Charge exchange spectroscopy

Preliminaries

Charge exchange spectroscopy is driven by reactions of the form

$$X^{+z_0} + D^0_{beam}(1) \rightarrow X^{+z_0}(nl) + D^+_{beam}$$
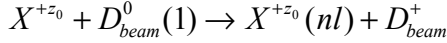
in which an electron is captured from a donor atom in its ground (or an excited) state. The principal application is usually to capture by the bare nuclei of impurity atoms in the plasma from the ground state of deuterium, helium or lithium atoms in fast neutral beams. Subsequently the hydrogen-like impurity ion radiates as

$$X^{+z_0-1}(n'l') \rightarrow X^{+z_0-1}(n''l'') + h\nu$$
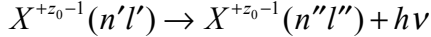
Composite spectral line features of the form $n' \rightarrow n''$ are observed made up from unresolved $n'l' \rightarrow n''l''$ multiplet components. Charge exchange line features often involve high principal quantum shells and occur over wide spectral ranges including the visible range. In general the populations of receiver levels are modified by redistributive collisions with plasma ions and electrons and by fields before radiation emission occurs

The programs of series ADAS3 are associated with neutral beams of hydrogen or helium isotopes and there are two streams of modelling. The first stream is concerned with modelling and detailed spectral line emission from hydrogen-like impurity ions in a plasma following charge transfer from fast neutral beams. It commences with a collection of state selective charge transfer cross-section data at n, nl or nlm resolution (type ADF01) spanning an extended region of collision energies and n-shells and in some cases different sources. For interpretation of charge exchange emission lines, effective emission coefficients for relevant spectral lines emitted by the receiver are required. These are archived in ADAS data format ADF12. They require special collisional-radiative population calculations for their evaluation. There are two collisional-radiative processing options, namely for calculations in the *bundle-nl* (ADAS308) or *bundle-nlj* (ADAS306) approximations. The programs ADAS308 and ADAS306 predict data for arbitrary lines at a fixed set of conditions and show extensive detail of the line emission. It is convenient to have available more automatic codes which generate ony tables of ADF12 coefficients over ranges of plasma parameters without the intervening displays. This capability is provided by ADAS309 and ADAS307 for the bundle-nlj and bundle-nl pictures respectively. The latter are termed scanning versions of the codes. The associated codes for interrogation of the fundamental state selective cross-section database and the effective charge exchange emission coefficient database are ADAS301 and ADAS303 respectively.

The ADAS data formats format

The various relevant classes of data are

adf01	bundle-n and bundle-nl charge exchange cross-sections
adf02	ion impact cross-sections with named participant
adf12	charge exchange effective emission coefficients
adf21	effective beam stopping coefficients
adf26	bundle-n populations of excited states in beams

ADF01

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}. For $n \geq n_{max}$ extrapolation is assumed of the form

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

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

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

Explicit l-subshell cross-sections $\sigma_{nl}(E_i)$ are tabulated for $n_{min} \le n \le n_{max}$ and $0 \le l \le n-1$. 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

$$\sigma_{nl}(E_i) = \begin{cases} \sigma_{n_{max}l}(E_i)(\sigma_n(E_i)/\sigma_{n_{max}}(E_i)) & for\ l \le n_{max}-1 \\ 0 & for\ l \ge n_{max} \end{cases}$$

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

$$\sigma_{nl}(E_i) \sim \begin{cases} (2l+1)^{pl2} & for\ l < xlcr \\ \exp(-(l-xlcr)^{pl3}) & for\ l < xlcr \end{cases}$$

The normalisation

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

is maintained while the sharpness of the switching between the two forms varies with the *l*-type. A detailed description is given in ADAS107.
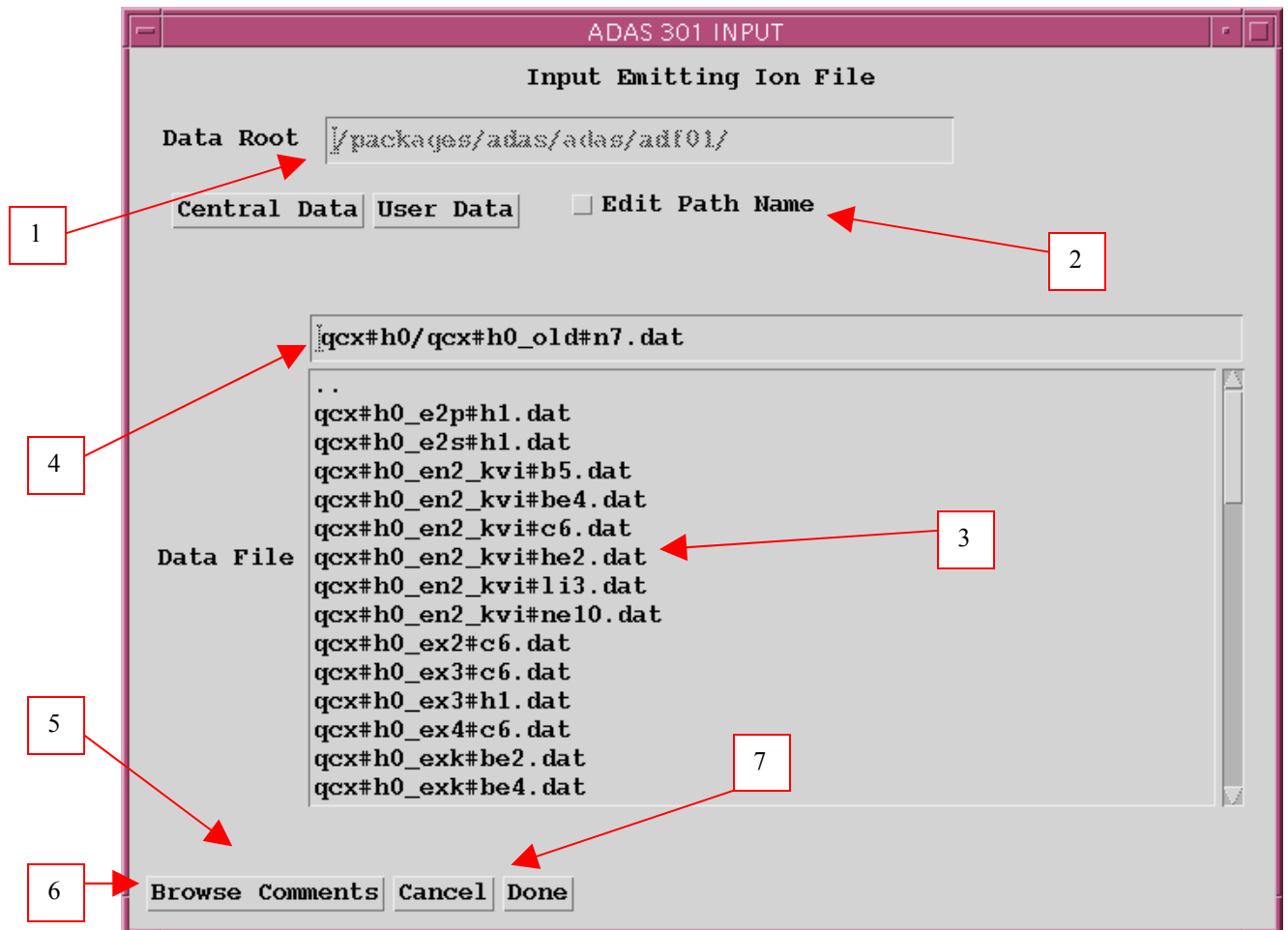
A typical ADF01 organisation is shown for H^0 donor to He^2 receiver

ADAS301

The code interrogates state selective charge exchange cross-section files of type ADF01. Data may be extracted for capture to a selected n-, nl-or nlm-shell of a hydrogen-like or lithium-like receiving ion depending on the ADF01 file. The data may be interpolated using cubic splines to provide cross-sections at arbitrarily chosen impact energies. A minimax polynomial approximation is also made to the source data. The source and interpolated cross-section data are displayed and a tabulation prepared. The tabular and graphical output may be printed and include the minimax polynomial approximation.

The **file selection window** is shown below.

ADAS 301 INPUT

Input Emitting Ion File

Data Root `/packages/adas/adas/adf01/`

Central Data   User Data   ☐ Edit Path Name

`qcx#h0/qcx#h0_old#n7.dat`

```
..
qcx#h0_e2p#h1.dat
qcx#h0_e2s#h1.dat
qcx#h0_en2_kvi#b5.dat
qcx#h0_en2_kvi#be4.dat
qcx#h0_en2_kvi#c6.dat
qcx#h0_en2_kvi#he2.dat
qcx#h0_en2_kvi#li3.dat
qcx#h0_en2_kvi#ne10.dat
qcx#h0_ex2#c6.dat
qcx#h0_ex3#c6.dat
qcx#h0_ex3#h1.dat
qcx#h0_ex4#c6.dat
qcx#h0_exk#be2.dat
qcx#h0_exk#be4.dat
```

Data File

Browse Comments   Cancel   Done

1. Data root 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 – ADF01 in this case. 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.

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. There are a large number of these, stored 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. 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 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. 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. 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.

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

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* again allows display of the information field section at the foot of the selected dataset, if it exists.

2.   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

3.   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. The program recovers the output velocities/energies you used when last executing the program.
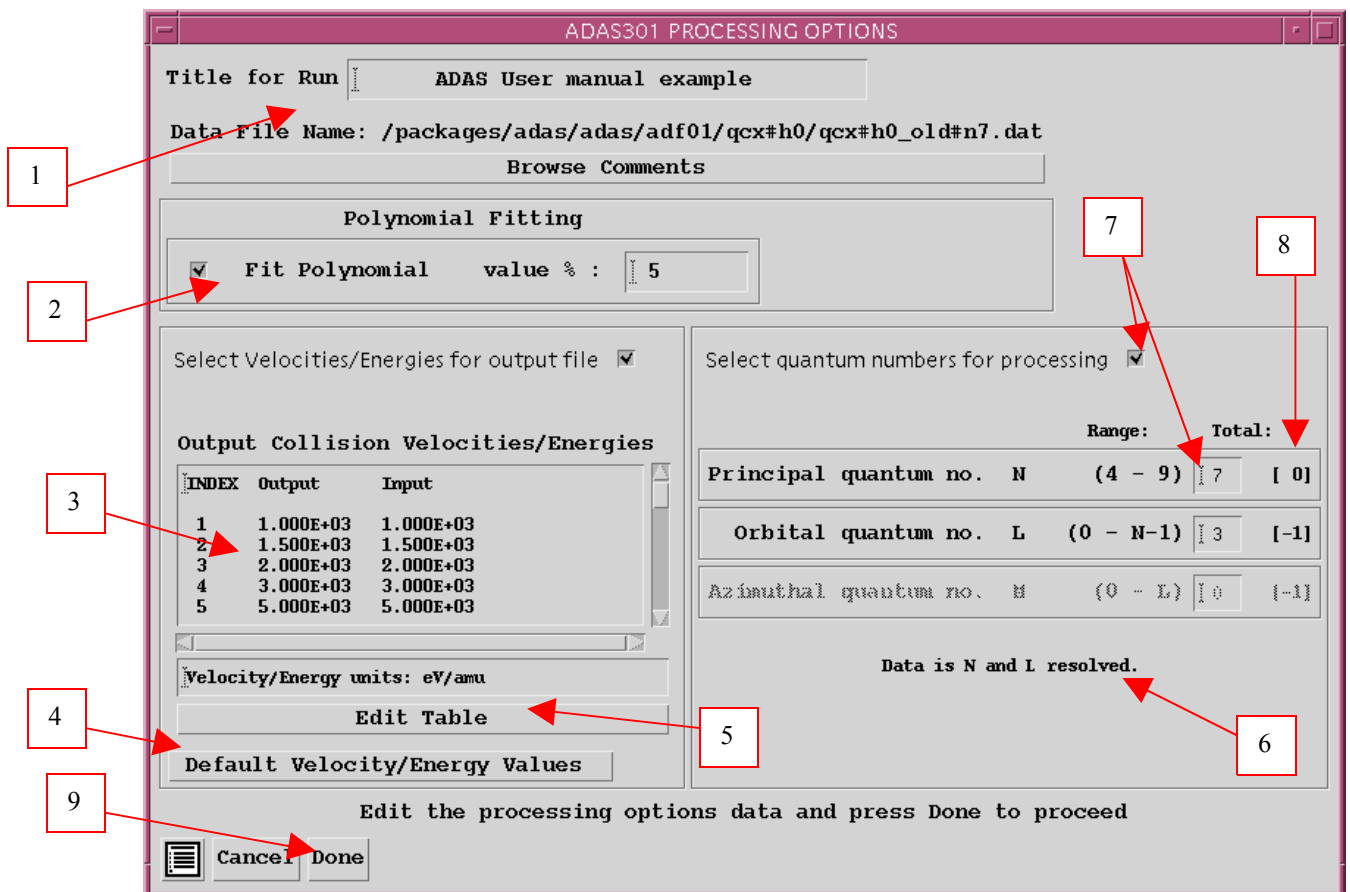
4.   Pressing the *Default Velocity/Energy values* button inserts a default set of velocities/energies equal to the input velocities/energies

5.   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.

6.   The specific cross-section data to be extracted is specified by the window to the right. The level or resolution of the data source is shown.

7.   Activate the *Select quantun numbers for processing* button to allow new settings of these quantum numbers. The values in the three smaller windowsbecome editable depending also on the resolution of the dataset. Note that the *Range* of the data in the dataset is displayed.

8.   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 │ ADAS User manual example

Data File Name: /packages/adas/adas/adf01/qcx#h0/qcx#h0_old#n7.dat

Browse Comments

Polynomial Fitting

☑ Fit Polynomial   value % : │ 5

Select Velocities/Energies for output file ☑

Output Collision Velocities/Energies

INDEX	Output	Input
1	1.000E+03	1.000E+03
2	1.500E+03	1.500E+03
3	2.000E+03	2.000E+03
4	3.000E+03	3.000E+03
5	5.000E+03	5.000E+03

Velocity/Energy units: eV/amu

Edit Table

Default Velocity/Energy Values

Select quantum numbers for processing ☑

	Range:	Total:
Principal quantum no. N	(4 − 9) │7	[0]
Orbital quantum no. L	(0 − N−1) │3	[−1]
Azimuthal quantum no. M	(0 − L) │0	[−1]

Data is N and L resolved.

Edit the processing options data and press Done to proceed

Cancel Done

1. 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** is shown below

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.

2. Graphical display is activated by the *Graphical Output* button. 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.

3. 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. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a 'pop-up' window issues a warning.

5. 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.

6. 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.
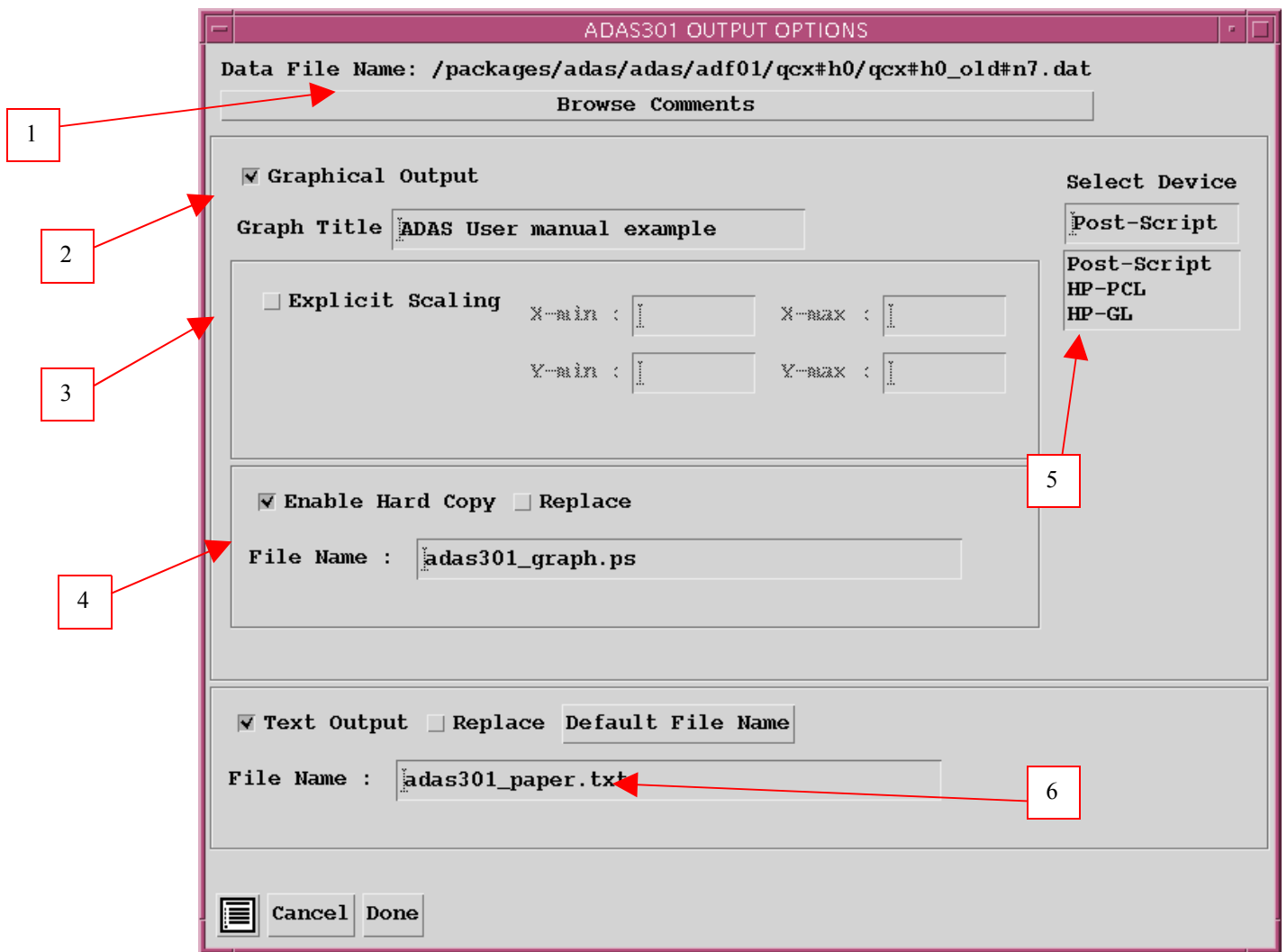
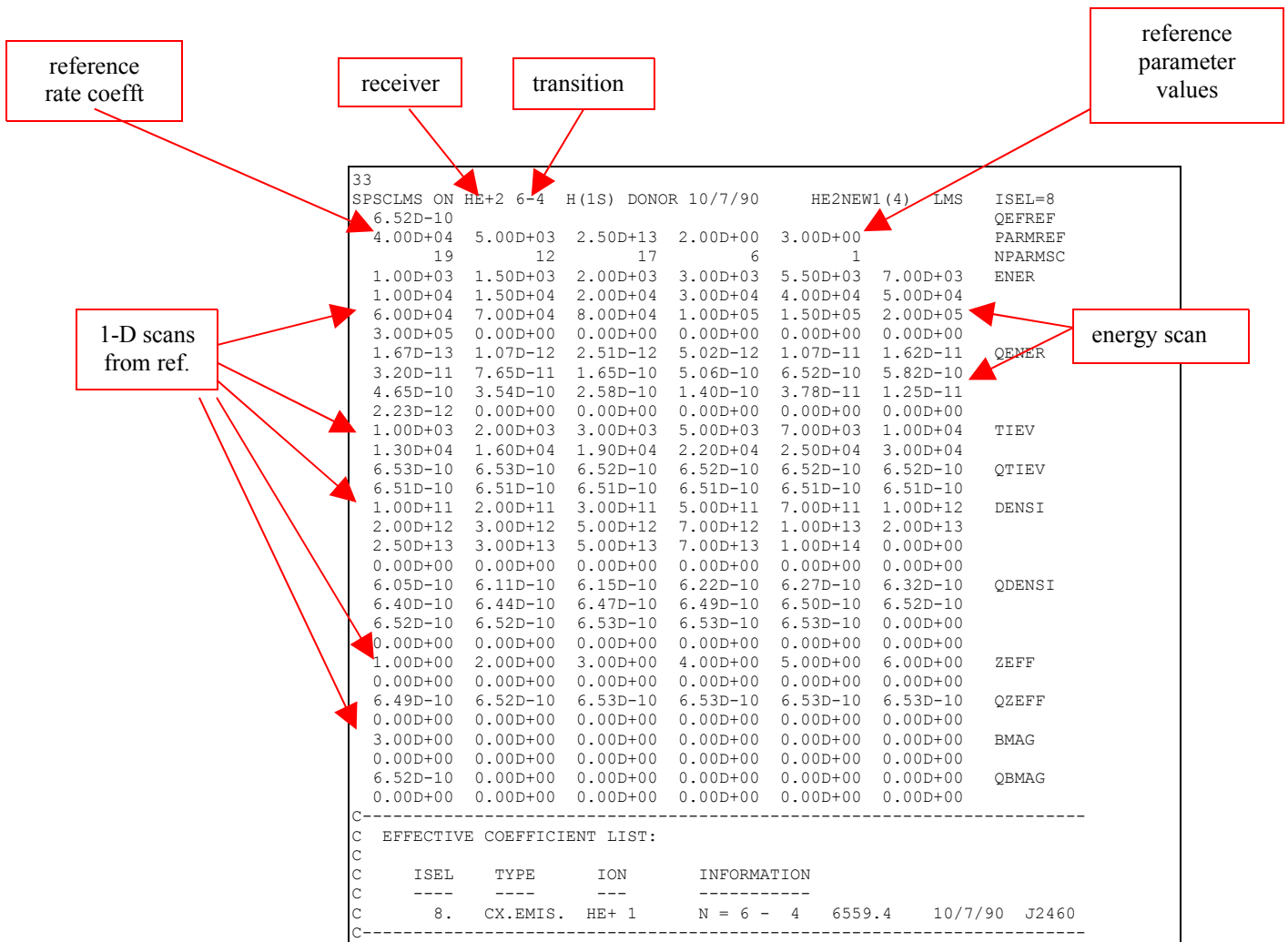The **Graphical output window** is shown below

1. Printing of the currently displayed graph is activated by the *Print* button.
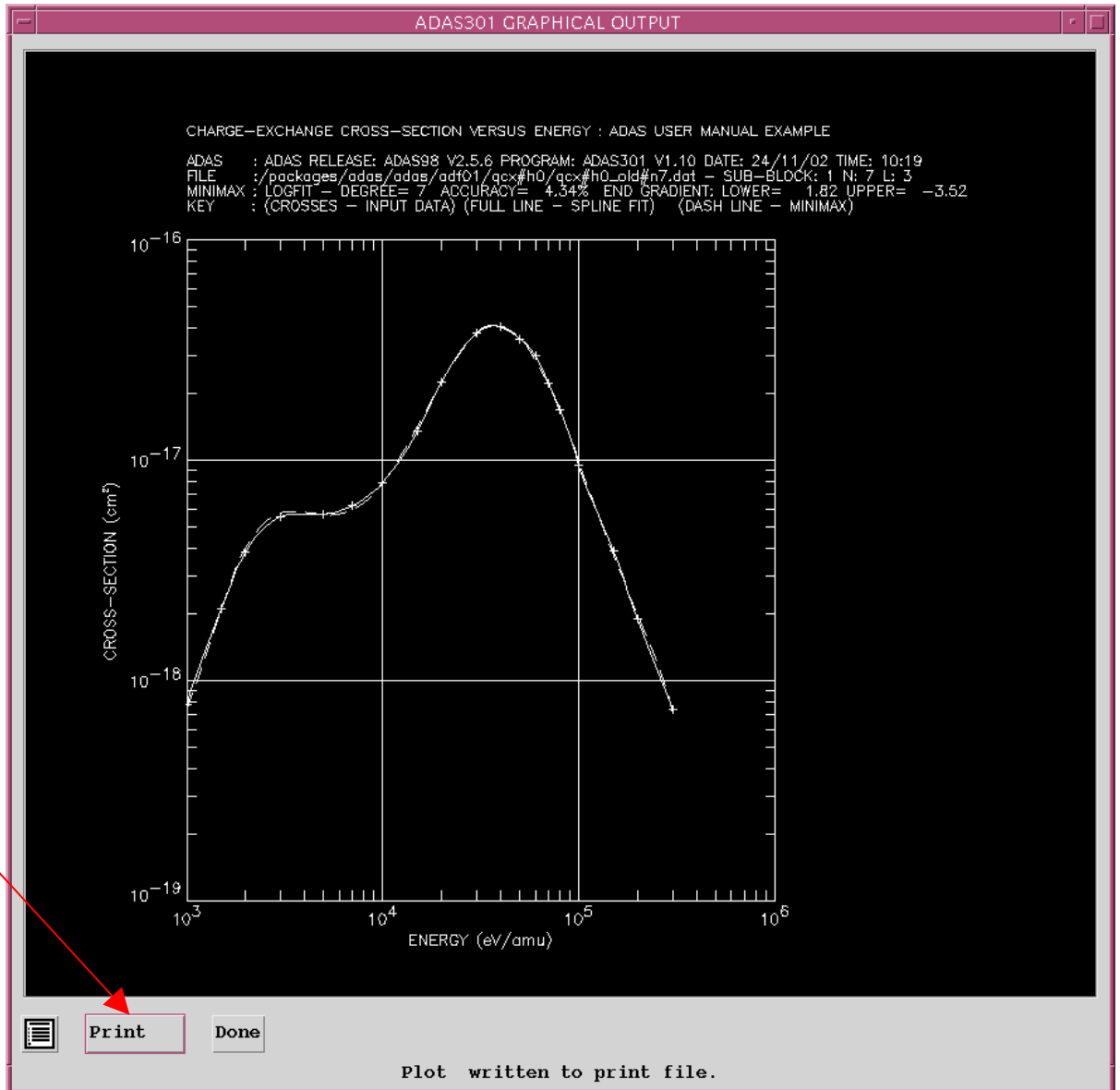
ADF12

Data from files of type ADF12 contain charge exchange effective emission coefficients for principal quantum shell transitions of hydrogen-like impurity ions, $q_{n \to n'}^{(eff)}$, at a reference beam/plasma condition of beam energy $E_u^{(ref)}$, plasma ion density $N_{zeff}^{(ref)}$, plasma ion temperature $T_{zeff}^{(ref)}$, plasma z effective $zeff^{(ref)}$ and magnetic field strength $B_{mag}^{(ref)}$. Also they contain the $q_{n \to n'}^{(eff)}$ at varying plasma conditions obtained by keeping all the parameters except one at the reference conditions. These are called one-dimensional scans and there are $q_{n \to n'}^{(eff)}$ sets at the following parameter sets:

$$\{E_{u,i}:i=1,I_E\}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, zeff^{(ref)}, B^{(ref)} \quad \text{with } E_u^{(ref)} \in \{E_{u,i}:i=1,I_E\},$$
$$E_u^{(zeff)}, \{N_{zeff}:i=1,I_N\}, T_{zeff}^{(ref)}, zeff^{(ref)}, B^{(ref)} \quad \text{with } N_{zeff}^{(ref)} \in \{N_{zeff}:i=1,I_N\},$$
$$E_u^{(ref)}, N_{zeff}^{(ref)}, \{T_{zeff,i}:i=1,I_T\}, zeff^{(ref)}, B^{(ref)} \quad \text{with } T_{zeff}^{(ref)} \in \{T_{zeff,i}:i=1,I_T\},$$
$$E_u^{(ref)}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, \{zeff_i:i=1,I_{zeff}\}, B^{(ref)} \quad \text{with } zeff^{(ref)} \in \{zeff_i:i=1,I_{zeff}\},$$
$$E_u^{(ref)}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, zeff^{(ref)}, \{B_i:i=1,I_B\} \quad \text{with } B^{(ref)} \in \{B_i:i=1,I_B\}.$$

reference rate coefft

receiver

transition

reference parameter values

1-D scans from ref.

energy scan

```
33
SPSCLMS ON HE+2 6-4  H(1S) DONOR 10/7/90     HE2NEW1(4)  LMS    ISEL=8
 6.52D-10                                                      QEFREF
 4.00D+04  5.00D+03  2.50D+13  2.00D+00  3.00D+00             PARMREF
      19        12        17         6         1              NPARMSC
 1.00D+03  1.50D+03  2.00D+03  3.00D+03  5.50D+03  7.00D+03   ENER
 1.00D+04  1.50D+04  2.00D+04  3.00D+04  4.00D+04  5.00D+04
 6.00D+04  7.00D+04  8.00D+04  1.00D+05  1.50D+05  2.00D+05
 3.00D+05  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
 1.67D-13  1.07D-12  2.51D-12  5.02D-12  1.07D-11  1.62D-11   QENER
 3.20D-11  7.65D-11  1.65D-10  5.06D-10  6.52D-10  5.82D-10
 4.65D-10  3.54D-10  2.58D-10  1.40D-10  3.78D-11  1.25D-11
 2.23D-12  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
 1.00D+03  2.00D+03  3.00D+03  5.00D+03  7.00D+03  1.00D+04   TIEV
 1.30D+04  1.60D+04  1.90D+04  2.20D+04  2.50D+04  3.00D+04
 6.53D-10  6.53D-10  6.52D-10  6.52D-10  6.52D-10  6.52D-10   QTIEV
 6.51D-10  6.51D-10  6.51D-10  6.51D-10  6.51D-10  6.51D-10
 1.00D+11  2.00D+11  3.00D+11  5.00D+11  7.00D+11  1.00D+12   DENSI
 2.00D+12  3.00D+12  5.00D+12  7.00D+12  1.00D+13  2.00D+13
 2.50D+13  3.00D+13  5.00D+13  7.00D+13  1.00D+14  0.00D+00
 0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
 6.05D-10  6.11D-10  6.15D-10  6.22D-10  6.27D-10  6.32D-10   QDENSI
 6.40D-10  6.44D-10  6.47D-10  6.49D-10  6.50D-10  6.52D-10
 6.52D-10  6.52D-10  6.53D-10  6.53D-10  6.53D-10  0.00D+00
 0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
 1.00D+00  2.00D+00  3.00D+00  4.00D+00  5.00D+00  6.00D+00   ZEFF
 0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
 6.49D-10  6.52D-10  6.53D-10  6.53D-10  6.53D-10  6.53D-10   QZEFF
 0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
 3.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00   BMAG
 0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
 6.52D-10  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00   QBMAG
 0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
C----------------------------------------------------------------------
C   EFFECTIVE COEFFICIENT LIST:
C
C    ISEL     TYPE      ION       INFORMATION
C    ----     ----      ---       -----------
C     8.    CX.EMIS.   HE+ 1     N = 6 -  4   6559.4    10/7/90  J2460
C----------------------------------------------------------------------
```

ADAS303

The program interrogates charge exchange spectroscopy effective emission coefficient data sets of type ADF12 associated with a particular neutral donor. The ADF12 data set collections are for the relevant hydrogen-like n-n' spectrum lines grouped according to the recombining ion. The code and data organisation allows the emission coefficient to be obtained (by interpolation using cubic splines) at plasma conditions and at relative collision energies of choice. A minimax polynomial approximation can also be made to the interpolated data. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and include the polynomial approximation.

The **file selection window** appears first and has the appearance shown below.

1. Data root 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. Note that each type of data is stored according to its ADAS data format (*adf* number). *adf12* is the appropriate format for use by the program ADAS303. Details of the organisation of such data is given in the *appxa-12*. 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. There are a large number of these. They are stored in sub-directories by donor which is usually neutral but not necessarily so (eg. *qef93#h*). The individual members are identified by the subdirectory name, a code and then fully ionised receiver (eg. *qef93#h_be4.dat*). The data sets generally contain many individual spectrum lines. Scroll bars appear if the number of entries exceed the file display window size. Such data is generally stored by year number (eg. *93*) with the most recent data to be preferred. 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. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.

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

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.

6. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window
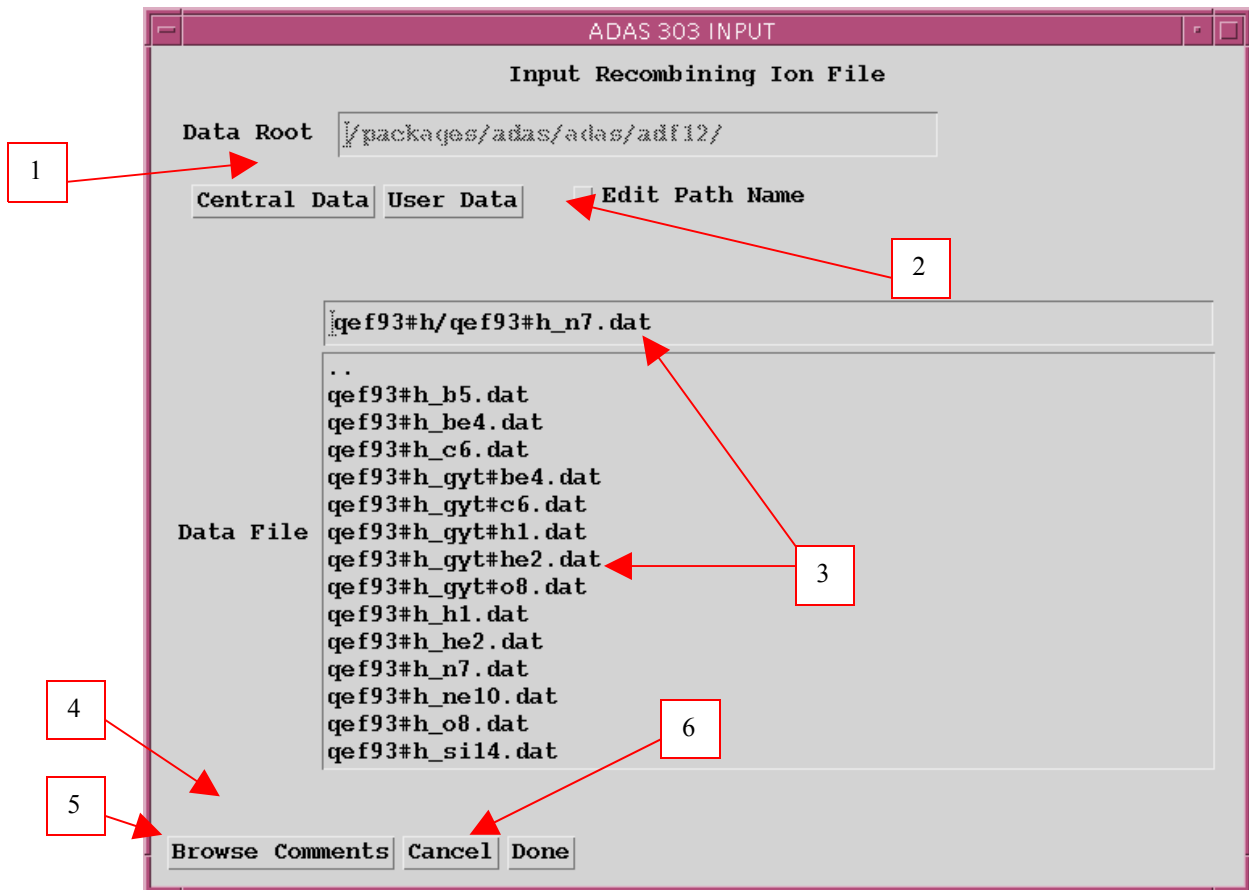
The **processing options window** is shown below:

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* again allows display of the information field section at the foot of the selected dataset, if it exists.

2. The output data extracted from the datafile may be fitted with a polynomial. 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.

3. Transitions available in the data set are displayed in the transition list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a transition to select it. The selected transition appears in the selection window just above the transition list display window.
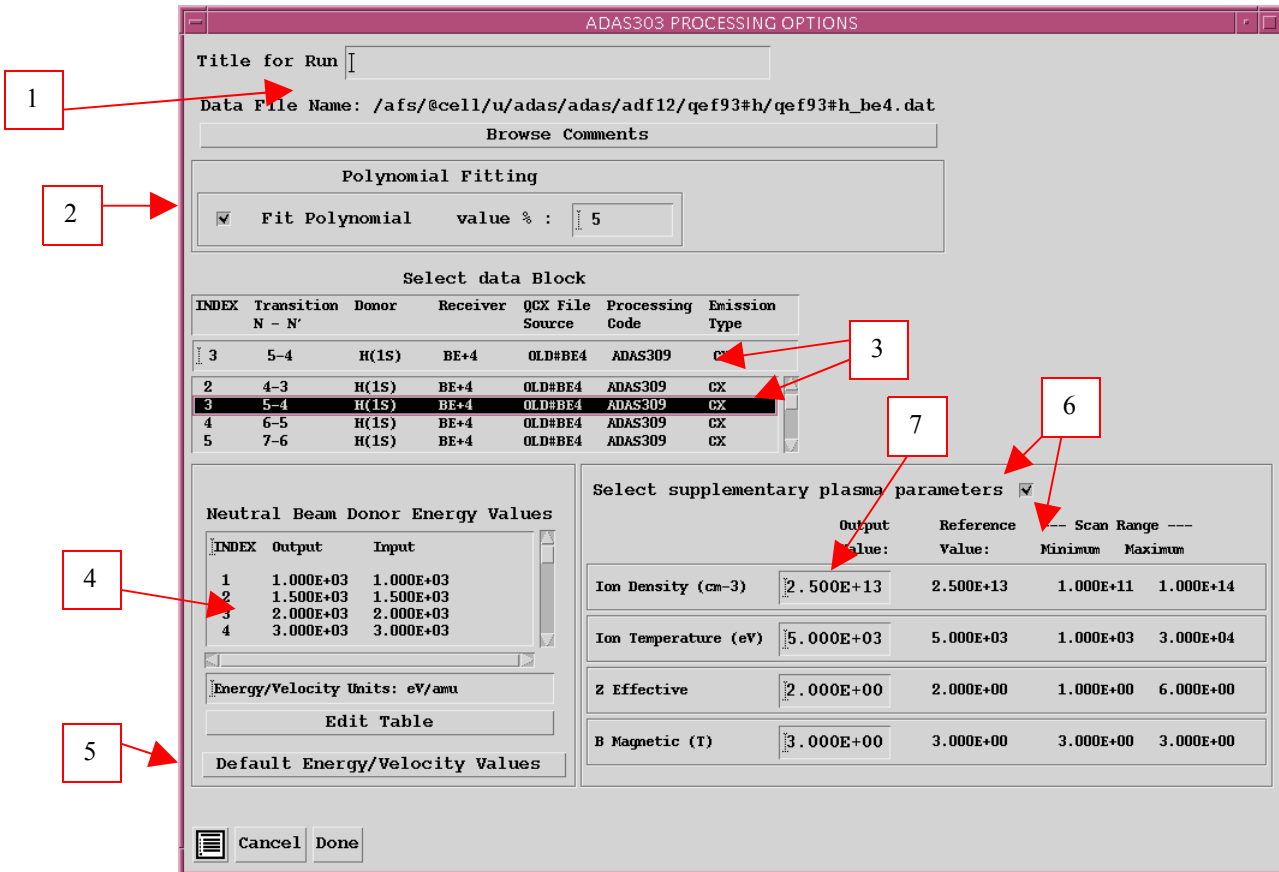
4. Energies/velocities for the neutral donor are displayed. The particular choice of units in use is shown below the table. Your settings of beam energy/velocity (output) are shown in the display window. The beam energy/velocity values at which the effective emission coefficients are stored in the datafile (input) are also shown for information. Click the *Edit Table* button to drop-down the ADAS Table Editor. Within Table Editor you can select which units to use as well as entering you energy/velocity values for output. Note that final graphed results are of effective emission coefficient versus beam energy (eV/amu).

5. The program recovers the output energies/velocities you used when last executing the program. Pressing the *Default Energy/Velocity values* button inserts a default set of energies/velocities equal to the input values

6. Effective emission coefficients for the ADF12 database are calculated at one-dimensional scans in various plasma parameters relative to a reference set of plasma conditions. Details are given in *appxa-12*. To alter the settings, activate the *Select supplementary plasma parameters* button.

7. The sub-windows become active with the output data entry box in each editable. For information, the reference value of each plasma parameter is given together with the range of the parameter in its one-dimensional scan. Values outside the range should not be entered. For

data prepared using processing code ADAS309, the B magnetic field parameter has no effect, but is simply used for place holding. The scan in *B Magnetic* is of zero length.

The **output options window** is shown below
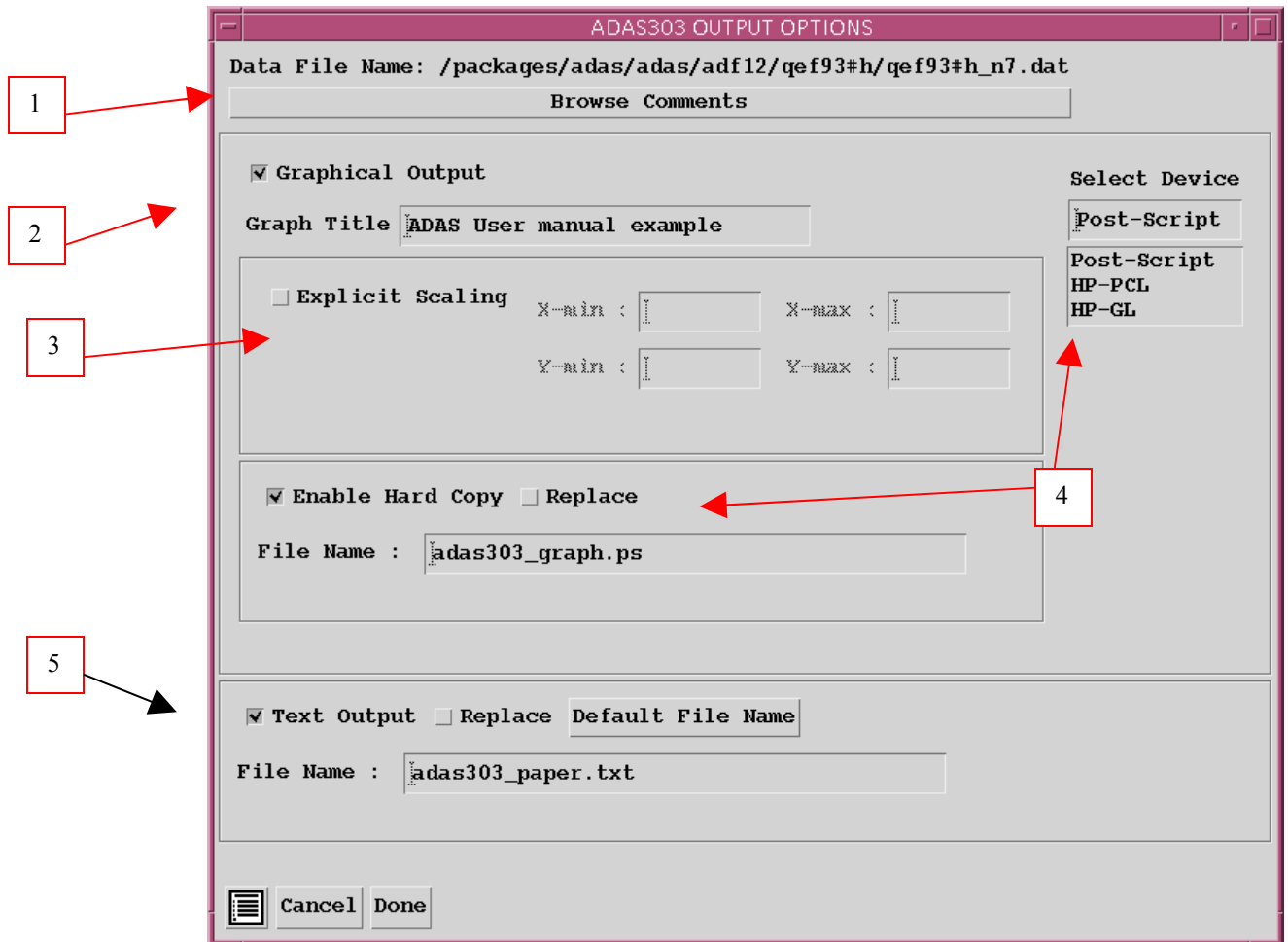
7. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.

8. Graphical display is activated by the *Graphical Output* button. 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.

9. 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.

10. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a 'pop-up' window issues a warning. 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.

11. 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.

The **Graphical output window** is shown below

2. Printing of the currently displayed graph is activated by the *Print* button.
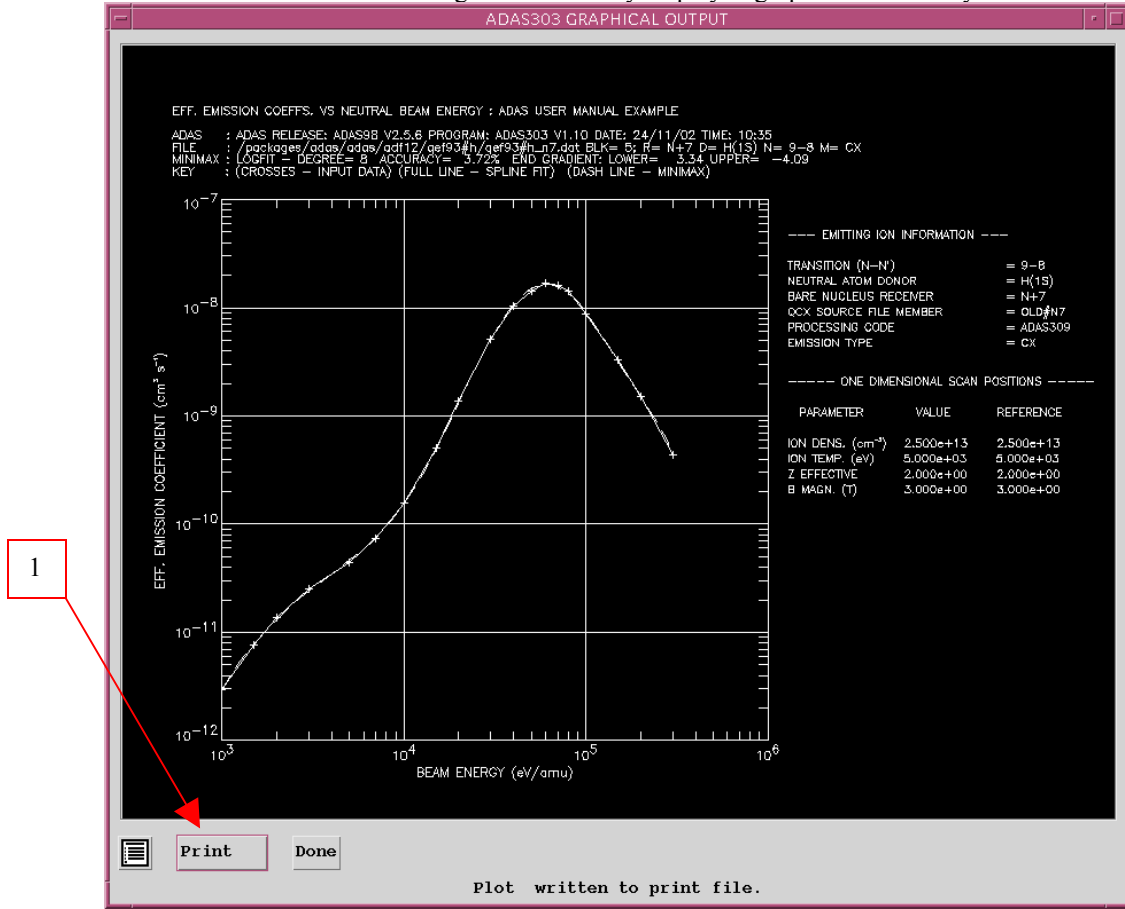
Calculating CXS effective emission coefficients

The line-of-sight integrated photon emissivity of a charge exchange driven line may be written as

$$I_{n \to n'}^{(z_0-1)} = \sum_{l,l'} I_{nl \to n'l'}^{(z_0-1)}$$

$$= \int_S \sum_{l,l'} A_{nl \to n'l'} N_{nl}^{(z_0-1)} ds$$

$$= \int_S [\sum_{l,l'} A_{nl \to n'l'} (N_{nl}^{(z_0-1)} / N_D N^{(z_0)})] N_D N^{(z_0)} ds$$

$$= \int_S [\sum_{l,l'} q_{nl \to n'l'}^{(eff)}] N_D N^{(z_0)} ds$$

$$= \int_S q_{n \to n'}^{(eff)} N_D N^{(z_0)} ds$$

$$\approx q_{n \to n'}^{(eff)} \int_S N_D N^{(z_0)} ds$$

where S is the path length through the neutral beam / plasma intersection along a spectrometer line-of-sight. N_D is the neutral donor number density and $N^{(z_0)}$ is the number density of fully ionised impurity atoms. $q_{n \to n'}^{(eff)}$ is the *effective emission coefficient* for the whole $n \to n'$ principal quantum shell transition and $\int_S N_D N^{(z_0)} ds$ is the *emission measure*. The mean transition energy is

ADAS Course at ITER   1-3 December 2010

$$\Delta E_{n,n'} = (\sum_{l,l'} \Delta E_{nl,n'l'} q_{nl \to n'l'}^{(eff)}) / q_{n \to n'}^{(eff)}$$

where $\Delta E_{nl,n'l'}$ is the line component transition energy and $q_{nl \to n'l'}^{(eff)}$ is the component effective emission coefficient. The effective emission coefficient $q_{n \to n'}^{(eff)}$ may be calculated theoretically. If it is approximately constant over the emitting volume, then measurement of a charge exchange line intensity $I_{n \to n'}^{(z_0-1)}$ allows deduction of the emission measure $\int_S N_D N^{(z_0)} ds$. If neutral beam attenuation to the observed volume is known or calculable then local impurity density may be inferred.

With the effective emission coefficients calculated theoretically, comparison with one observed charge exchange line intensity allows deduction of the emission measure. Then all other line intensities are predictable. If more than one line intensity is observed, then a mean emission measure may be deduced and some comment may be made on the ratios of experimental to theoretical effective emission coefficients. The organisation of the collisional-radiative modelling in ADAS308 is specifically designed to allow such comparison. The following points and assumptions are made:
(i) From the theoretical point-of-view the direct capture cross-sections to levels are more fundamental quantities for comparison with experiment that the effective emission coefficients.
(ii) The dominant fundamental processes modifying the initial distribution of capture are redistribution within an n-shell and radiative cascade in low and moderate density plasmas. Limiting the collisional-radiative theory to these dominant processes allows a compact invertable relationship to be established between column emissivities of charge exchange spectrum lines and direct capture cross-sections.
(ii) It is of most practical value to target experiment / theory comparisons on the n-shell distribution of capture (including the n-shell decrement) in fusion studies. This may be achieved by imposing theoretical information on the l sub-shell distribution of capture.

Consider the monoenergetic direct capture rate coefficients to nl sub-levels $q_{nl}^{(CX)}$ from the initial neutral donor state $D^0(1)$ by the fully stripped impurity ion with number density $N^{(z_0)}$, denoted more compactly by N^+.

$$q_{nl}^{(CX)}(E_u) = v\, \sigma_{nl}^{(CX)}(v)$$

where E_u is the relative collision energy per atomic mass unit so that $v = \sqrt{2 E_u / m_p}$ is the relative collision speed, with m_p the proton mass and σ the capture cross-section.

It is supposed that

$$q_{nl}^{(CX)}(E_u) = f_{(n)l}^{(theor)} q_n^{(CX)}(E_u)$$

Since no collisional excitation from lower to higher n-shells is allowed, the populations of the lj sublevels of the principal quantum shell $n' \geq n + 1$ may be written as

$$N_{n'l'} = N_D N^+ \sum_{n^{iv} \geq n+1} W_{n'l',n^{iv}} q_{n^{iv}}^{(CX)}$$

Then the equations determining the populations of the sub-shells of the principal quantum shell n are

$$\sum_{l''} M_{(n)l,l''} N_{nl''} = N_D N^+ f_{(n)l}^{(theor)} q_n^{(CX)} + \sum_{n' \geq n+1} A_{nl,n'l'} N_{n'l'}$$

so that

$$N_{nlj} = N_D N^+ W_{nlj,n} q_n^{(CX)} + N_D N^+ \sum_{n^{iv} \geq n+1} W_{nlj,n^{iv}} q_{n^{iv}}^{(CX)}$$

with

$$W_{nlj,n} = [\sum_{l''j''} M_{(n)lj,l''j''}^{-1} f_{(n)l''j''}^{(theor)}] q_n^{(CX)}$$

and

$$W_{nlj,n^{iv}} = \sum_{l'',j'',l',j'} M_{(n)lj,l''j''}^{-1} A_{nl''j'',n'l'j'} W_{n'l'j',n^{iv}}$$

The solution can proceed recursively downwards in n with compact vector and array storage.

Tabulations of experimental or theoretical state selective charge exchange cross-section data span a range of principal quantum shells $\sigma_{nlj}^{(CX)}(v) : n_0 \leq n \leq n_1$. Cascade from levels $n > n_1$ may contribute significantly to the populations of lower levels especially at high collision energies when the decrease of the direct charge exchange cross-sections with n is slow ($\sigma_n \sim n^{-\alpha}$ and $\alpha \sim 3$). However,

redistribution amongst lj sub-levels of the higher n-shells is high, approaching statistical in most circumstances. Therefore the cascade solution is initiated at some n_{max} (~20 typically) for complete n-shell populations only (matrices $W^{(high)}$), with subshells implicitly statistically populated, down to n_1 whereupon the lj resolved solution (matrices $W^{(low)}$) is commenced.

In general observable spectrum lines are associated with upper principal quantum shells $n \leq n_1$. If M_{rep}, lines are identified each with a distinct upper n-shells $\bar{n}_{irep} : irep = 1,..., M_{rep}$, then a 'condensation' may be imposed such that

$$q_n^{(CX)} = \sum_{irep=1}^{M_{rep}} L_{n,irep} q_{\bar{n}_{irep}}^{(CX)} \qquad \text{for } n_0 \leq n \leq n_1$$

and

$$q_n^{(CX)} = (n/n_1)^\alpha q_{n_1}^{(CX)} \qquad \text{for } n > n_1$$

giving, after integration along the line-of-sight, a matrix relation

$$\begin{bmatrix} I_{\bar{n}_1 \to \bar{n}_1'} \\ . \\ I_{\bar{n}_{M_{rep}} \to \bar{n}_{M_{rep}}'} \end{bmatrix} = (\int_S N_D N^+ ds) \begin{bmatrix} a_{11} \cdot & . & a_{1M_{rep}} \\ . & . & . \\ a_{M_{rep}1} & . & a_{M_{rep}M_{rep}} \end{bmatrix} \begin{bmatrix} q_{\bar{n}_1}^{(CX)} \\ . \\ q_{\bar{n}_{M_{rep}}}^{(CX)} \end{bmatrix}$$

The coefficients of the matrix are theoretically calculated quantities. The equations may be solved for the the $q_{\bar{n}_i}^{(CX)}$ and the emission measure $\int_S N_D N^+ ds$ subject to the constraint

$$\sum_{irep=1}^{M_{rep}} q_{\bar{n}_{irep}}^{(CX)} = \sum_{irep=1}^{M_{rep}} q_{\bar{n}_{irep}}^{(CX)(theor)}$$

ADAS308

The code analyses *column* (line-of-sight integrated) emissivity observations of charge exchange spectroscopy lines from hydrogenic impurities, occuring through neutral beam / plasma interaction, in terms of emission measure. It predicts the column intensities of spectral components of the charge exchange lines, the Doppler broadened line shapes and effective emission coefficients for arbitrary lines in an l-resolved picture.

The **file selection window** is shown below.

1. Data root 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 – ADF01 in this case. 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.

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. 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. The ADF01 file nmaes 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 newer data such as *kvi*. Additional codes are used for excited donors such as *ex2* for hydrogen n=2. Click on a name 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 all have the termination *.dat*.

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

1.
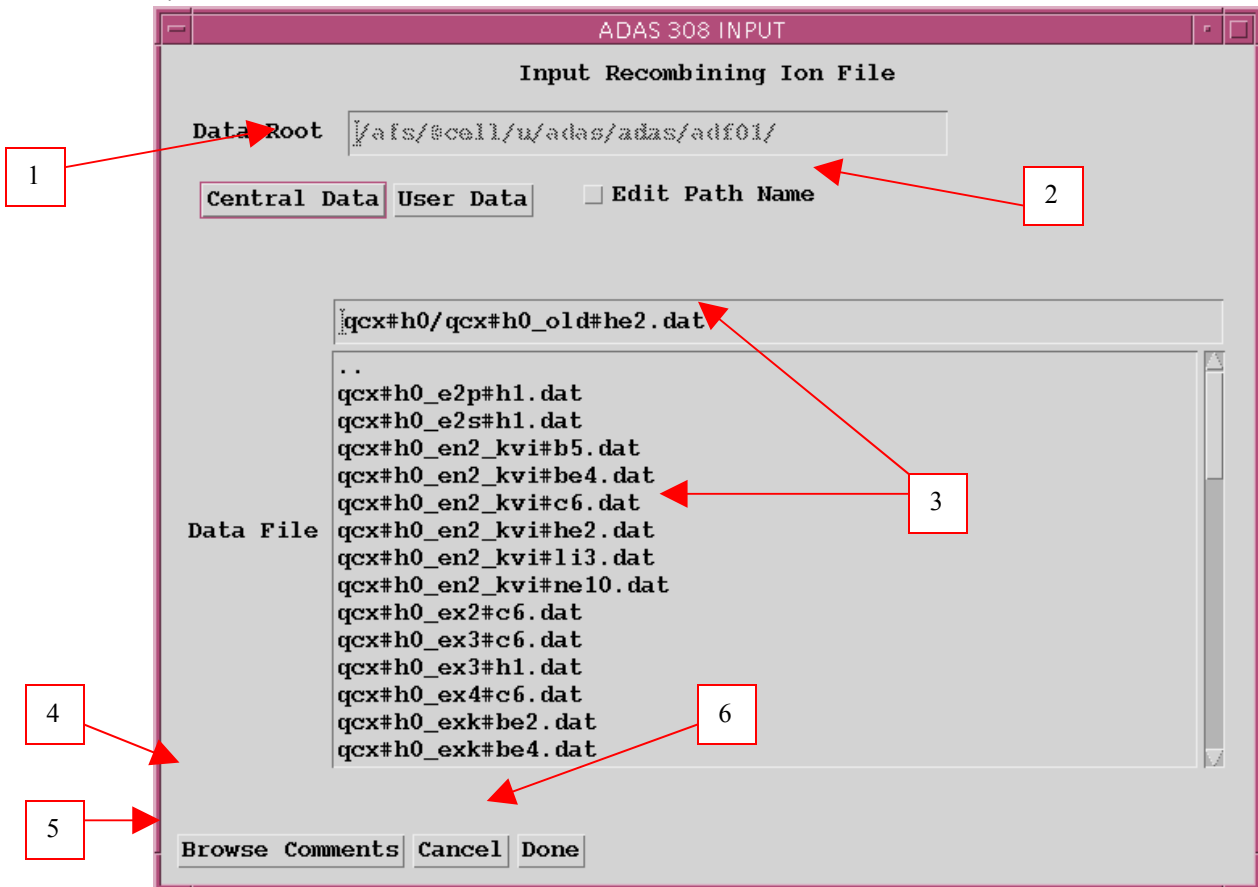
5. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what has gone into the dataset and the attribution of the dataset. The possibility of browsing the comments appears in the subsequent main window also.

6. 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

9. 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.

10. Information is given on the fully ionised impurity receiver and the neutral beam donor. The atomic mass of the receiver must be entered.

11. The specification of beam parameters, details of observed line of sight spectral emissivities to be analysed and emissivities to be predicted are required. Input data of each of these three types may be

addressed in turn by activation of the relevant button. The window below the button list then presents the appropriate table.

12. *The Required emissivity predictions* button is displayed. This activates the predictive part of the code which becomes possible once the observed lines have been analysed in terms of emission measure. Then any set of lines within the N-shell limits may be predicted. The standard output includes the mean wavelength and effective emisison coefficient, but for up to five lines an extended tabulation of line component emissivities may be produced. Graphs may be produced for two selected line. Indicate these selections in the *Key* columnThe table may be edited by clicking on the *Edit Table* button.

13. The *Observed spectrum lines* table allows introduction of a number of observed intensities. It is possible to enter values which do not allow a consistent solution. The code advises of this but it is the responsibility of the user to check that the data is unblended etc. It is also a usual practice to enter just one line, possibly with a fictitious emissivity merely to obtain effective emission coefficients and line component details.

14. The *Beam parameter information* button causes display of the third editable table in the sub-window. Note that no check is made that the various beam energy fractions sum to unity. This is the responsibility of the user.
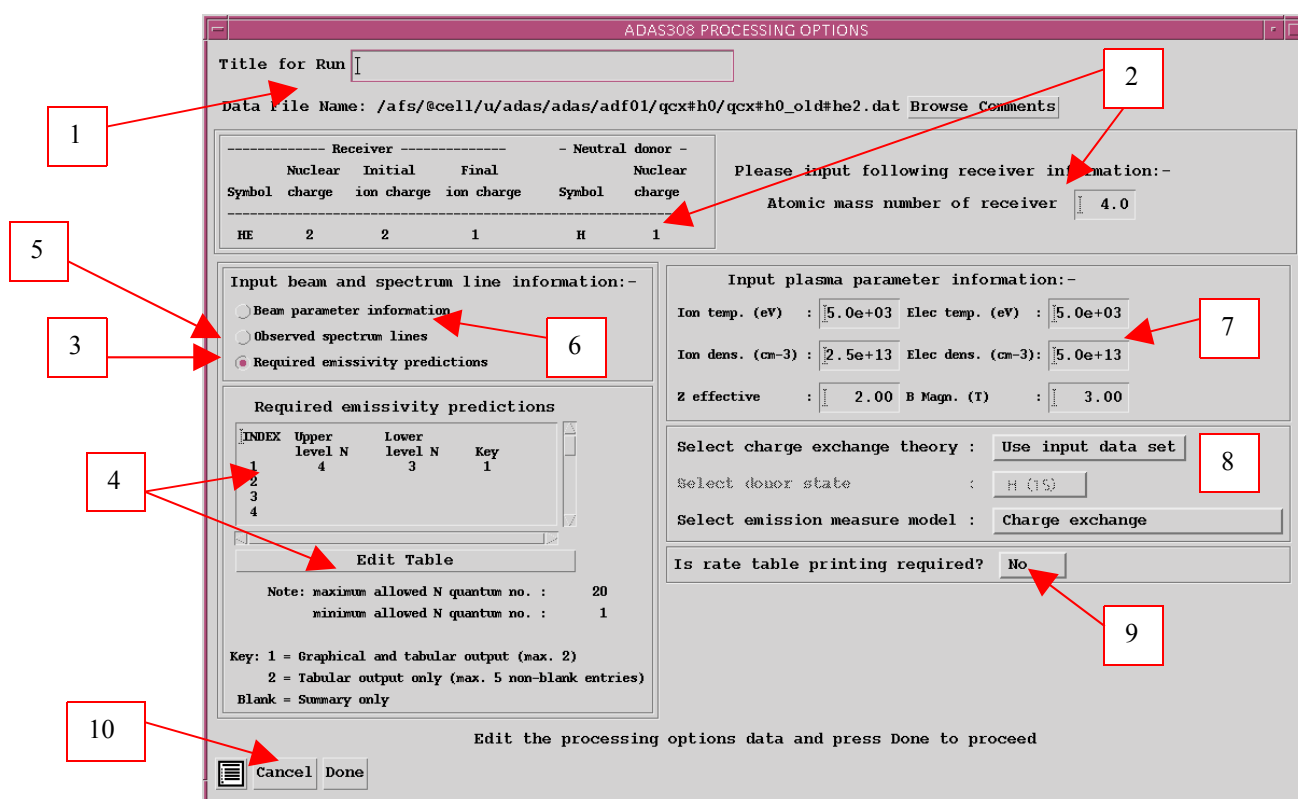
15. Enter the plasma environment parameters. These determine the collisional redistribution of the populations of the recombined plasma ion. For ADAS308, *B Magn*. has no effect, but a value should be entered as a place holder.

16. The final sub-window allows model and theory choices. Details are given in the ADAS Manual. For each type, clicking on the selection window drops down a short menu of choices. Click on the appropriate choice. The ADAS data base source numerical data of type ADF01 is the most usual, that is the *Use input data set* choice button. Note that

the *Select emission measure* model choice includes *Electron impact excitation* as well *as Charge exchange*.

17. Extended information on the rates used in the populaiton modelling may be printed.

18. 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** is shown below. Note that two plots are produced if required. The *Plot A* is the stick diagram of component line-of-sight emissivities. The *Plot B* is of the Doppler broadened profile of the line at the plasma ion temperature.

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.

2. Graphical display is activated by the *Graphical Output* button. 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.

3. 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. Plot A axes limits refer to the 'stick diagram and Plot B axes limits to the Doppler broadened profile.

4. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable 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. 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*.

The **Graphical output window** is shown below

3. Printing of the currently displayed graph is activated by the *Print* button.
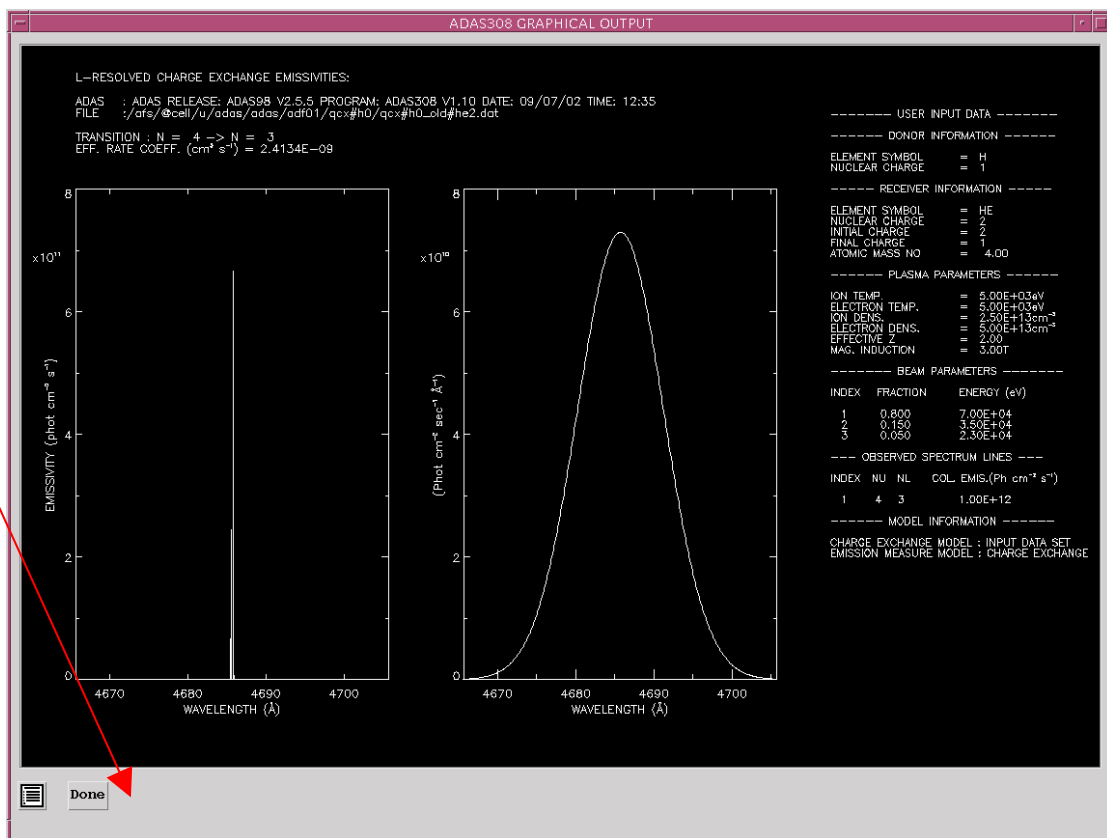
Extended CXS capabilities

The charge exchange spectroscopy modelling capabilities of ADAS are still extending. This is largely motivated by the need to cope with heavier receiver ions beyond argon, which may be partially ionized. Attention is drawn to two new codes ADAS315 and ADAS316. Many subroutines have been added or modified to accommodate the new capabilities. The user should check the detailed release notes in item 4. A number of subroutines have modified parameter sets.

ADAS315: Preparation and extraction of universal adf49/adf01 CX cross-section data

This is a straightforward code which creates and ADF01 file for a specific ion of an element from a z-scaleable universal dataset of format ADF49. There are only two datasets of AD49 format corresponding to H(n=1) and H(n=2) donor respectively. The input screen is shown below followed by the output screen. A choice is possible of output energies. It is to be noted that in the level of approximation of the universal ADF49 data and the bundle-n application models, only the residual charge of the recombining ion is relevant. For the high n-shells of importance, the Rydberg electron is effectively in a hydrogenic state in the Coulomb field of the residual charge. The ADF49 datasets are subject to change as more fiducial data becomes available and the opimising of the z-scaling paramterisation is reworked. At this stage ADAS315 and ADAS316 are enabling a first look at the heavy ion CXS.
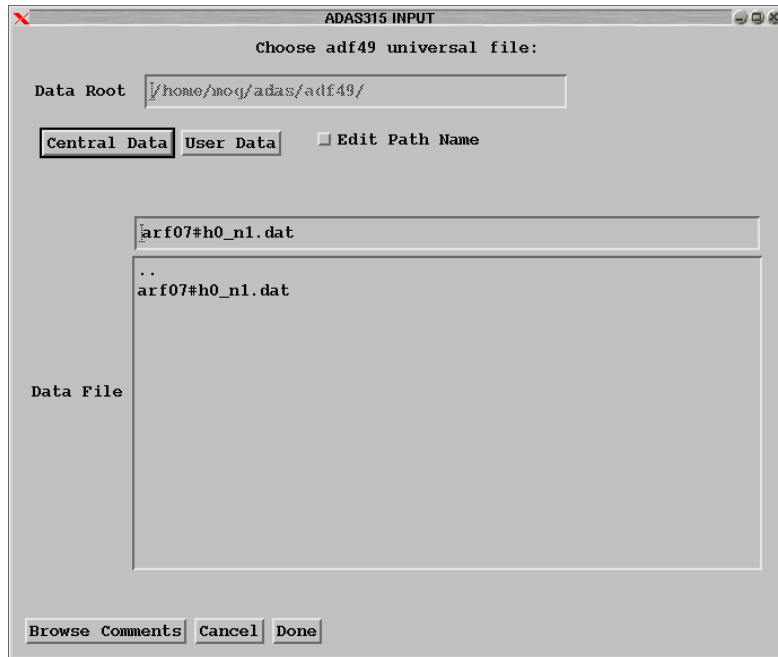

Running ADAS315 (an IDL only) code, available also at the command line, in a script allows output ADF01 files to be generated rapidly for a set of ions of an element.
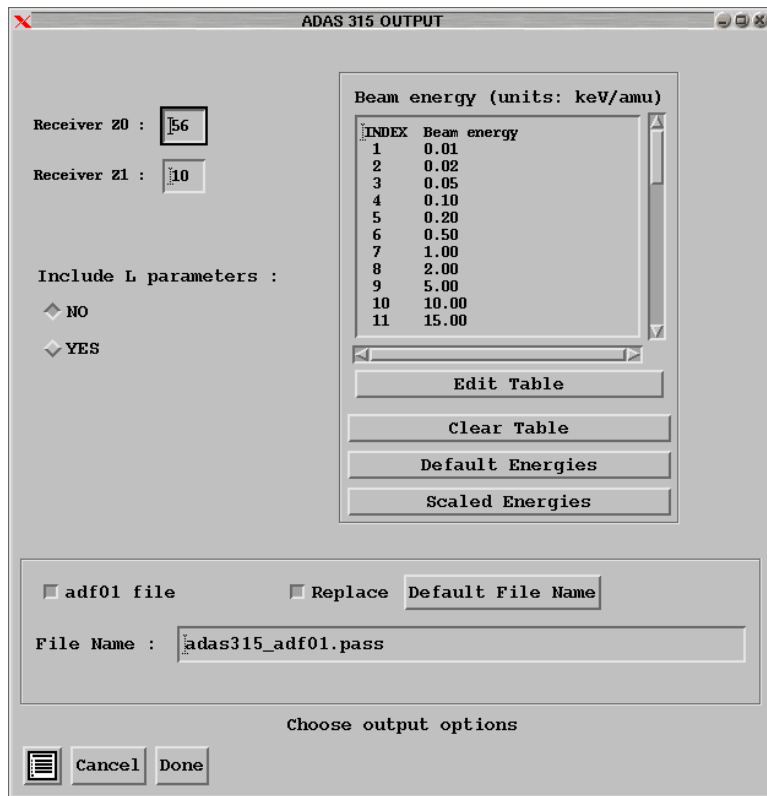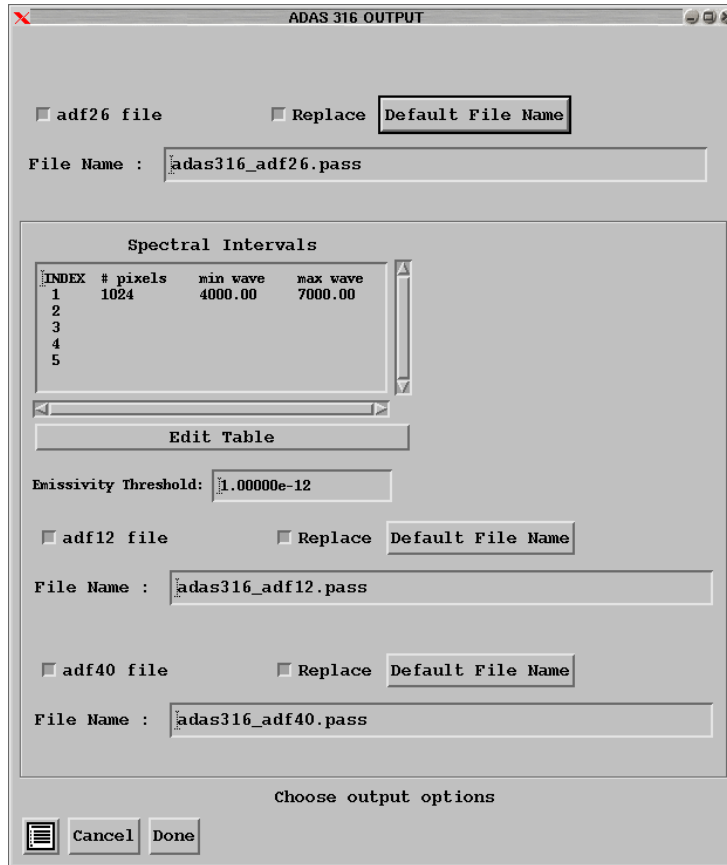
ADAS316: Charge exchange spectroscopy – process effective coefficients: bundle-n

The code calculates charge exchange effective emission coefficients of format ADF12 from and input ADF01 file, probably created by ADAS315.
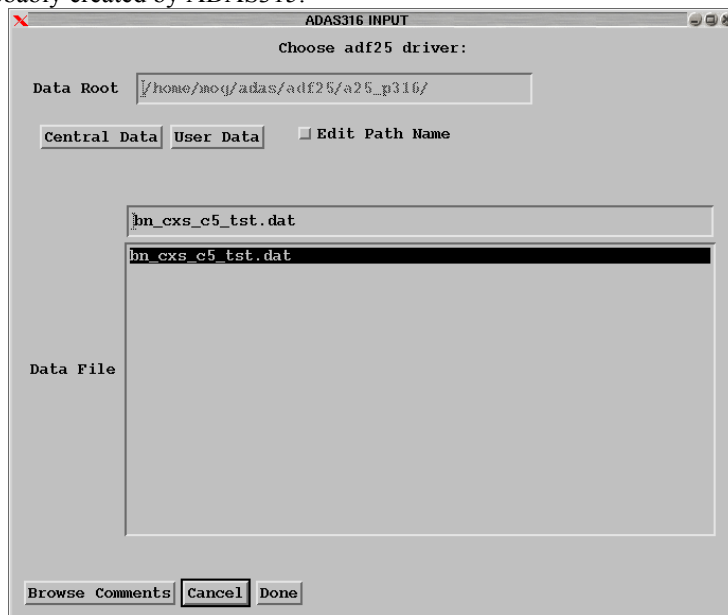
The code requires a driver data set and, for bundle-n in ADAS, these have historically been archived in ADF25.

A new sub-directory /a25_p316 has been assigned and a complete redesign of the driver has been carried out. Also a new read routine exploits the new drivers fully. We would like to move to this type of driver in the future, where there is substantial guidance to the user in the fields and mnemonics used in the driver. The driver allows scans over parameters to be specified. In fact the driver is quite versatile and appropriate to all type of bundle-n calculation . We shall exploit it further for Bremsstrahlung + free-bound continuum iand quasi-continuum high Rydberg line contributions in the future.

The output screen follows a usual pattern. Output ADF26 (the bundle-n population solution), ADF12 (charge exchange effective emission coefficients) and ADF40 (feature emissivity coefficients) may be produced. For heavy species CXS, because of the very large number of transitions between highly excited states, the ADF40 format becomes more useful that ADF12. A graph of the bundle-n-population solution, at the reference plasma parameters (usually at the centroid of the scans) is generated and shown with the free–electron capture and charge exchange capture parts separated – as illustrated below.