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## ADAS807: Prepare cross-referencing files

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. Added extra features now allow all the intermediate and cross-referencing files and data blocks required in the 'GCR Project' to be generated automatically

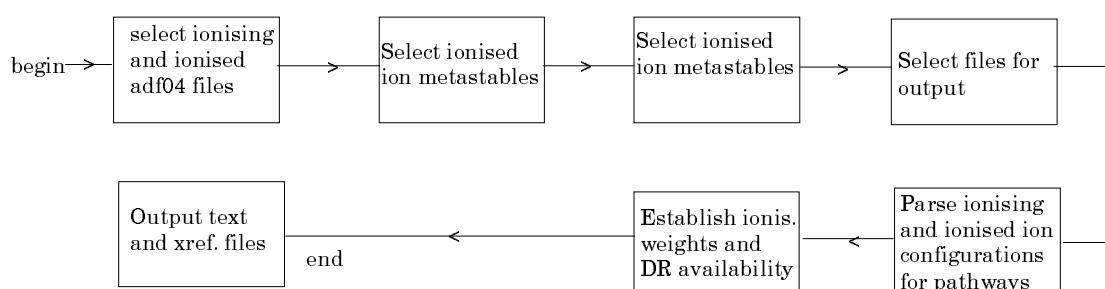
### Background theory:

The theory is described in the main codes of ADAS series 2 and 4..

### Program steps:

These are summarised in figure 9.07.

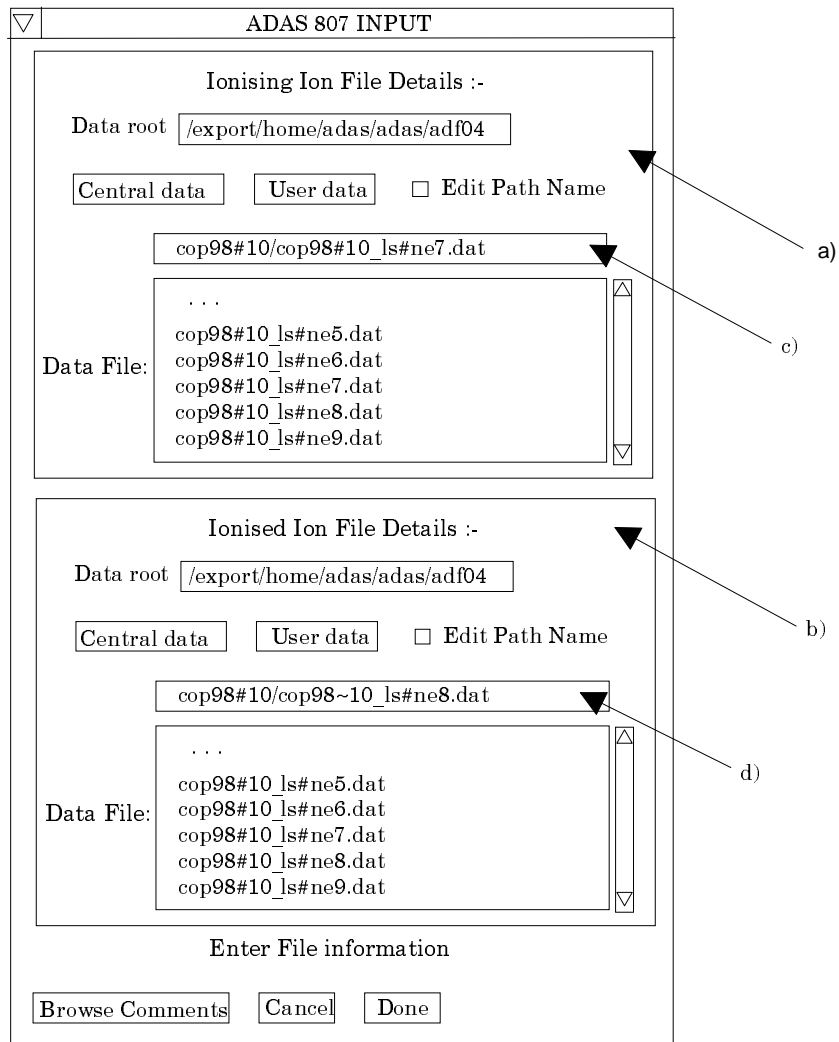
Figure 9.07



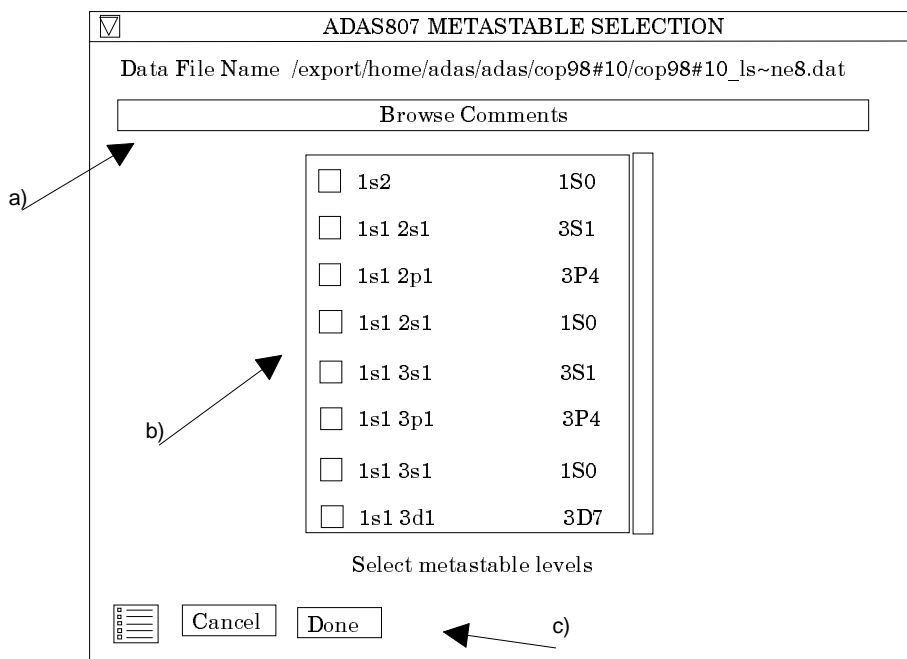
### Interactive parameter comments:

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-riden 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.
9. Note that the code now makes an automatic initial selection of the metastable levels. This may be overridden by the user

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

ADAS807 OUTPUT OPTIONS

Text Output     Replace    Default File Name

File Name : paper.txt

a)

Ionisation Pathways     Replace    Default File Name

File Name : /home/mog/adas/pass/adas807\_adf04.pass

b)

Ionisation Rates (S-lines)     Replace    Default File Name

File Name : /home/mog/adas/pass/adas807\_adf04\_sline.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

f)

Choose output options

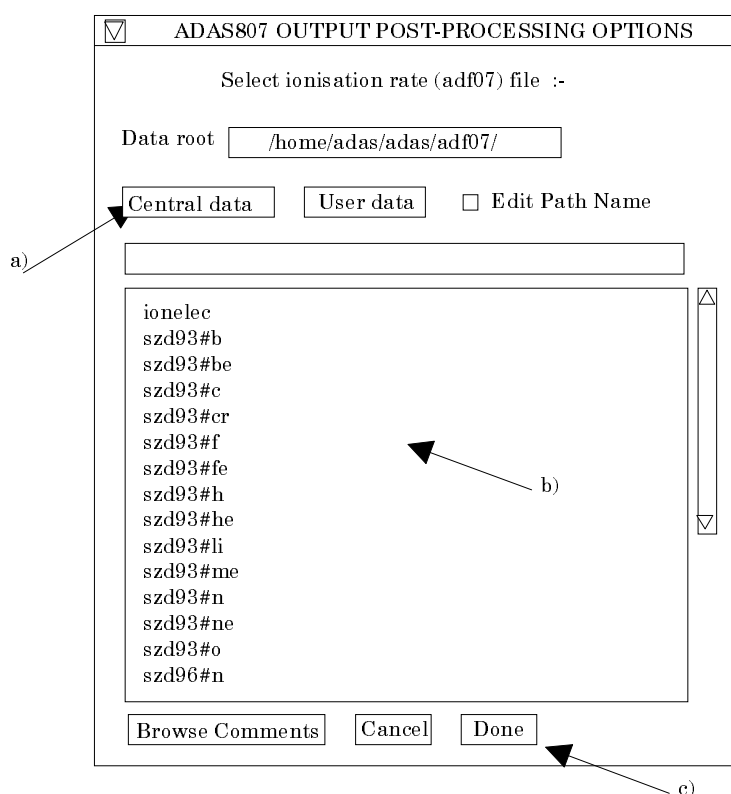
Cancel Done

g)

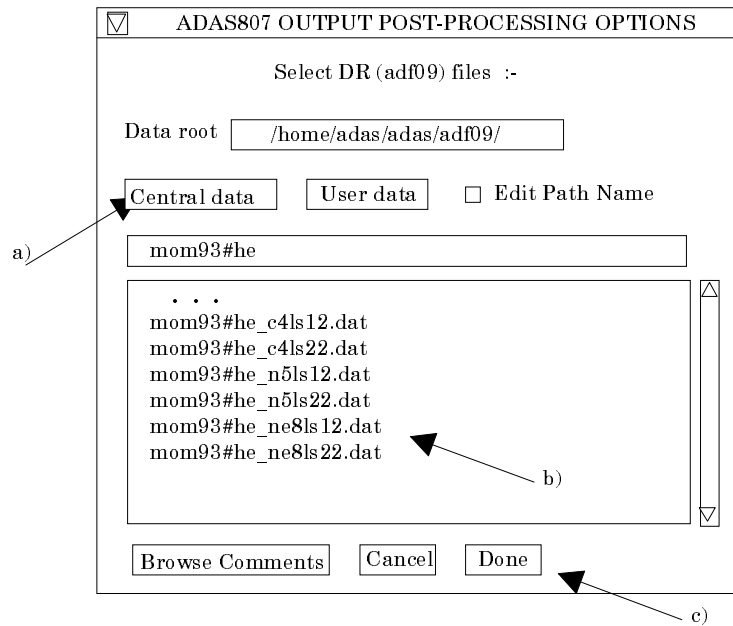
10. At a) output of the tabular record of the interrogation may be enabled. This is usually called *paper.txt* and it is created in the directory from which ADAS was launched.
11. Four cross-reference, template and augmented files can be created. At b) the ionising *adf04* file, with ionisation pathways added, is specified for output..
12. At c) the option to add electron impact ionisation rate coefficient data to the output *adf04* file as 'S-lines' is given. As indicated in the comments for code ADAS208, S-lines can include true excited levels as well as ground and metastable levels.

Within the ADAS databases, we have only explicit data for electron impact ionisation from ground and metastables. Ionisation from true excited states is included in ADAS population codes but via internal subroutines (reflecting fairly simple approximate methods such as ECIP or fits). This does correspond to reality in that there is almost no high quality theoretical data and no experimental data for excited state ionisation.

13. Selection at c) pops up an input file selection widget as shown below. It points to the adf07 formatted section of the adas database where ionisation rate tabulations are located. It is metastable resolved initial and final state ionisation data which is relevant here.
14. Select by element. It is important to *Browse Comments* and verify that the data set chosen is appropriate. The provision of initial and final state resolved ionisation data is an important issue which we have been working on extensively. Details are given the new data description part of the bulletin below, but note that we have prescriptions for creating approximate resolved data form unresolved stage-to-stage data for 1<sup>st</sup> and 2<sup>nd</sup> period iso-electronic series.
15. At d), 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.



16. At e), the automatic creation of the mapping file of type adf18/a09\_a04, which carries state selective dielectronic data into the adf04 file as 'R-lines', is implemented. It pops up the widget shown below.
17. The mapping file is used in a subsequent execution of the mapping by ADAS212.



18. At f), 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.
19. At g), 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.
20. 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.

## Notes: