ADAS314: Convert QCX to effective cross-sections

The code converts state selective charge exchange cross-sections of ADAS data format *adf01,* for capture to form one electron ions, to averaged cross-sections over reactant distribution functions. There are a number of choices depending on whether the donor and/or receiver are mono-energetic or have Maxwellian speed distributions. The averaged data is returned in the same format as the original *adf01* file. Extreme care must be used in interpreting results using such a datafile in other ADAS series 3 programs.

Background theory:

Program steps:

These are summarised in the figure below.

Figure 3.14

Interactive parameter comments:

The program which makes use of data from archived ADAS data-sets initiates an interactive dialogue with the user in three parts, namely, input data file selection, entry of user data and disposition of output. The primary calculations may be conducted in foreground or background.

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 ADAS312 from the program selection menus in the usual manner.

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

1.   Data root a) shows the full pathway to the appropriate data subdirectories of type *adf01*. 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.

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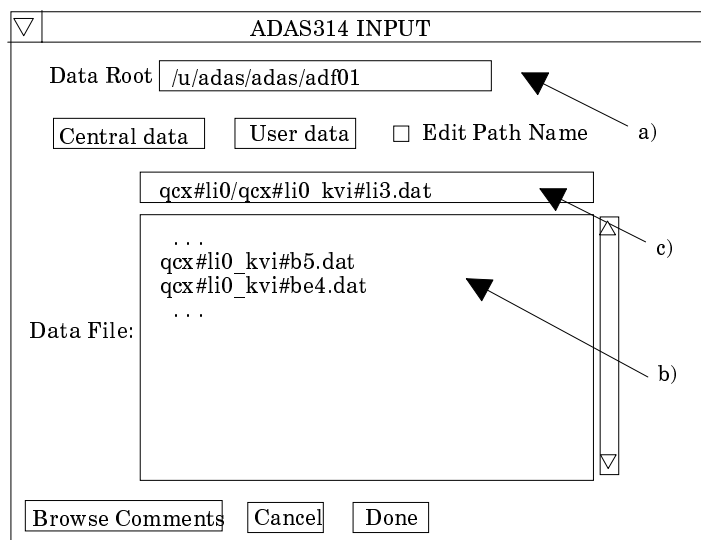
7.   Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

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

8.   An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being interrogated is also shown. The button *Browse comments* allows display of the information field section at the foot of the selected dataset, if it exists, in the usual manner.

9.   At a), enter the mass numbers of the donor and receiver reactants. These are used for conversions between energies and speeds.

10.   At b), the choice of particular form of averaging is made. There are four choices.

(i) <u>mono-energetic</u> - one collision partner static, other mono-energetic. The code essentially alters the energy range of the adf01 file tabulation. The effective cross-section, rate coefficient/moving partner speed is delivered as a function of moving partner energy in eV/amu.

(ii) <u>thermal donor</u> - monoenergetic receiver. A donor/receiver sub-widget entry box appears at d), receiver energy to be specified as a 'temp' in sub-widget in eV, donor thermal with energies entered in a table using Table Editor. The effective cross-section, rate coefficient/donor mean speed is delivered as a function of donor energy in eV/amu.

(iii) <u>thermal receiver</u> - monoenergetic donor. A donor/receiver sub-widget entry box appears at d), donor energy to be specified as a 'temp' in sub-widget in eV, receiver thermal with energies entered in a table using Table Editor. The effective cross-section, rate coefficient/receiver mean speed is delivered as a function of receiver energy in eV/amu.

(iv) <u>thermal thermal</u> - Donor and receiver thermal at the same temperature with temperatures entered in a table using Table Editor. The effective cross-section, rate coefficient/donor mean speed is delivered as a function of donor energy in eV/amu.

11.   At c), the temperatures/energies (the request title alters according to the selection at b)) at which you wish the output data are chosen. Table editor is available to enter this data and default temperatures (equal to the energies in the *adf01* file) may be chosen by button click as usual. Note that temperatures can be specified in terms of donor temperature (eV), receiver temperature(eV) or eV/amu. This scaling operates independently of the type of averaging selected.

12.   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 3 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

```
┌─────────────────────────────────────────────────────────────────────┐
│ ▽ │                    ADAS314  PROCESSING OPTIONS                    │
├───┴─────────────────────────────────────────────────────────────────┤
│                                                                       │
│      Title for Run      ┌───────────────────────────────────────┐     │
│                         └───────────────────────────────────────┘     │
│                                                                       │
│      Data File Name :  /u/adas/adas/adf01/qcx#li0/qcx#li0_kvi#li3.dat │
│      ┌──────────────────────────────────────────────────────────┐     │
│      │                    Browse comments                       │     │
│      ├──────────────────────────────────────────────────────────┤     │
│      │  Enter the reactant mass numbers   Donor :  ┌──────┐  Receiver  ┌──────┐ │
│      │                                             └──────┘           └──────┘ │
```



```
│      Select form of thermal average                                   │
│                                                                       │
│         ◇   Mono - energetic          ◇   Thermal - Thermal           │
│                                                                       │
│         ◇   Thermal Donor             ◇   Thermal Receiver            │
```

a)
b)
c)
d)

Enter Output Particle Energies
Output values

Index	Output	Input
1	5.000E+04	5.000E+04
2	7.000E+04	7.000E+04
3	1.000E+05	1.000E+05
4	1.500E+05	1.500E+05
5	2.000E+05	2.000E+05

Enter the Receiver Temp :

Temperature Units : eV (don.)

Edit Table

Default Temperatures

Cancel   Done

The **output options window** is shown below. There is no graphical output possibility but in addition to the usual text file, an output data file is always produced.

13.   The data output file at b) is of *adf01* format. It is usually sent to the pass directory as *adas314_adf01.pass* for checking and re-naming later. This is the default file name.

14.   At c) 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.

15.   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 3 menu. *Done* and *Cancel* take you back to the previous screen.

Illustration:

Table 3.14a.

Notes: