

ADAS301: State selective charge exchange data - graph and fit cross-section

The program interrogates state selective charge exchange cross-section files of type ADF01. Data is extracted for the capture to a selected n-shell of a hydrogen-like or lithium-like receiving ion. The data may be interpolated using cubic splines at selected relative collision energies. A minimax polynomial fit is made to the interpolated data. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the polynomial approximation.

Background theory:

The program only allows display of the total and n-shell charge exchange cross-sections. However the data sets can in general contain nl- or nlm subshell cross-sections. The full prescription of the data sets are given in the appendix.

For a specified relative collision energy E_i belonging to the tabulation, let the total cross section be $\sigma_{tot}(E_i)$ and the n-shell cross-sections be $\sigma_n(E_i)$. The latter are tabulated for $n_{min} \leq n \leq n_{max}$ for some n_{min} and n_{max} . Data can be displayed for $n \geq n_{max}$. To achieve this the program uses an extrapolation of the form

$$\sigma_n(E_i) = (n_{max}/n)^{\beta(E_i)} \sigma_{n_{max}}(E_i) \quad 4.1.1$$

The parameter $\beta(E_i)$ is deduced from $\sigma_{n_{max}-1}(E_i)$ and $\sigma_{n_{max}}(E_i)$. It is tabulated in the data set. The $\sigma_n(E_i)$ are normalised to the total cross-section so that

$$\sigma_{tot}(E_i) = \sum_{n=n_{min}}^{\infty} \sigma_n(E_i) \quad 4.1.2$$

using the extrapolation equation 4.1.1 for $n \geq n_{max}$.

Although there is no display option for l-subshell cross-sections, the underlying data subroutine operating on data sets of type ADF01 also returns these. Explicit l-subshell cross-sections $\sigma_{nl}(E_i)$ are tabulated for $n_{min} \leq n \leq n_{max}$ and $0 \leq l \leq n-1$. In extrapolation there are two cases.

Case 1: No l subshell subdivision parameters are given in the ADF01 dataset.. It is assumed that the l distribution for $n > n_{max}$ is the same as for n_{max} so that

$$\sigma_{nl}(E_i) = \begin{cases} \sigma_{n_{max}l}(E_i)(\sigma_n(E_i)/\sigma_{n_{max}}(E_i)) & \text{for } l \leq n_{max} - 1 \\ 0 & \text{for } l \geq n_{max} \end{cases} \quad 4.1.3$$

Case 2: l subshell parameters are given in the the ADF01 dataset. The parameters are obtained as a fit to l- subshell cross-section data for a particular n-shell using the program ADAS107. The parameterisation identifies an l-type , parameter $ltyp(E_i)$ and an approximate l (non integral) at which the cross-section behaviour changes from rising at low l to falling at high l, parameter $xlcr(E_i)$. The behaviour is then given by

$$\sigma_{nl}(E_i) \sim \begin{cases} (2l+1)^{pl^2} & \text{for } l < xlcr \\ \exp(-(l-xlcr)^{pl^3}) & \text{for } l > xlcr \end{cases} \quad 4.1.4$$

The normalisation

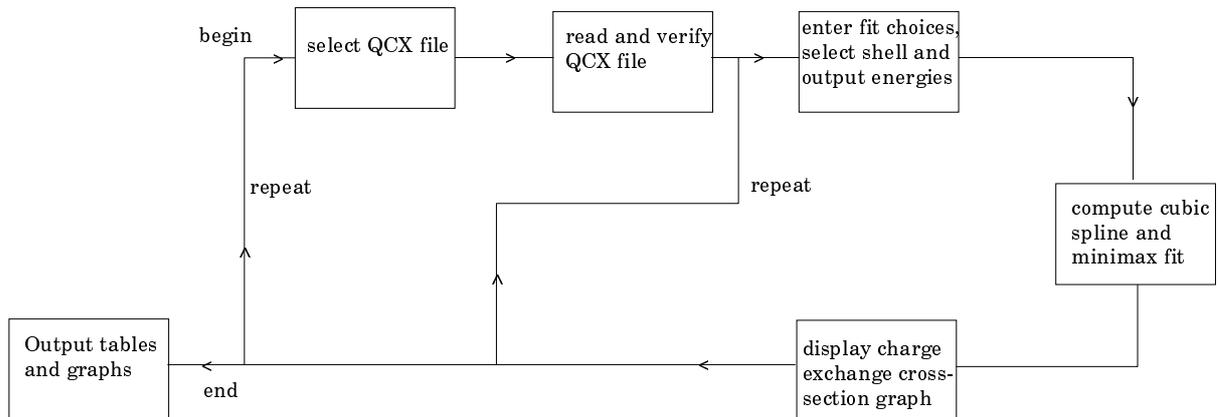
$$\sigma_n(E_i) = \sum_{l=0}^{n-1} \sigma_{nl}(E_i) \quad 4.1.5$$

is maintained while the sharpness of the switching between the two forms varies with the l-type. A detailed description is given in ADAS107.

Program steps:

These are summarised in figure 4.1.

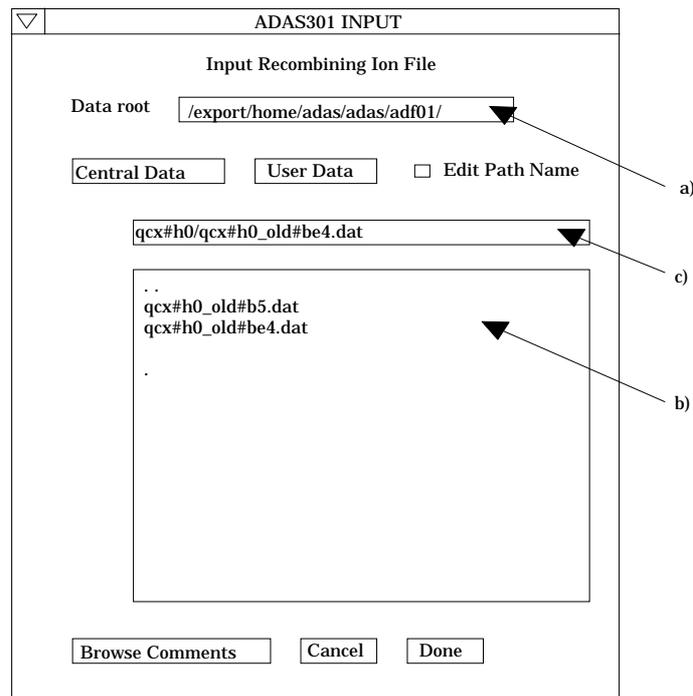
Figure 4.1



Interactive parameter comments:

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).

The **file selection window** appears first. Its appearance is as shown below.



1. Note that each type of data is stored according to its ADAS data format (*adf* number). *adf01* is the appropriate format for use by the program ADAS301. 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*.
2. 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. There are a large number of these. They are stored in sub-directories by donor which is usually neutral but not necessarily so (eg. *qcx#h0*). The individual members are identified by the subdirectory name, a code and then fully ionised receiver (eg. *qcx#h0_old#c6.dat*). The data sets generally contain *nl*-resolved cross-section data but *n*-resolved and *nlm*-resolved are handled. Resolution levels must not be mixed in datasets.

3. The codes distinguish different sources. The first letter *o* or the code *old* has been used to indicate that the data has been produced from JET compilations which originally had parametrised *l*-distribution of cross-sections. The nl-resolved data with such code has been reconstituted from them. Data of code *old* is the preferred JET data. Other sources codes include *ory* (old Ryufuku), *ool* (old Olson), *ofr* (old Fritsch) and *omo* (old molecular orbital). There are new data such as *kvi*.
4. Click on a file name in the file display window to select it. The selected name appears in the smaller selection window above the file display window. Then the individual datafiles are presented for selection. Datafiles, as distinct from directories, 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. It is important to use this facility to find out what has gone into the dataset and the attribution of the dataset. The possibility of browsing the comments appears in the subsequent main window also.
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 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.
9. The output data extracted from the datafile, a 'charge exchange cross-section', may be fitted with a polynomial. This is as a function of relative collision energy per atomic mass unit (eV/amu). Clicking the *Fit Polynomial* button 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. **Remember to press the return key on the keyboard to record the value.**
10. You may operate in velocity units or energy units as you find convenient. Your settings of collision velocity/energy (output) are shown in the display window. The velocity/energy values at which the charge exchange coefficients are stored in the datafile (input) are also shown for information.
11. The program recovers the output velocities/energies you used when last executing the program. Pressing the *Default Velocity/Energy values* button inserts a default set of velocities/energies equal to the input velocities/energies
12. The Velocity/Energy 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: It follows the same pattern of operation as described in the *18nov-94* bulletin.
13. The specific cross-section data to be extracted is specified by the window to the right at a). The level or resolution of the data source is shown at c). Activate the *Select quantun numbers for processing* button to allow new settings of these quantum numbers. The values in the three smaller windows b) become editable depending also on the resolution of the dataset. Note that the *Range* of the data in the dataset is displayed. There are special codes to be used to obtain summed cross-sections over sub-quantum numbers. These are indicated in brackets under the *Total* column and should be entered into the editable window if required.

ADAS301 PROCESSING OPTIONS

Title for Run

Data File Name : /export/home/adas/adas/adf01/qcx#h0/qcx#h0_c6.dat

Polynomial fitting

Fit Polynomial value % :

Select velocities/energies for Output File

Output Collision velocities/energies

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

Velocity/Energy units :

Select quantum numbers for processing

Range	Total
Principal quantum no. N (1-12) <input type="text" value="0"/>	[0]
Orbital quantum no. L (0-N-1) <input type="text" value="1"/>	[-1]
Azimuthal quantum no. M (0-L) <input type="text" value="1"/>	[-1]

Data is N and L resolved

Edit the processing options data and press Done to continue

14. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

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

15. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
16. 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 b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.
17. 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.
18. A choice of output graph plotting devices is given in the Device list window d). Clicking on the required device selects it. It appears in the selection window above the Device list window.
19. 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.

ADAS301 OUTPUT OPTIONS

Data file name : /export/home/adas/adas/adf01/qcx#h0/qcx#h0_old#be4.dat

Browse comments

Graphical Output Default Device

Graph Title :

Explicit Scaling

X-min : X-max :

Y-min : Y-max :

Enable Hard Copy Replace

File name :
HP-PCL
HP-GL

Text Output Replace

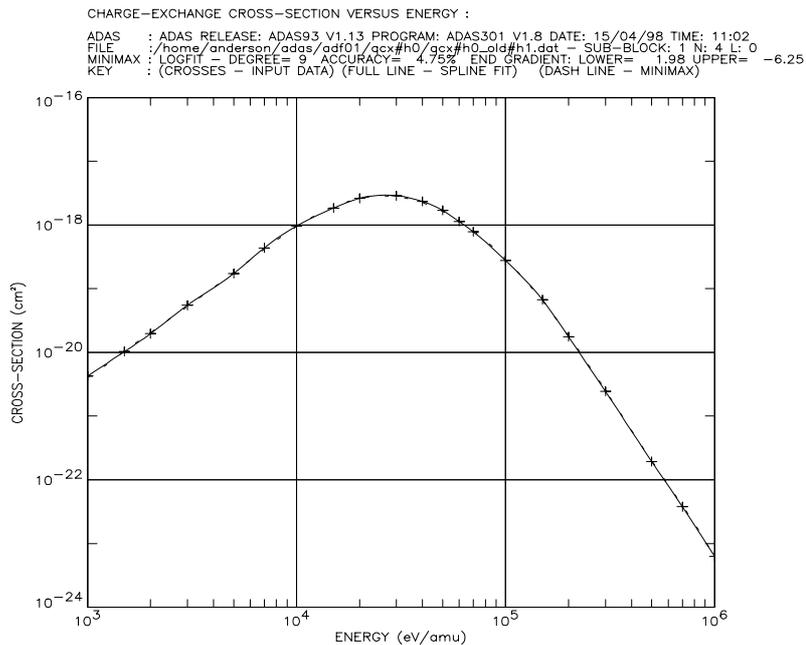
File name :

20. The graph itself is displayed in a following **Graphical Output** window.

Illustration:

The output from the programme is illustrated in figure 2.1a for capture by H^+ from a deuterium beam atom in its ground state $D^0(1s)$, into the $n=4$ shell. Input values in the source data set are shown as crosses. The spine curve is the continuous line and the minimax polynomial fit is the dashed curve.

Figure 2.1a



The tabular output is shown in table 2.1a. Output data which requires extrapolation beyond the range of the original data in the source QCX file are indicated by * when necessary. The rate coefficient is obtained from the cross-section by simply multiplying by the collision speed.

Table 4.1a

```

ADAS RELEASE: ADAS93 V1.13 PROGRAM: ADAS301 V1.8 DATE: 15/04/98 TIME: 11:02
**** TABULAR OUTPUT FROM CHARGE EXCHANGE CROSS-SECTION INTERROGATION PROGRAM: ADAS301
- DATE: 15/04/98 *****
-----
                CHARGE EXCHANGE CROSS-SECTIONS AS A FUNCTION OF ENERGY
-----
                DATA GENERATED USING PROGRAM: ADAS301
-----
/home/anderson/adas/adf01/qcx#h0/qcx#h0_old#h1.dat                - SUB-B
FILE IS L RESOLVED
PRINCIPAL QUANTUM N-SHELL = 4
ORBITAL QUANTUM L-SHELL = 0
-- ENERGY -- ----- VELOCITY ----- ----- CROSS-SECTION ----- RATE COEFFT
   eV/amu   at.units   cm/sec           cm**2      pi*(a0**2)   cm**3/sec
-----
 1.000D+03   2.008D-01   4.393D+07   4.240D-21   4.820D-05   1.863D-13
 1.500D+03   2.459D-01   5.380D+07   1.030D-20   1.171D-04   5.542D-13
 2.000D+03   2.840D-01   6.212D+07   1.960D-20   2.228D-04   1.218D-12
 3.000D+03   3.478D-01   7.609D+07   5.480D-20   6.229D-04   4.170D-12
 5.000D+03   4.490D-01   9.823D+07   1.720D-19   1.955D-03   1.690D-11
 7.000D+03   5.313D-01   1.162D+08   4.360D-19   4.956D-03   5.067D-11
 1.000D+04   6.350D-01   1.389D+08   9.640D-19   1.096D-02   1.339D-10
 1.500D+04   7.777D-01   1.701D+08   1.840D-18   2.092D-02   3.130D-10
 2.000D+04   8.980D-01   1.965D+08   2.610D-18   2.967D-02   5.127D-10
 3.000D+04   1.100D+00   2.406D+08   2.870D-18   3.262D-02   6.905D-10
 4.000D+04   1.270D+00   2.778D+08   2.340D-18   2.660D-02   6.501D-10
 5.000D+04   1.420D+00   3.106D+08   1.690D-18   1.921D-02   5.250D-10
 6.000D+04   1.555D+00   3.403D+08   1.130D-18   1.284D-02   3.845D-10
 7.000D+04   1.680D+00   3.675D+08   7.790D-19   8.855D-03   2.863D-10
 1.000D+05   2.008D+00   4.393D+08   2.760D-19   3.137D-03   1.212D-10
 1.500D+05   2.459D+00   5.380D+08   6.700D-20   7.616D-04   3.605D-11
 2.000D+05   2.840D+00   6.212D+08   1.750D-20   1.989D-04   1.087D-11
 3.000D+05   3.478D+00   7.609D+08   2.450D-21   2.785D-05   1.864D-12
 5.000D+05   4.490D+00   9.823D+08   1.930D-22   2.194D-06   1.896D-13
-----
KEY: a0 => Bohr radius = 5.29177D-11 m
-----
MINIMAX POLYNOMIAL - TAYLOR COEFTS: LOG10(X-SEC<cm**2>) vs. LOG10(ENGY<eV/amu>)
-----
      A( 1) =  5.568210682D+04          A( 2) = -1.194505768D+05
      A( 3) =  1.128699357D+05          A( 4) = -6.168654737D+04
      A( 5) =  2.149226561D+04          A( 6) = -4.951451870D+03
      A( 7) =  7.544920835D+02          A( 8) = -7.334742753D+01
      A( 9) =  4.129134057D+00          A(10) = -1.025897794D-01
LOGFIT - DEGREE= 9 ACCURACY= 4.75% END GRADIENT: LOWER= 1.98 UPPER= -6.25
-----

```

Notes