	3p1(2)1(0.5)	1	5
C + 3	312.4	2s1(2)0(0.5) -	3p1(2)1(1.5)	1	6
C + 3	384.032	2p1(2)1(0.5) -	3d1(2)2(1.5)	2	7
C + 3	384.2	2p1(2)1(1.5) -	3d1(2)2(1.5)	2	8
C + 3	384.165	2p1(2)1(1.5) -	3d1(2)2(1.5)	0	9
C IV	419.718	2p1(2)1(1.5) -	3s1(2)0(0.5)	0	-4
=====					

(contd.)

=====		
observed wavelength	observed intensity	uncert.
----- ----- -----		
312.429	14.2	7.2
312.429		
384.032	8.6	3.3
384.65	9.5	2.5
419.718	12.4	2.5
=====		

7.3.7. The observed intensity can be given either in *egs cm-2 s-1*, as in the example above, or in *photons cm-2 s-1*. The program will recognise the units from the magnitude. Units can be mixed in the same input data file.

7.3.8. The abundance file is of the simple structure shown below:

O	2.470E-04
NE	3.530E-05
SI	3.920E-05
MG	4.470E-05
S	8.630E-06
FE	3.920E-05
CA	2.940E-06

- 7.3.9. Abundances can be given either as a fraction $N(Z)/N_H$, as in the example above, or in log scale with $\log(N_H)=12.0$. In this latter case, 'H 12.0' must appear in the data (see the abundance file example *.../abund.anders_grevesse*).
- 7.3.10. The kernel file is of the form produced directly as the collection file from ADAS506. Note that you must keep to precisely the same formatting conventions for your personal files of these types.
- 7.4. The **Temperature** action drops down the menu shown at b) above. When you click on this, the temperature sub-window at c) in the control window is reproduced with the boxes editable. Note that entry of any one of the fields causes consistent modification of the others.
- 7.5. The **Weight** action drops down the menu shown at c) above. Click your choice for weighting of the observed intensities. The last choice from the data file uses the variance estimate of the intensity measurement usually provided as part of the observed intensity data (see the structure of an intensity file). This is the default if no selection is made.
- 7.6. The **Smoothing** action drops down the menu shown at d) above
- 7.7. The **Noise** action drops down the menu shown at e) above.
- 7.8. The **Plot** action drops down the menu shown at f) above. Clicking the graphical selection button pops up the standard ADAS output options window below:

ADAS601 OUTPUT OPTIONS

Graphical Output
 Graph Title

Explicit Scaling

X-min

X-max

Y-min

Y-max

Enable Hard Copy Replace
 File name :

Default Device

Post-script
 HP-PCL
 HP-GL

Text Output Replace
 File name :

- 7.8.1. Click the plot kernel button to show a simple graph of the G(Te) functions available in the kernel file.
- 7.8.2. A valid DEM plot is available once the integral inversion has been performed once.

- 7.9. The **Run** action drops down the menu shown at g) above.
 - 7.9.1. Click on the execute integral inversion button to initiate the integral inversion calculation.
 - 7.9.2. After completion of at least one calculation the differential emission measure becomes available for plotting as above.

Additional data has been placed in the ADAS data base. This includes *adf04* specific ion file sub-directories - *copsm#h*, *copha#he*, each with several members. The *adf18* data class is now being built up. Such data sets are of the cross-referencing type enabling data to be transferred from one data class to another and into various programs when some sort of level re-indexing is necessary. Thus there are sub-directories *a17_p208* (containing mappings from *adf17* to the program ADAS208), *a09_a04* (containing mappings from *adf09* to *adf04*) and *a09_p204* (containing mappings from *adf09* to the program ADAS204). These data sets mostly relate to the so called '93' data. You will have noticed '93' appearing widely in directory names. I use the generic '93' name for derived data of the metastable resolved form produced in the 93-95 period. We are working hard on a big '96' data revision for an extended range of light elements which will increase the level sets included for each ion and use finer grids in temperature and density. We hope to release it in about two months. Note also the new data classes *adf24* and *adf25*. *adf24* is state selective charge exchange cross-section data for partially stripped ions at low energy. Only data for carbon ions are issued at this time - this is a growth area. ADAS509 is the interrogation code on this data class. *adf25* contains driving data sets for the code ADAS204. ADAS407 can produce such data sets automatically but we usually view these as a starting point and manually adjust the data sets to our taste. I hope to include ADAS204 in the next release and so shall delay further discussion on these data sets until that time.

H. P. Summers
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