In this release there are four new codes, ADAS414, ADAS415, ADAS801 and ADAS807. ADAS414 and ADAS415 are concerned with the type of soft X-ray filters used in measurements of radiated power from fusion plasmas. Rather simplistic treatments of this have been usual in fusion and incorporated in ADAS . However, the absorption coefficient tables of Henke are available on the internet and are accessed by both fusion and astrophysics users. Under the prompting and support of Ralph Dux, Martin O'Mullane has now introduced the computation of Henke filters and has made ADAS408 consistent with their use. ADAS801 is the start of a new series on atomic structure and creation directly of baseline adf04 files. It is is again MartinO'Mullane's effort and stems from the background code, which we call Cowan/O'Mullane, used extensively in support of ADAS. Now it is available to everyone online. We had hoped to add a number of utility codes to series 8 in this release which aid in the construction of the full, adjusted and augmented adf04 files from the baseline adf04 file. Only the first of these, ADAS807, is ready for this release. Ralph Dux has been the prime mover for this code with assistance from Martin.
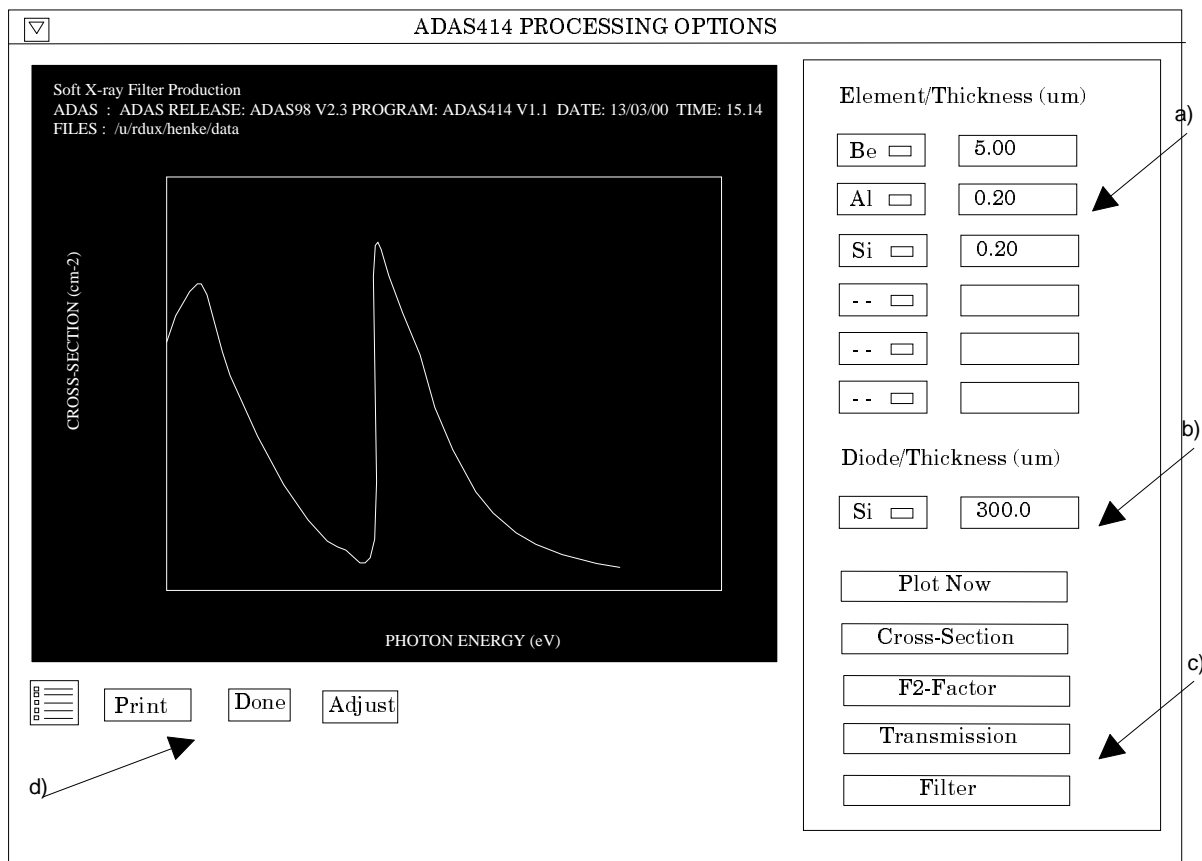
ADAS414   The code generates a numerical representation of the characteristics of thin window filter/diode soft X-ray detectors used in measurements of radiant power from fusion plasmas. Filter/diode detectors have been in general use in fusion for measurements of the radiated power from the high temperature plasma. The devices have a characteristic pass band in the soft X-ray region determined by the transmission of sub-micron deposited metallic layers on a thin window and the absorption in the semiconductor diode substrate. In ADAS modelling of the populations and ionisation state of impurities in plasmas, the radiant power (cf. *plt*, *prb*, *prc* dataset libraries) is an important output quantity. Also, recognising the nature of radiant power measurements, radiant power datasets modified by simple cut-off or Be/Si filter representations have been introduced (cf. ADAS408, ADAS208). These representations are now felt to be too crude for present work, especially if discrimination of the broad transition array features from different heavy metals is to be achieved. A better representation is sought. The spectral absorption characteristics of elements have been collected and tabulated by Henke et al. (1993). These data are maintained for internet access (*http://xray.uu.se*) and provide all necessary information for the present purpose. ADAS414 prepares a numerical representation of a filter/diode combination from Henke absorption data in a form suitable for subsequent ADAS use. The filter is created interactively with graphical display and the final output file may be used by the appropriate ADAS power codes.

   The **file selection window** has the appearance shown below
1. Data root a) shows the full pathway to the subdirectory of Henke cross-section data, *adf35*. 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.

2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window.

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

Soft X-ray Filter Production
ADAS : ADAS RELEASE: ADAS98 V2.3 PROGRAM: ADAS414 V1.1 DATE: 13/03/00 TIME: 15.14
FILES : /u/rdux/henke/data

CROSS-SECTION (cm-2)

PHOTON ENERGY (eV)

Element/Thickness (um)   a)

Be	5.00
Al	0.20
Si	0.20
--	
--	
--	

Diode/Thickness (um)   b)
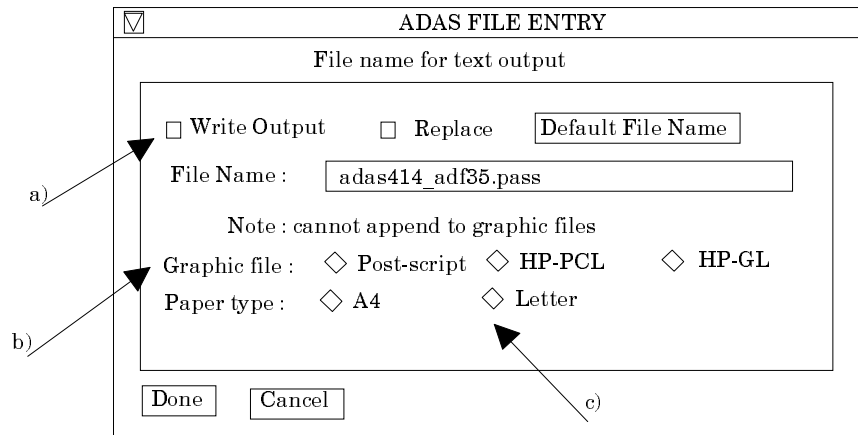
| Si | 300.0 |

Plot Now

Cross-Section

F2-Factor   c)

Transmission

Filter

Print   Done   Adjust

d)

4. The specification of the thin window layers is made at a). Click on the left drop-down list button to see the available elements and select an element. The layer thickness in micros is then entered in the editable box to the right. Up to six layers can be selected.

5. At b), the diode substrate absorbing thickness is specified in the same manner. The choice of substrate is restricted to silicon and germanium.

6. The displayable quantities are selected at c). Make the appropriate choice and finally press *Plot Now* to see the graph.

7. The buttons at d) allow printing of the graph, adjustment of the graph and progression to the final output of the numerical filter file.

8. The *Print* button pops up the File Entry widget as shown below. Specify the output file in the usual manner.

9. The *Adjust* button pops-up the Graph Control widget as shown below. This allows choices of logarithmic or linear plotting and X & Y axes minimum and maximum values.

10. 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 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

ADAS FILE ENTRY

File name for graphical output

☐ Write Output   ☐ Replace   Default File Name

a)

File Name :   adas414_graph.pass

Note : cannot append to graphic files

b)

Graphic file :   ◇ Post-script   ◇ HP-PCL   ◇ HP-GL

Paper type :   ◇ A4   ◇ Letter

c)

Done   Cancel

GRAPH CONTROL

Axes :   X Log / Y Linear

a')

X-units :   (eV)

X :   ☐   ☐

b')

Y :   ☐   ☐

Cancel
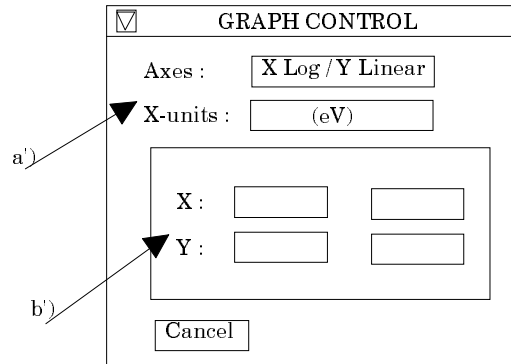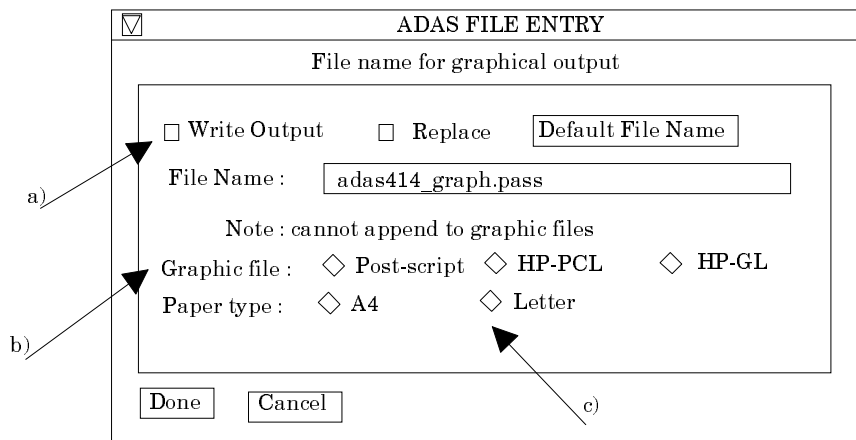
The **text file options window** appearance is shown below

ADAS FILE ENTRY

File name for text output

☐ Write Output   ☐ Replace   Default File Name

a)

File Name :   adas414_adf35.pass

Note : cannot append to graphic files

b)

Graphic file :   ◇ Post-script   ◇ HP-PCL   ◇ HP-GL

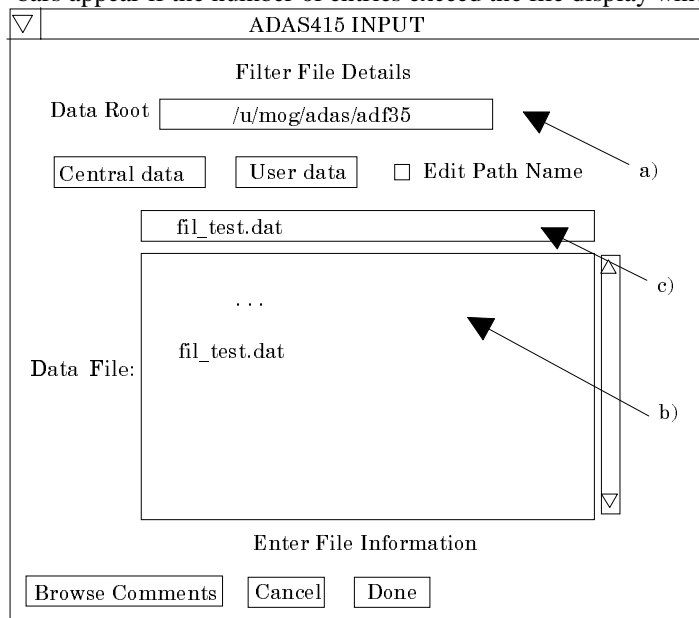Paper type :   ◇ A4   ◇ Letter

c)

Done   Cancel

ADAS415   Th The code displays a numerical filter transmission function from a filter file of type *adf35* created by the code ADAS414 or by other means.

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

1. Data root a) shows the full pathway to the appropriate data subdirectories of type *ad35*. 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.

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

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

```
┌─┬──────────────────────────────────────────────────────┐
│▽│                    ADAS415 INPUT                       │
├─┴──────────────────────────────────────────────────────┤
│                    Filter File Details                    │
│                                                           │
│   Data Root ┌──────────────────────────┐                 │
│             │    /u/mog/adas/adf35       │    ▼            │
│             └──────────────────────────┘                 │
│                                                    a)     │
│   ┌──────────────┐   ┌──────────────┐  □ Edit Path Name   │
│   │ Central data │   │  User data   │                     │
│   └──────────────┘   └──────────────┘                     │
│          ┌──────────────────────────────┐                 │
│          │  fil_test.dat              ▼  │                 │
│          └──────────────────────────────┘                 │
│          ┌──────────────────────────┐ ┌─┐                 │
│          │                          │ │△│    c)           │
│          │        . . .             │ │ │                 │
│          │                        ▼ │ │ │                 │
│          │   fil_test.dat           │ │ │                 │
│   Data File:│                       │ │ │    b)           │
│          │                          │ │ │                 │
│          │                          │ │ │                 │
│          │                          │ │▽│                 │
│          └──────────────────────────┘ └─┘                 │
│                  Enter File Information                    │
│  ┌────────────────┐ ┌──────┐ ┌──────┐                     │
│  │ Browse Comments│ │Cancel│ │ Done │                     │
│  └────────────────┘ └──────┘ └──────┘                     │
└───────────────────────────────────────────────────────────┘
```

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 the notation used for radiative recombination data file names, that is, *<ion>ls* with *<ion>* the recombining ion. *ls* indicates that the radiative recombination data is at LS-resolution.

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

6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile.

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

There is no processing options window.

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

8. 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.

9. Graphical display is activated by the *Graphical Output* button at 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.

10. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button at b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.

11. Hard copy is activated by the *Enable Hard Copy* button at 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.

12. A choice of output graph plotting devices is given in the Device list window to the right. Clicking on the required device selects it. It appears in the selection window above the Device list window.

13. At d) output of the tabular record of the interrogation may be enabled. This is usually called *paper.txt* and it is created in the directory from which ADAS was launched.

14. 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 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

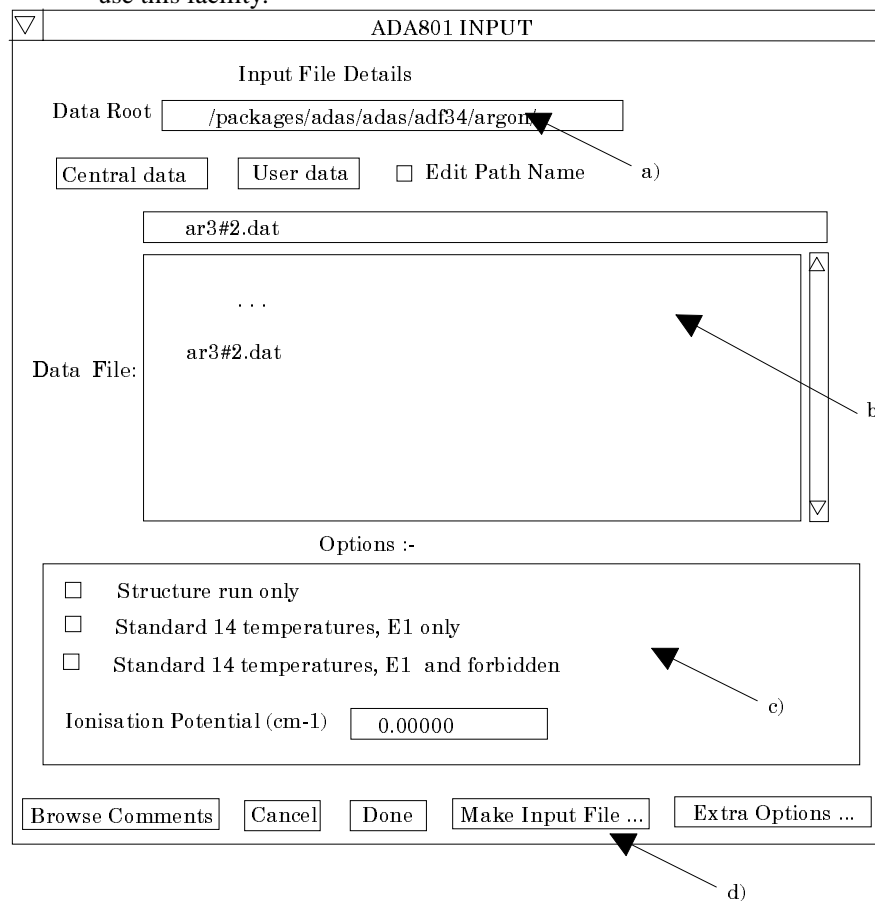The **Graphical Output window** appearance is shown below.
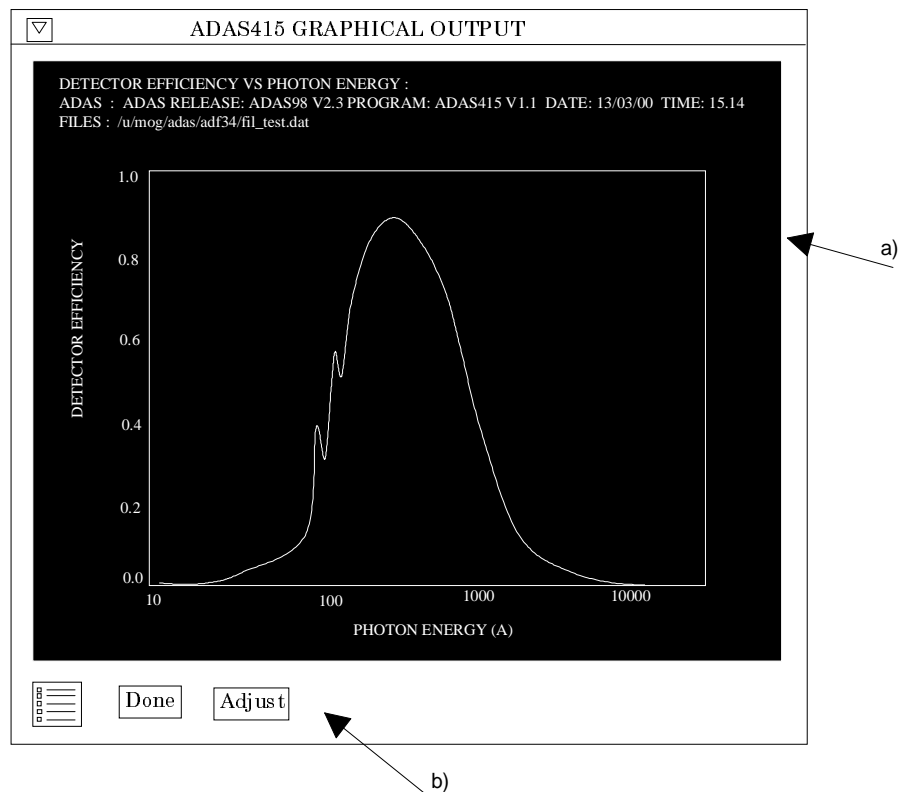
15. Click the *Adjust* button to alter the plotting style (logarithmic or linear) and the maxima and minima for the axes. This is achieved by a pop-up widget as described of the code ADAS414.

16. Click *Done* to return to the Output Options window or the *Exit to Menu* to return to the series 4 menu.

ADAS801   The code solves the Schrodinger equation for a multi-electron atom in a multi-configuration expansion approximation with relativistic corrections treated perturbatively. The eigensolutions are used to evaluate radiative transition probabilities of electric dipole, electric quadrupole and magnetic dipole type and to evaluate electron impact collision cross-sections and Maxwell averaged rate coefficients in a plane-wave Born approximation. The code used here is that developed by Cowan. It has been adjusted by O'Mullane for use in ADAS to provide output in *adf04* format. Also choices of state bundling and state identification have been introduced as necessary for futher manipulations within ADAS.

The **Input Option window** has the appearance shown below

1. Data root a) shows the full pathway to the appropriate data subdirectories of type *adf34*. 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.

```
┌─┬──────────────────────────────────────────────────────────────┐
│▽│                        ADA801 INPUT                          │
├─┴──────────────────────────────────────────────────────────────┤
│                      Input File Details                          │
│                                                                  │
│   Data Root    ┌──────────────────────────────────┐             │
│                │ /packages/adas/adas/adf34/argon▼  │             │
│                └──────────────────────────────────┘             │
│   ┌──────────────┐   ┌─────────────┐   □ Edit Path Name    a)   │
│   │ Central data │   │  User data  │                             │
│   └──────────────┘   └─────────────┘                             │
│              ┌───────────────────────────────────────────┐      │
│              │ ar3#2.dat                                  │      │
│              └───────────────────────────────────────────┘      │
│              ┌─────────────────────────────────────────┬─┐      │
│              │                                         △│      │
│              │     . . .                               │ │      │
│              │                                       ▼  │ │      │
│              │     ar3#2.dat                           │ │      │
│   Data  File:│                                         │ │ b)   │
│              │                                         │ │      │
│              │                                         │ │      │
│              │                                       ▽│ │      │
│              └─────────────────────────────────────────┴─┘      │
│                        Options :-                                │
│   ┌──────────────────────────────────────────────────────┐      │
│   │  □   Structure run only                               │      │
│   │  □   Standard 14 temperatures, E1 only                │      │
│   │  □   Standard 14 temperatures, E1  and forbidden  ▼   │      │
│   │                                              c)       │      │
│   │  Ionisation Potential (cm-1)  ┌──────────┐            │      │
│   │                               │ 0.00000  │            │      │
│   │                               └──────────┘            │      │
│   └──────────────────────────────────────────────────────┘      │
│ ┌─────────────────┐ ┌────────┐ ┌──────┐ ┌───────────────┐ ┌──────────────┐ │
│ │ Browse Comments │ │ Cancel │ │ Done │ │ Make Input File ...│ │ Extra Options ...│ │
│ └─────────────────┘ └────────┘ └──────┘ └───────────────┘ └──────────────┘ │
│                                       ▼                          │
│                                          d)                      │
└──────────────────────────────────────────────────────────────────┘
```

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

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

4. Once a data file is selected, the set of buttons at c) become active. Make the appropriate selection. The standard temperatures are those z-scaled temperatures used in *adf04* files designed for iso-electronic sequences studies. Once can choose to include only electric dipole or elelctrc dipole and forbidden transition probabilities. The latter choice can lead to a large expansion of the output *adf04* file.

5. It is necessary to enter the ionisation potential for the ion. That is the energy (cm-1) to ionise from the ground state to the ground state of the next ion. Note that this value is only written to the output *adf04* file.

6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile.

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

8. The *Make Input File* button generates a pop-up widget which gives guided creation of an input file. **This is not yet operational**.

9. The Extra Options button generates the pop-up widget shown below and allows more more access to the options of the code.

10. At a) sub-selection of the forbidden transition probability output is possible. This may usefully reduce the size of the output *adf04* file.

11. At b), scale factors can be altered to improve the final energy levels and transition probabilities. The values displayed when the widget opens are those from the previous case. There is no other prescription and any such alteratons are a matter for the user.

12. At c), an editable table of output temperatures for the electron impact collisional rate coefficients in the *adf04* file is offered. Buttons at d) allow default choices and switching between normal and reduced forms for the temperatures. There is also a *Clear* button which empties the table.

The **output options window** has the appearance shown below.

13. There is no graphical display.

14. At a) and b) output adf04 file names are selected or specified. The buttons allow choice of level (IC) and/or term (LS) format of the output *adf04* file. In the usual manner *Default File Names* may be selected.

15. There are large files of intermediate data created by the code which can be directed to the user /pass directory. Also a summary text file can be output. The choices are at c).

16. The program can be run in foreground by clicking *Run Now* at d) or it can *be Run in Batch*. **Batch is not yet operational**.

17. In foreground mode, the pop-up widget shown below gives information on the progress of the calculation. The steps in the calculation described in the program section are highlighted in turn and the thermometer shows the progress in that step.

18. Examples of the output adf04 file are available in the ADAS database under the directories */.../adas/adas/adf04/copmm#<element symbol>*.

ADAS807 The code prepares the set of augmented, cross-reference and template files which are required for complete generalised collisional radiative modelling using the codes of ADAS series 2 and 4.

The **file selection window** appears first as illustrated below. *adf04* is the appropriate format for use by the program ADAS807 ADAS807 requires two such files, namely, for the

'Ionising Ion' and the 'Ionised Ion'. If you wish to use personal data of this type, then as usual it should be held in a similar file structure to central ADAS with your identifier replacing the first *adas*, but in addition it must have the configuration fields in 'Eissner' notation and the orbital binding energy fields not empty.

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

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

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

4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual data-files are presented for selection. Data-files all have the termination *.dat*. Note that data-sets in sub-directories of the form */cop98* and */copmm* are the only ones guaranteed to work.

5. When an ionising ion has been chosen, then the corresponding ionised ion has to be chosen in sub-window b). ADAS807 creates the expected file name and displays it at d) if it exists. This name can be over-ridden in the usual manner.
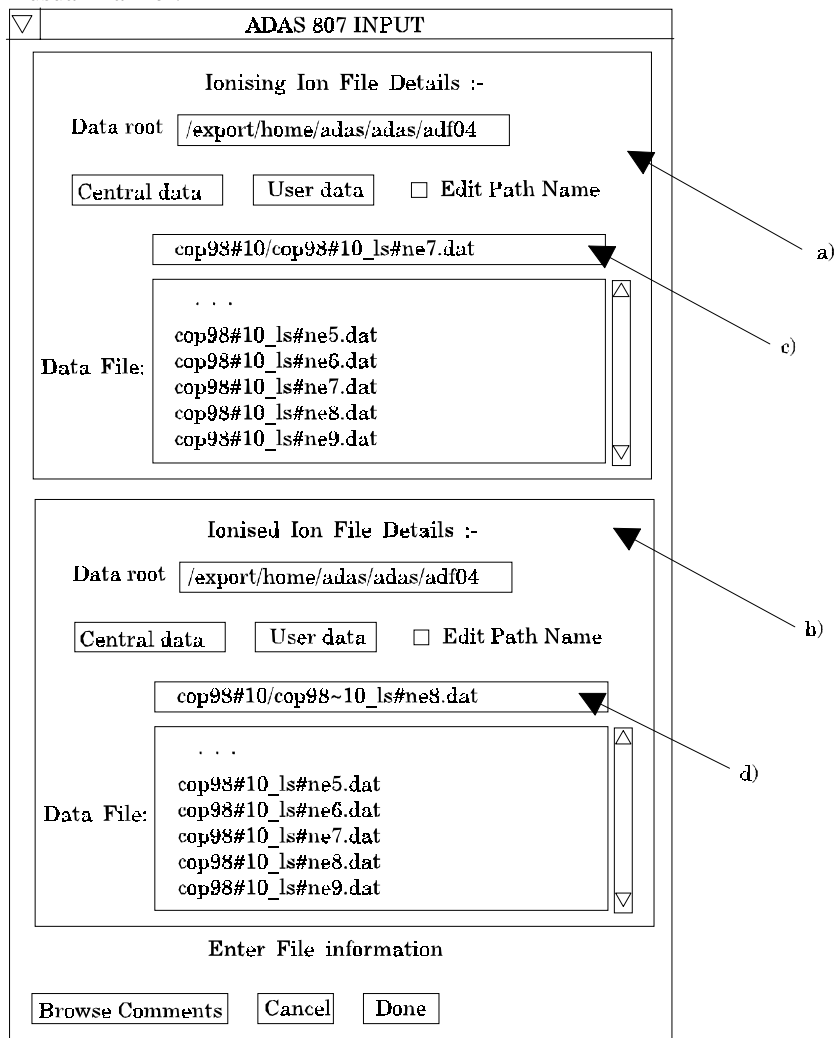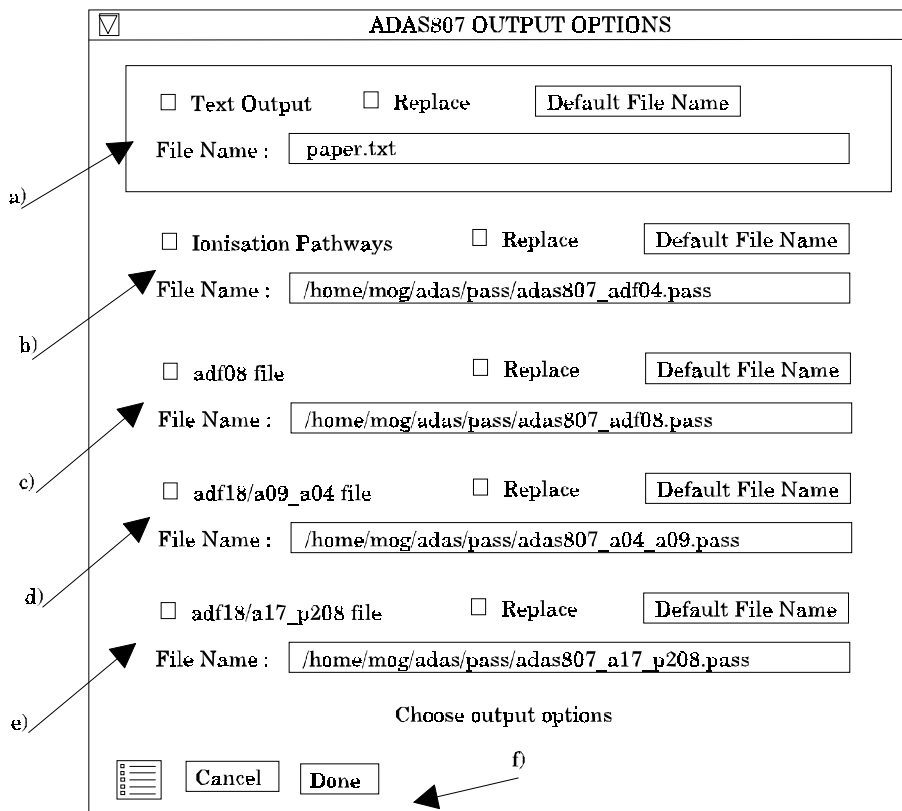
The **metastable selection** window is as shown below. The metastables are to be chosen for the ionised ion.
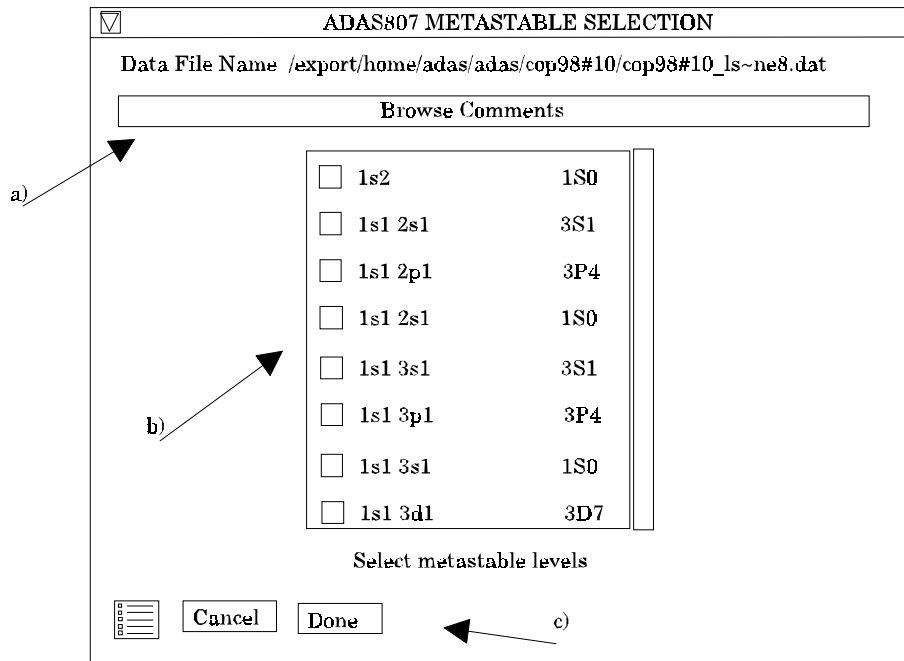
6. The ionised ion data file name is displayed at a) and the comments section of the file can be browsed in the usual manner.
7. At b), a scrollable table of the levels present in the data file is presented with buttons to select levels required as metastables.
8. Clicking the *Done* button at c) moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window. The *Exit to Menu* icon button is also present.

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

ADAS807 OUTPUT OPTIONS

a) Text Output   Replace   Default File Name
File Name : paper.txt

b) Ionisation Pathways   Replace   Default File Name
File Name : /home/mog/adas/pass/adas807_adf04.pass

c) adf08 file   Replace   Default File Name
File Name : /home/mog/adas/pass/adas807_adf08.pass

d) adf18/a09_a04 file   Replace   Default File Name
File Name : /home/mog/adas/pass/adas807_a04_a09.pass

e) adf18/a17_p208 file   Replace   Default File Name
File Name : /home/mog/adas/pass/adas807_a17_p208.pass

Choose output options

Cancel   Done   f)

9. At a) output of the tabular record of the interrogation may be enabled. This is usually called *paper.txt* and it is created in the directory from which ADAS was launched.

10. Four cross-reference, template and augmented files can be created. At b) the ionising *adf04* file, with ionisation pathways added, is specified for output..

11. At c), the template *adf08* file for state selective recombination data is specified for output. This file can then act as the input to the code ADAS211 which calculates the actual recombination coefficients.

12. At d), the cross-referencing file, which relates between the primary state selective dielectronic archives and the target *adf04* ionising file, is specified for output. This cross-referencing file is the necessary input file for the dielectronic mapping code ADAS212 which actually adds the dielectronic data to the *adf04* file.

13. At e), the cross-referencing file, which details the fractionation of the high bundle-n shell projection matrices over the resolved low levels of the ionising *adf04* file, is specified for output.

14. 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 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

There are a number of new ADAS data formats assosciated with the new codes. These are as follow

ADF34 Provides driver datasets for ADAS801 Cowan/O'Mullane atomic structure calculations. Data root = /.../adas/adas/adf34/; class library = /iso_nucl; sublibraries = /argon, /nickel, /xenon.
ADF35 Provides absorption source data and spectral filter data used byADAS408. Data root = /.../adas/adas/adf35/; class library = /henke.

H. P. Summers
18 Mar 2000