Charge exchange spectroscopy

- Preliminaries
- ADAS series 5/series2 - thermal charge transfer
- ADAS series 3 - charge transfer with neutral beams

Preliminaries

- We are concerned with the charge exchange reaction

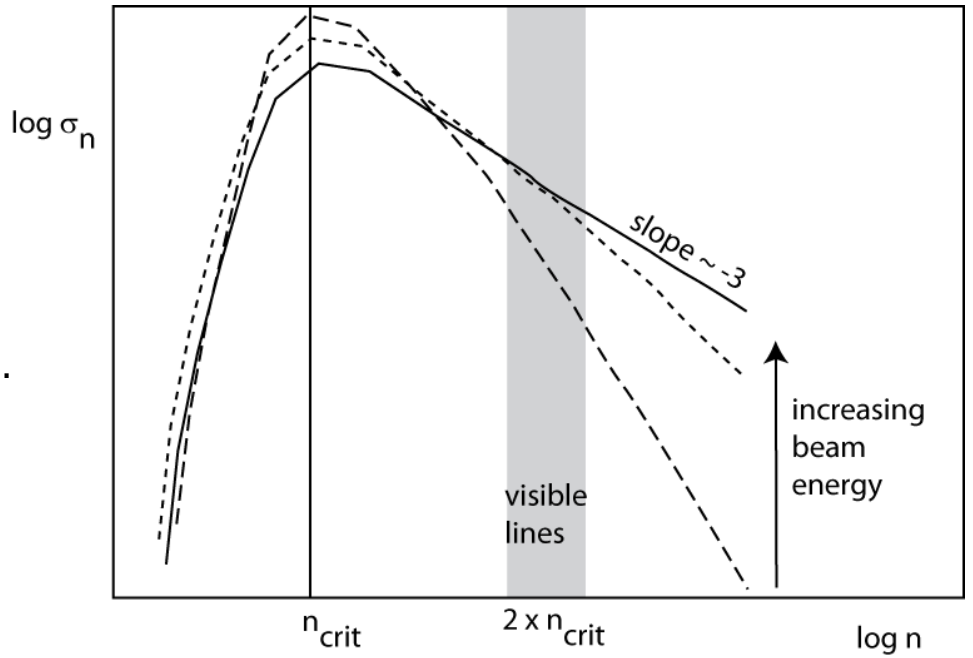
$$X^{+z_0} + D(1s) \rightarrow X^{+z_0-1}(i) + D^+$$

- It is state selective depending on the energy of the collision.

- Two regimes are of interest

  (a) Thermal hydrogen as the donor in thermal plasma – a near-edge plasma phenomenon. Partially stripped receivers and excited donors may be involved.

  (b) Hydrogen in fast beams – a core plasma phenomenon localised in the beams. Mostly stripped receivers and ground state donors are involved.



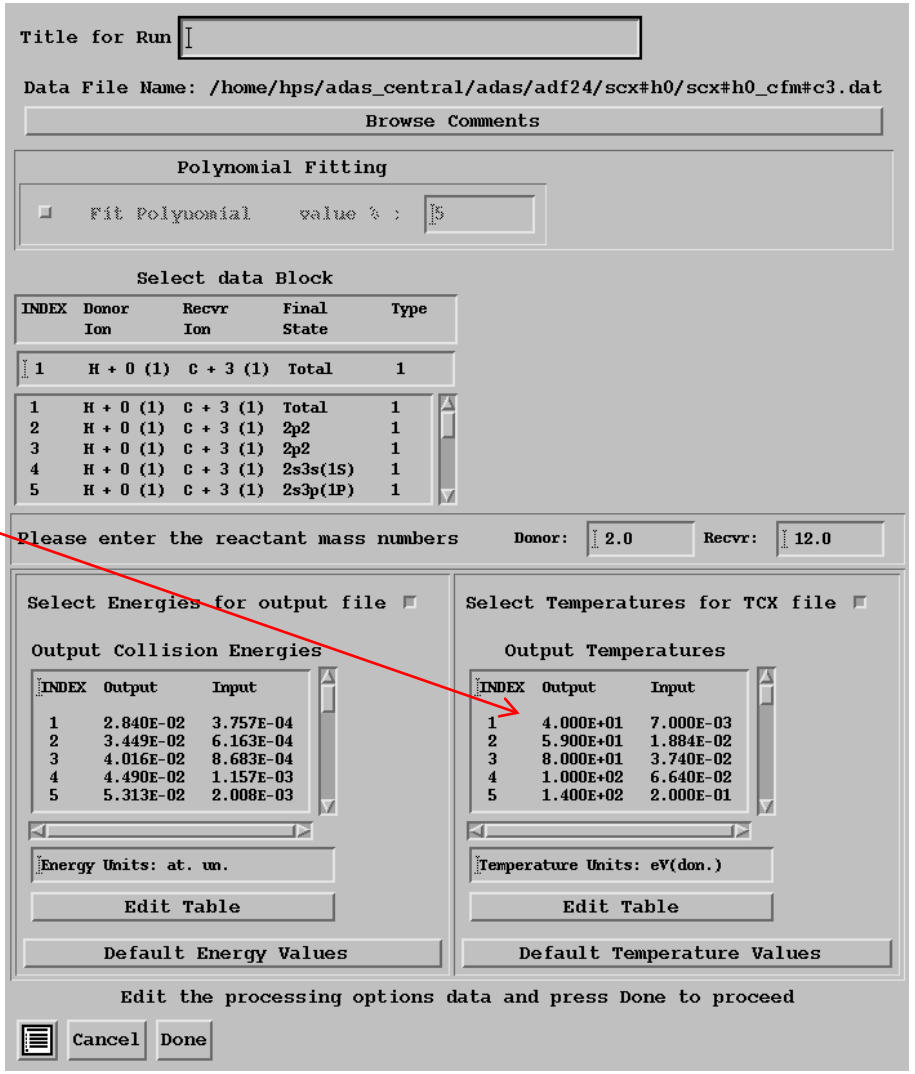
Thermal charge transfer

- State selective charge transfer cross-sections are stored in ADAS format ADF24.
- ADF24 data is organised as a simple indexed list of transitions with each cross-section a function of energy.
- The series 5 code ADAS509 interrogates data format ADF24. As well as display, it allows conversion to thermal-thermal rate and preparation of these in a new format ADF14.
- ADF14 is organised as a simple indexed list, but the tabulation of each transition is as a two dimensional array as a function of donor and receiver temperatures.
- The series 5 code ADAS505 interrogates data format ADF14.
- Data is transferred from there (by hand) into ADF04 - as a 1-dimensional locus through the 2-dimensional array – usually the donor and receiver temperatures are set equal.

Thermal charge transfer

Processing with ADAS509

Select temperatures for adf14 dataset



Thermal charge transfer

Extended ADF04 data format for CX

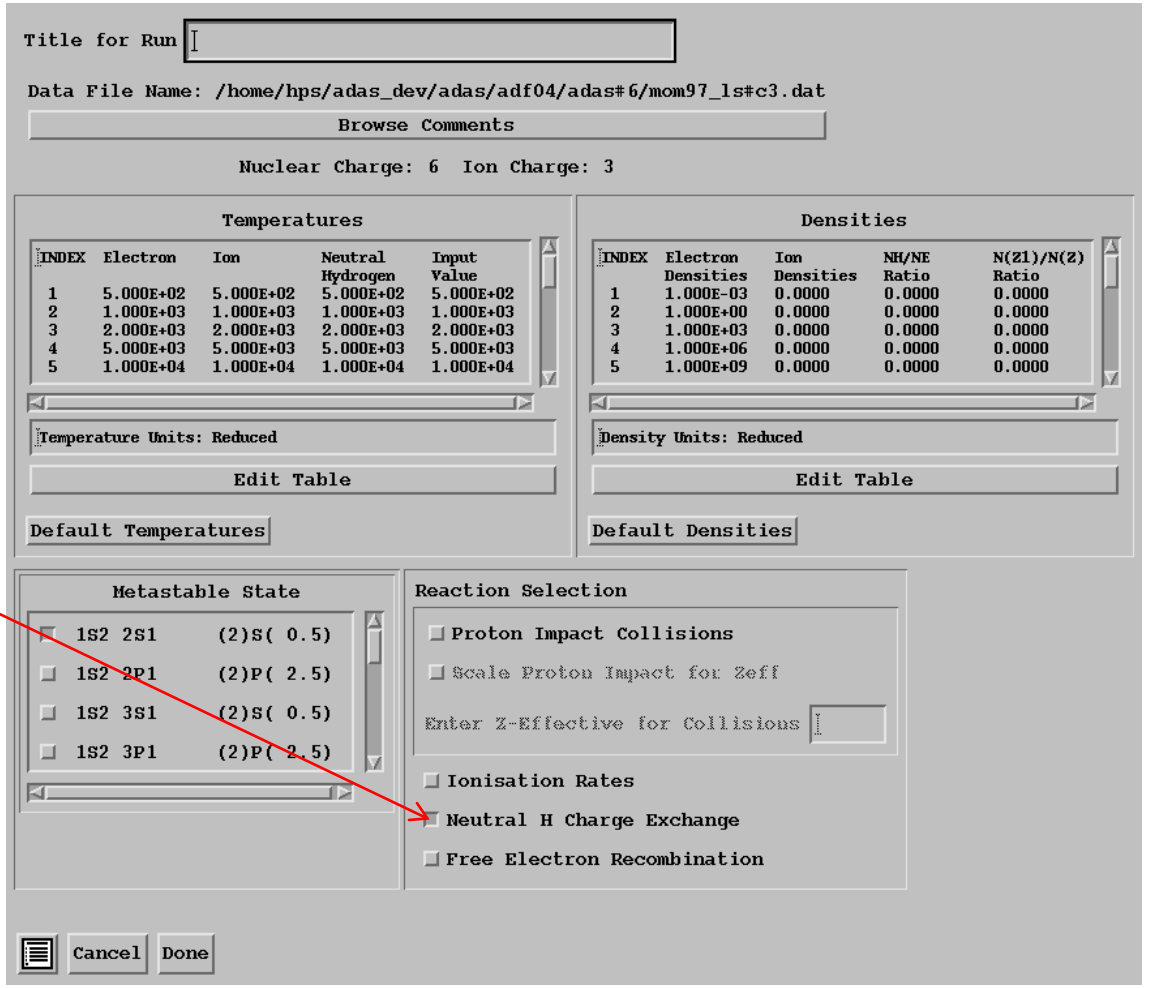
/home/adas/adas/adf04/adas#6/mom97_ls#c3.dat

```
C + 3         6         4        520178.4(1S)   2931440.0(3S)
    1 1S2 2S1           (2)0( 0.5)        0.0   {1}1.000 {2}1.500
    2 1S2 2P1           (2)1( 2.5)    64555.4   {1}1.000
    3 1S2 3S1           (2)0( 0.5)   302849.0   {1}1.000
    4 1S2 3P1           (2)1( 2.5)   320071.2   {1}1.000
    5 1S2 3D1           (2)2( 4.5)   324886.1   {1}1.000
    6 1S2 4S1           (2)0( 0.5)   401348.1   {1}1.000
    7 1S2 4P1           (2)1( 2.5)   408319.8   {1}1.000
    8 1S2 4D1           (2)2( 4.5)   410338.5   {1}1.000
    9 1S2 4F1           (2)3( 6.5)   410434.2   {1}1.000
   10 1S2 5S1           (2)0( 0.5)   445368.5   {1}1.000
   11 1S2 5P1           (2)1( 2.5)   448860.5   {1}1.000
   12 1S2 5D1           (2)2( 4.5)   449889.2   {1}1.000
   13 1S2 5F1           (2)3( 6.5)   449939.8   {1}1.000
   14 1S2 5G1           (2)4( 8.5)   449948.4   {1}1.000
   -1
  4.0    3       8.00+03 1.60+04 3.20+04 8.00+04 1.60+05 3.20+05 8.00+05 1.60+06 3.20+06 8.00+06 1.60+07
    3    1 1.00-30 5.68-01 5.49-01 5.16-01 4.46-01 3.96-01 3.84-01 3.87-01 3.83-01 3.83-01 3.85-01 3.86-01
    5    1 4.57+05 4.90-01 4.97-01 5.11-01 5.43-01 5.79-01 6.24-01 7.90-01 9.58-01 1.08+00 1.18+00 1.21+00
              .         .     .
H   3  +1          1.00-13 1.42-13 2.00-13 3.67-13 3.40-12 6.46-11 1.02-09 3.98-09 1.11-08 3.02-08 5.13-08
H   4  +1          5.50-12 2.47-11 1.41-10 9.53-10 3.16-09 8.82-09 2.15-08 3.45-08 4.91-08 6.01-08 6.13-08
H   5  +1          1.38-09 1.78-09 2.12-09 2.32-09 2.20-09 1.89-09 1.88-09 4.35-09 1.15-08 2.62-08 3.94-08
H   6  +1          2.12-17 3.00-17 4.25-17 8.52-17 4.76-16 6.14-15 2.00-13 2.74-12 3.10-11 3.01-10 9.08-10
H   7  +1          1.09-16 1.54-16 2.18-16 4.38-16 2.44-15 3.16-14 1.03-12 1.41-11 1.52-10 1.08-09 2.24-09
H   8  +1          3.22-17 4.56-17 6.45-17 1.29-16 7.23-16 9.33-15 3.01-13 4.14-12 5.26-11 8.12-10 3.18-09
H   9  +1          3.72-17 5.26-17 7.46-17 1.49-16 8.35-16 1.08-14 3.51-13 4.80-12 5.46-11 5.37-10 1.78-09
            .         .     .
  -1
  -1  -1
```

Thermal CX rate coeffts.

Thermal charge transfer

Processing with ADAS205 or ADAS208



Activate thermal CX

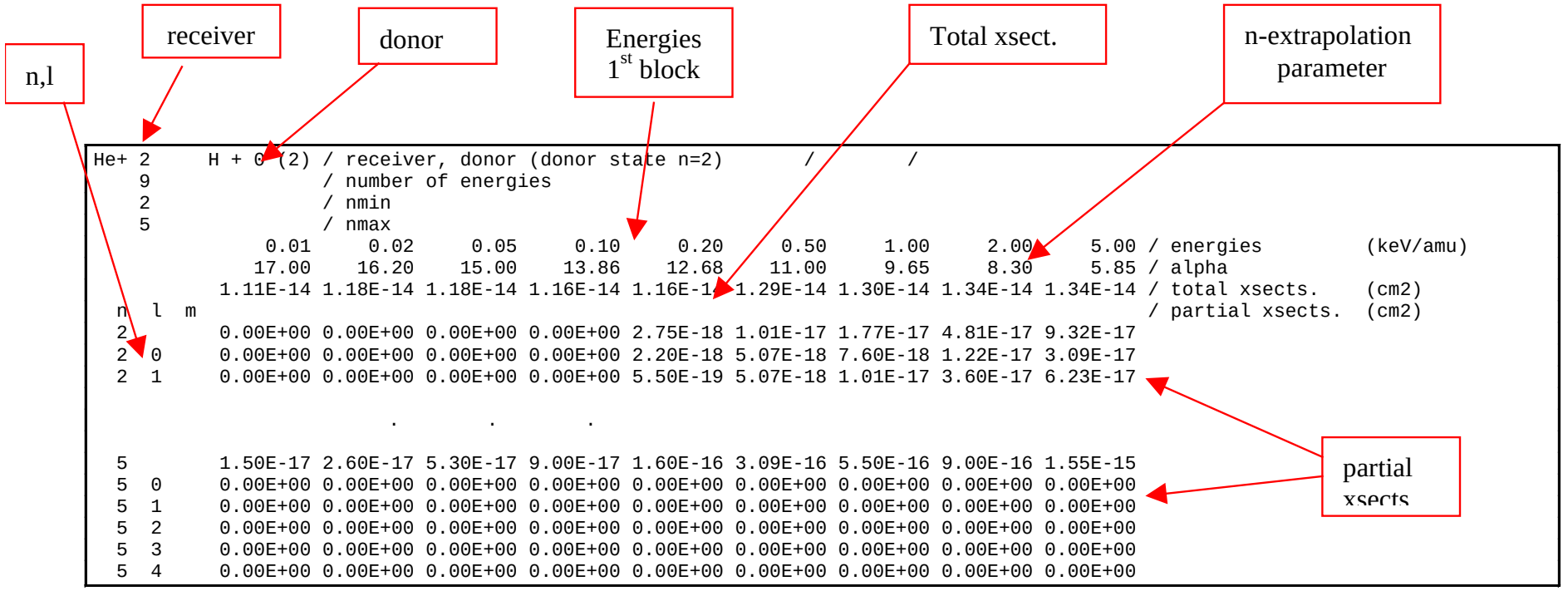
Charge transfer with neutral beams

- Interrogating state selective charge exchange cross-sections using ADAS301.
- Interrogating CXS effective emission coefficients using ADAS303.
- Calculating and examining effective emission coefficients using ADAS308.

Interrogating charge exchange cross-sections

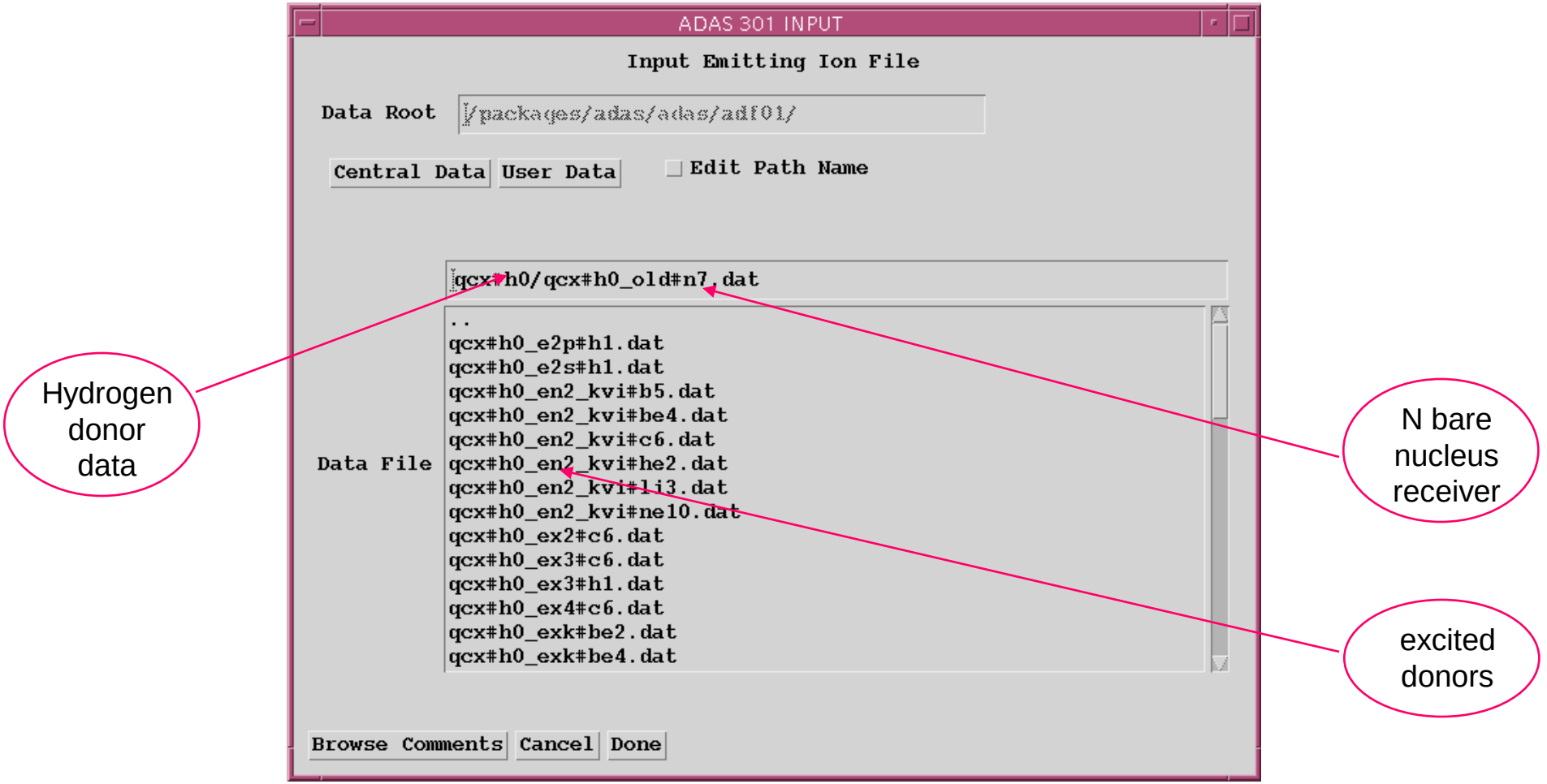
- Datasets of class ADF01 contain state selective charge exchange xsect. (qcx) data as a function of energy.
- These data for bare nucleus light impurity receivers into nl-shells in general.
- The donors may be H, He or Li and can include donation from ground state and excited state. There are separate data sets for each excited donor state.
- Code ADAS301 interrogates ADF01 data sets and displays results at energies of your choice.

ADF01 charge exchange cross-sections

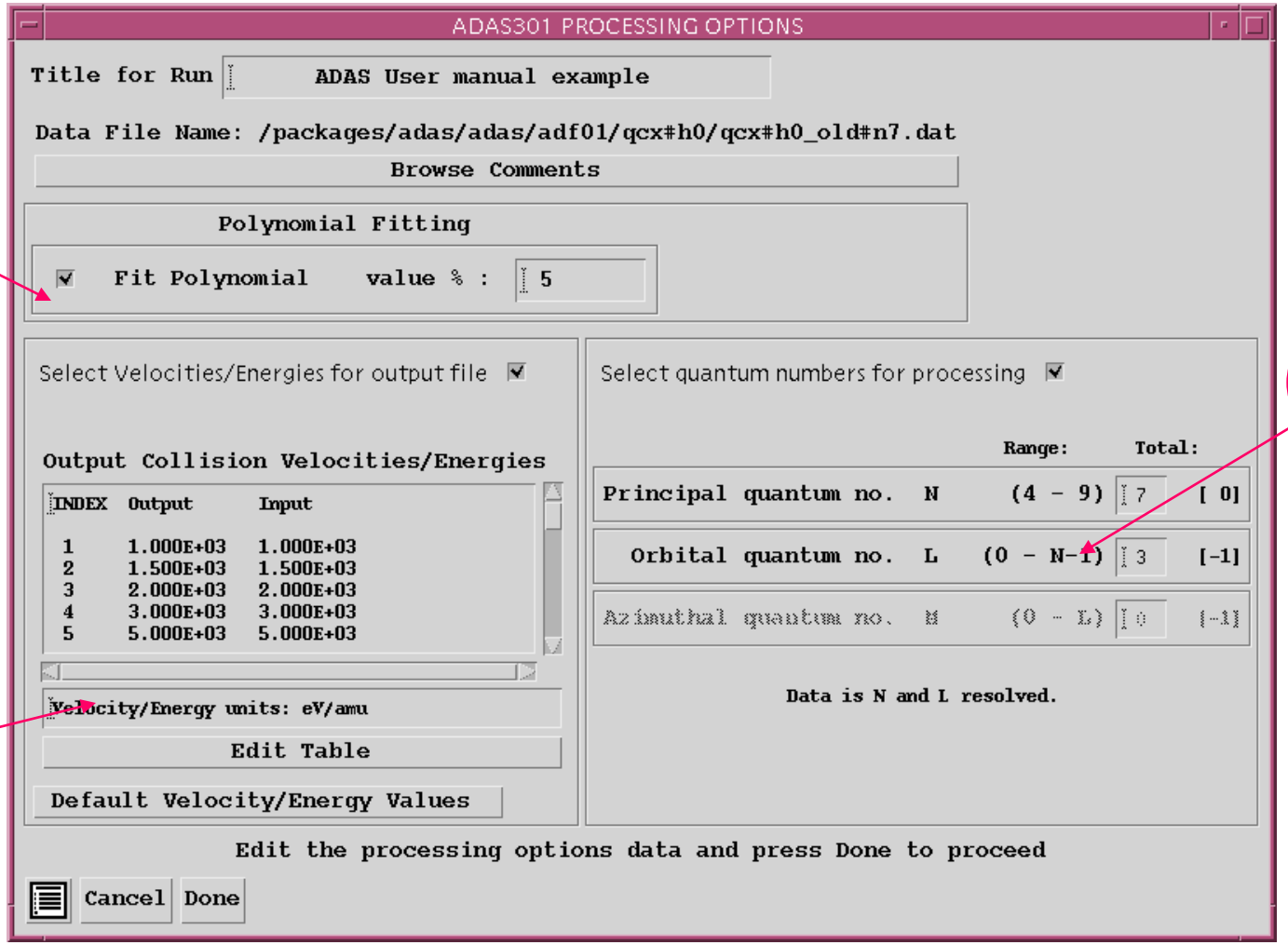



```
He+ 2     H + 0 (2) / receiver, donor (donor state n=2)       /        /
    9               / number of energies
    2               / nmin
    5               / nmax
              0.01     0.02     0.05     0.10     0.20     0.50     1.00     2.00     5.00 / energies         (keV/amu)
             17.00    16.20    15.00    13.86    12.68    11.00     9.65     8.30     5.85 / alpha
          1.11E-14 1.18E-14 1.18E-14 1.16E-14 1.16E-14 1.29E-14 1.30E-14 1.34E-14 1.34E-14 / total xsects.    (cm2)
  n   l  m                                                                                 / partial xsects.  (cm2)
  2        0.00E+00 0.00E+00 0.00E+00 0.00E+00 2.75E-18 1.01E-17 1.77E-17 4.81E-17 9.32E-17
  2  0     0.00E+00 0.00E+00 0.00E+00 0.00E+00 2.20E-18 5.07E-18 7.60E-18 1.22E-17 3.09E-17
  2  1     0.00E+00 0.00E+00 0.00E+00 0.00E+00 5.50E-19 5.07E-18 1.01E-17 3.60E-17 6.23E-17

                        .        .        .

  5        1.50E-17 2.60E-17 5.30E-17 9.00E-17 1.60E-16 3.09E-16 5.50E-16 9.00E-16 1.55E-15
  5  0     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  1     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  2     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  3     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  4     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
```

ADAS301 input



ADAS302 Processing

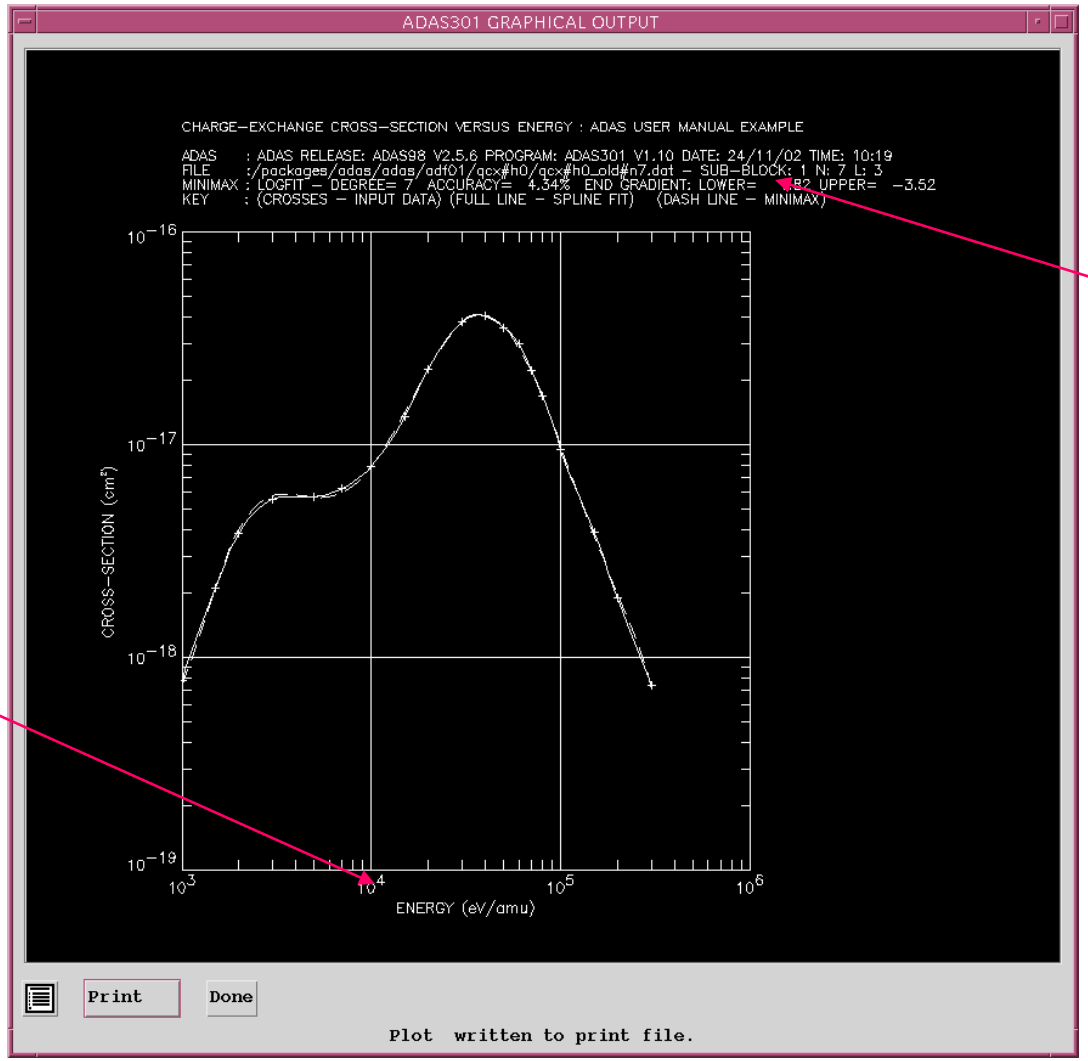


Polynomial fit

Specify energies & units

select partial xsect

ADAS301 graph



specification of extracted xsect.

graph is a function of energy

Charge exchange effective emission

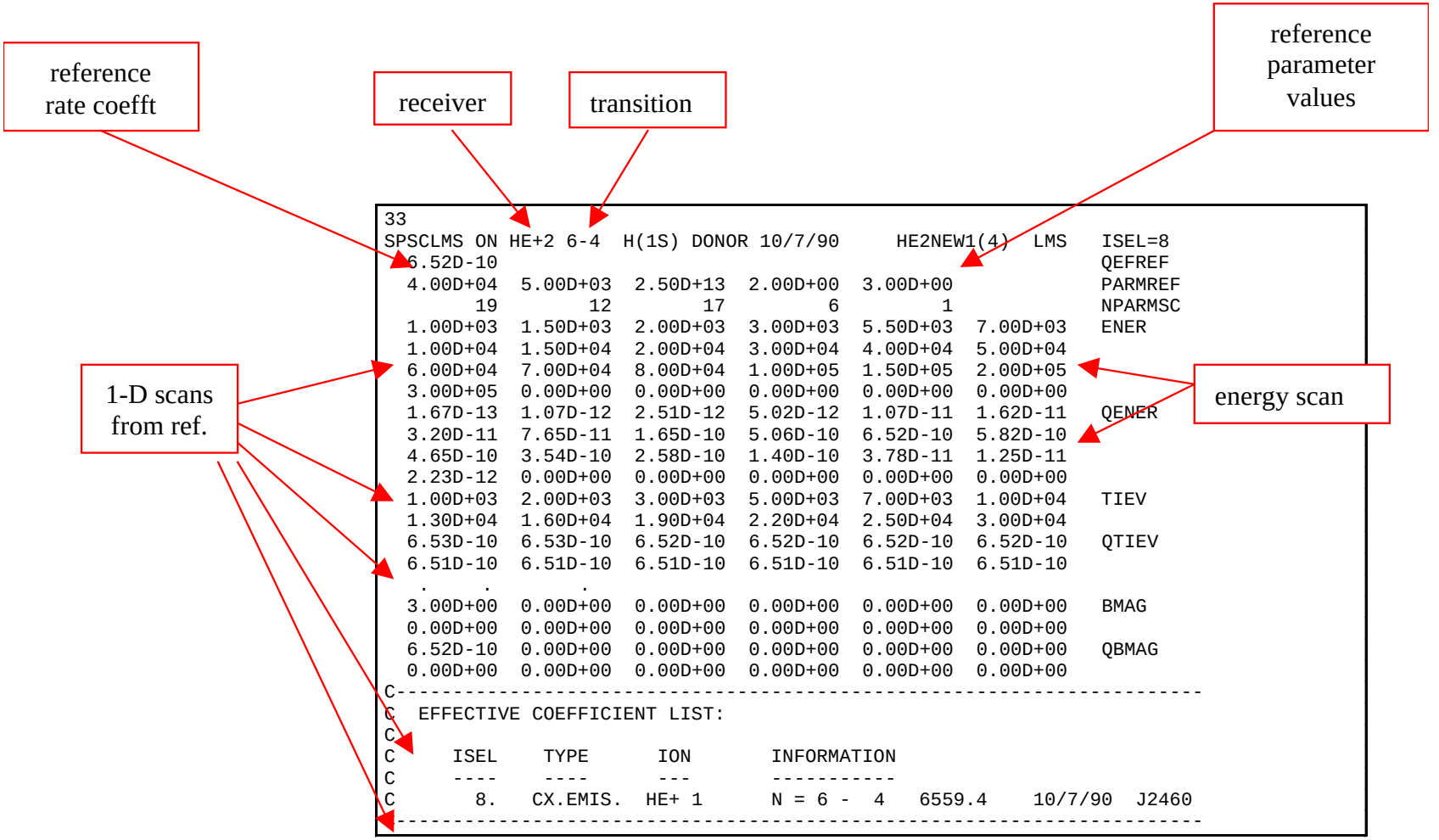
The line-of-sight integrated photon emissivity of a charge exchange driven line may be written as

$$
\begin{aligned}
I_{n\to n'}^{(z_0-1)} &= \sum_{l,l'} I_{nl\to n'l'}^{(z_0-1)} \\
&= \int_S \sum_{l,l'} A_{nl\to n'l'} N_{nl}^{(z_0-1)} ds \\
&= \int_S [\sum_{l,l'} A_{nl\to n'l'} (N_{nl}^{(z_0-1)} \ / \ N_D N^{(z_0)})] N_D N^{(z_0)} ds \\
&= \int_S [\sum_{l,l'} q_{nl\to n'l'}^{(eff)}] N_D N^{(z_0)} ds \\
&= \int_S q_{n\to n'}^{(eff)} N_D N^{(z_0)} ds \\
&\approx q_{n\to n'}^{(eff)} \int_S N_D N^{(z_0)} ds
\end{aligned}
$$

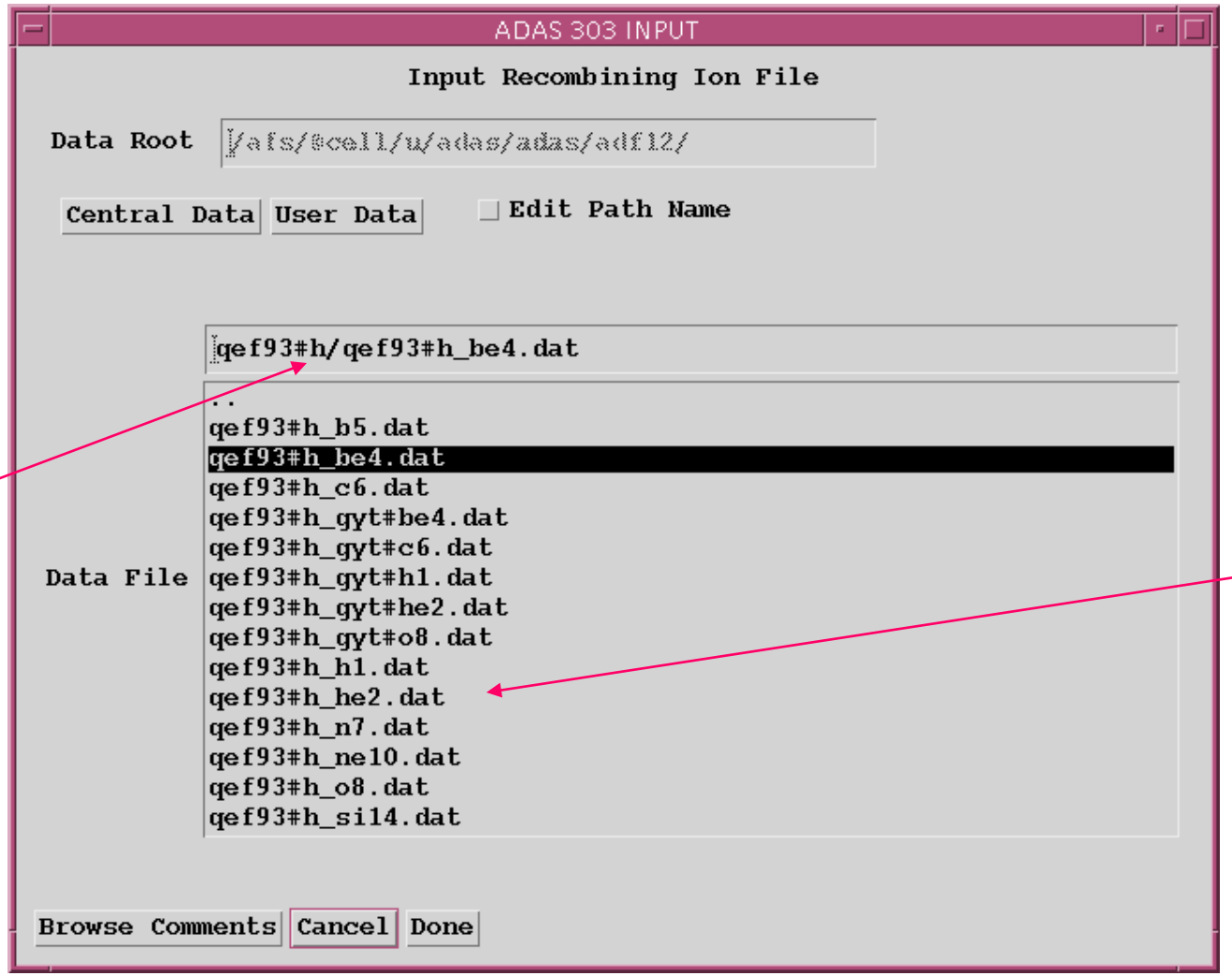
Interrogating CXS effective emission coefficients

- Datasets of class ADF12 contain CXS effective emission (qef) data as a function of beam and plasma parameters.
- These coefficients include the effect of collisional redistribution of nl-substate populations of the receiver ion in the plasma.
- The individual components of the n->n' CX transition are not resolvable for bare nucleus receivers so only whole transition arrays are given.
- Code ADAS303 interrogates ADF12 data sets and displays results at beam and plasma conditions of your choice.

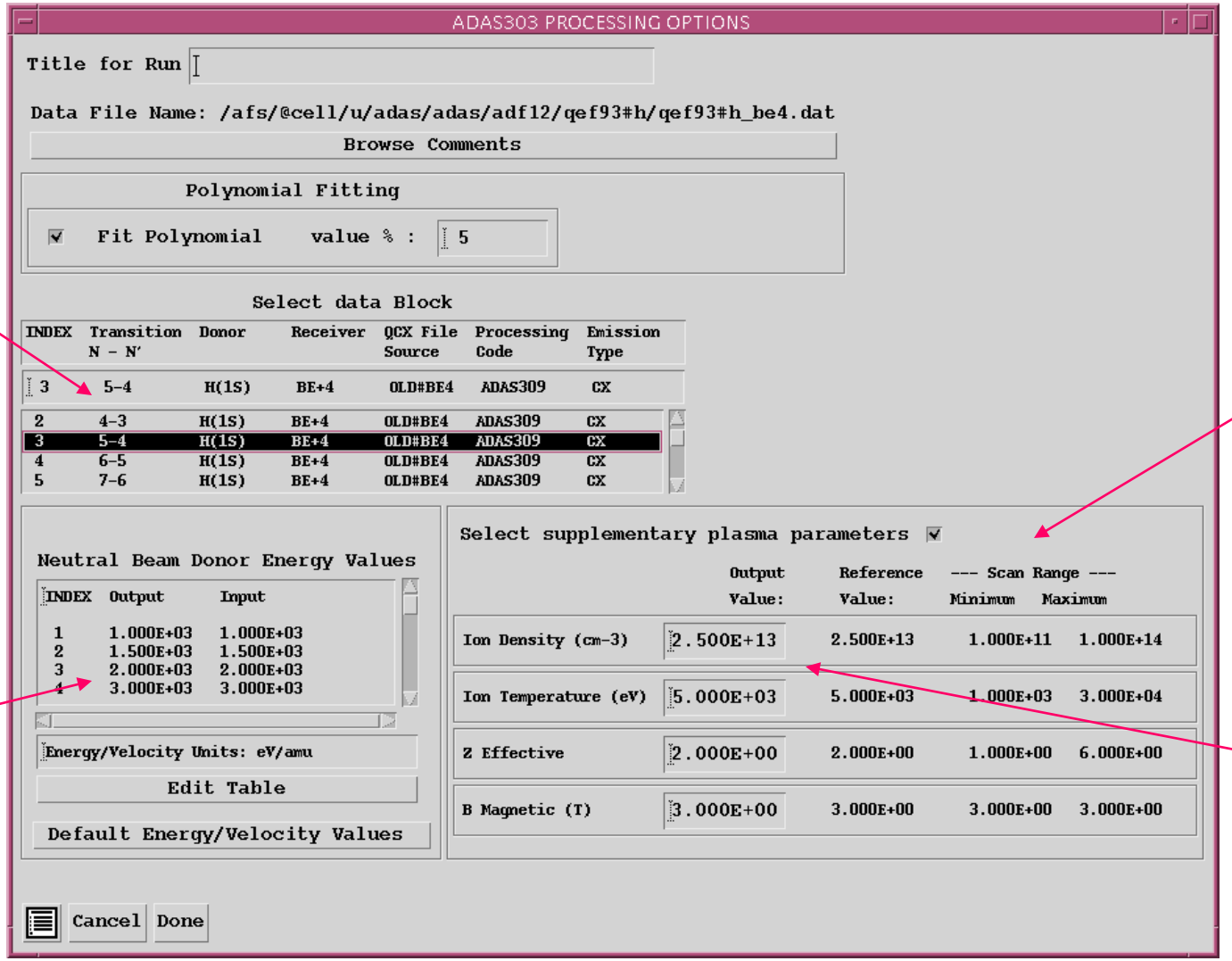
ADF12 charge exchange cross-sections



ADAS303 input



ADAS303 Processing



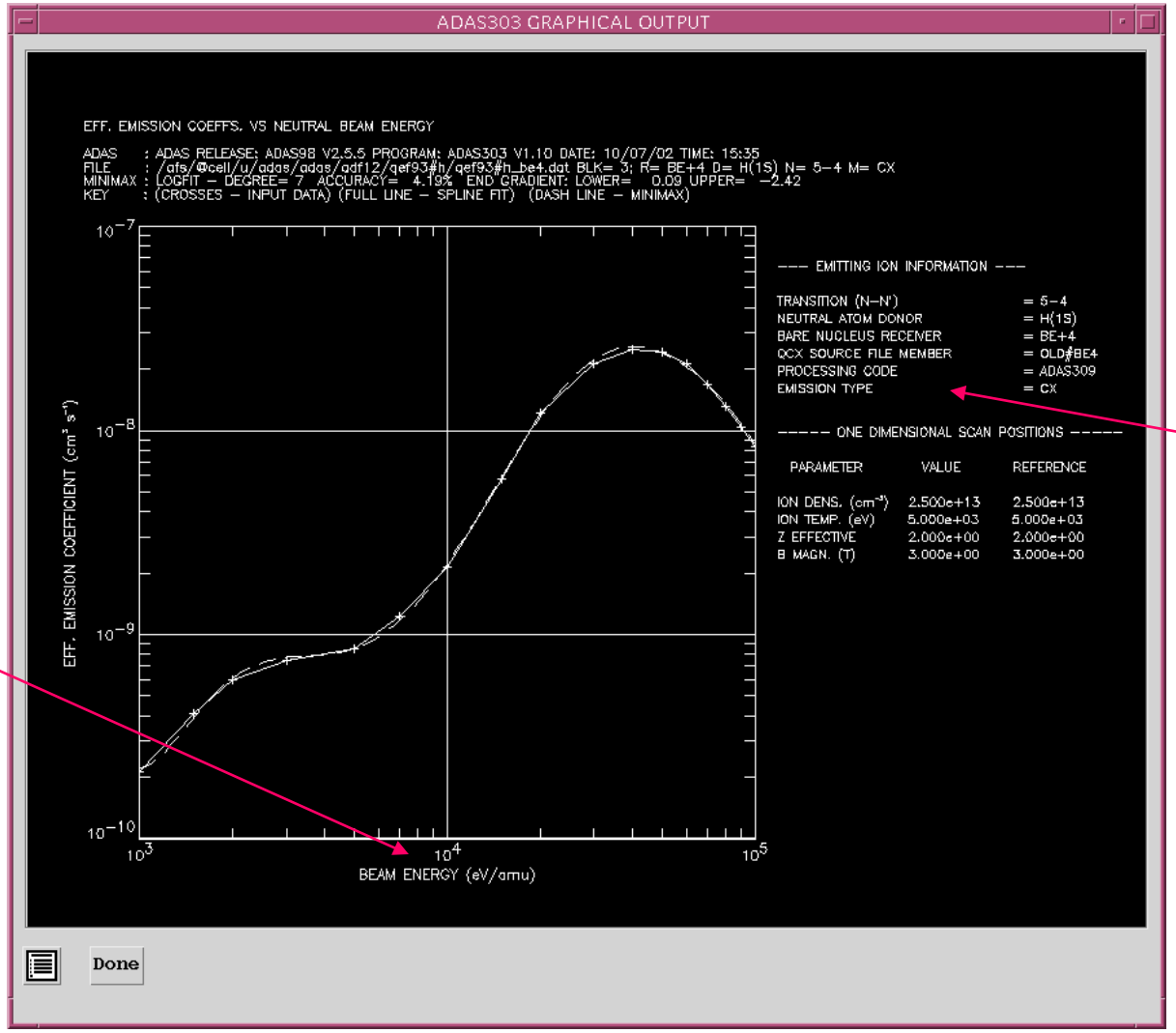
Select transition

Specify donor energies

Scan range and reference

Select plasma conditions

ADAS303 graph



graph is a function of beam energy

plasma and beam conditions for graph

Calculating CXS effective emission

- Datasets of class ADF01 state selective charge exchange cross-section data for capture by fully ionised ions.

- Code ADAS308 computes effective emission coefficients, predicts CXS line positions and profiles and deduces the beam plasma emission measure.

Calculating CXS effective emission (contd.)

- The driving reactions are

$$X^{+z_0} + D^0_{beam}(1s) \rightarrow X^{+z_0-1}(nl) + D^+_{beam}$$

- The effective emission coefficient for n-n' transition is

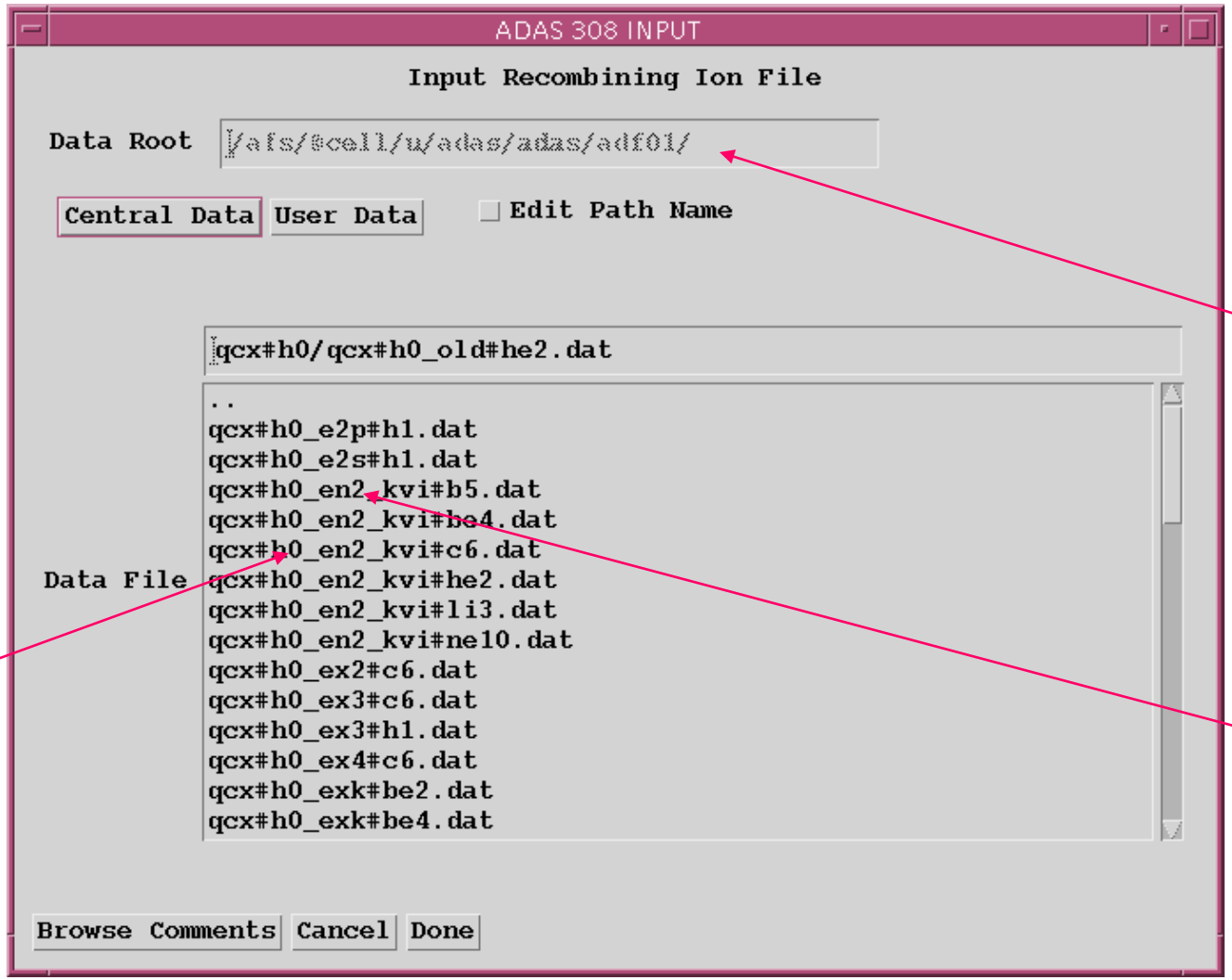
$$q^{(eff)}_{n\rightarrow n'} = \sum_{l,l'} A_{nl\rightarrow n'l'}(N^{(z_0-1)}_{nl} / N_D N^{(z_0)})$$

- Thus a collisional-radiative, resolved-nl population calculation is required to determine the effective emission coefficients.

Calculating CXS effective emission (contd.)

- File selection
  - » The fundamental state selective charge exchange x-sect data is format ADF01. These data are resolved into the nl shells of the receiver.
  - » Note that there are sub-directories for different donors and separate data sets for ground and excited donor states.
- Processing options
  - » *Beam parameter, observed spectrum lines and required emissivity predictions must be entered using Table Editor.*
  - » *Then plasma conditions must be entered.*
  - » *Finally model for emission measure is chosen.*
- Output options
  - » Graphical display of the spectral position, intensity and shape of a designated n-n' transition is given.
  - » Tabulations of predicted intensities of other lines are given together with the estimated emission measure.

ADAS308 Input



Calculating CXS effective emission (contd.)

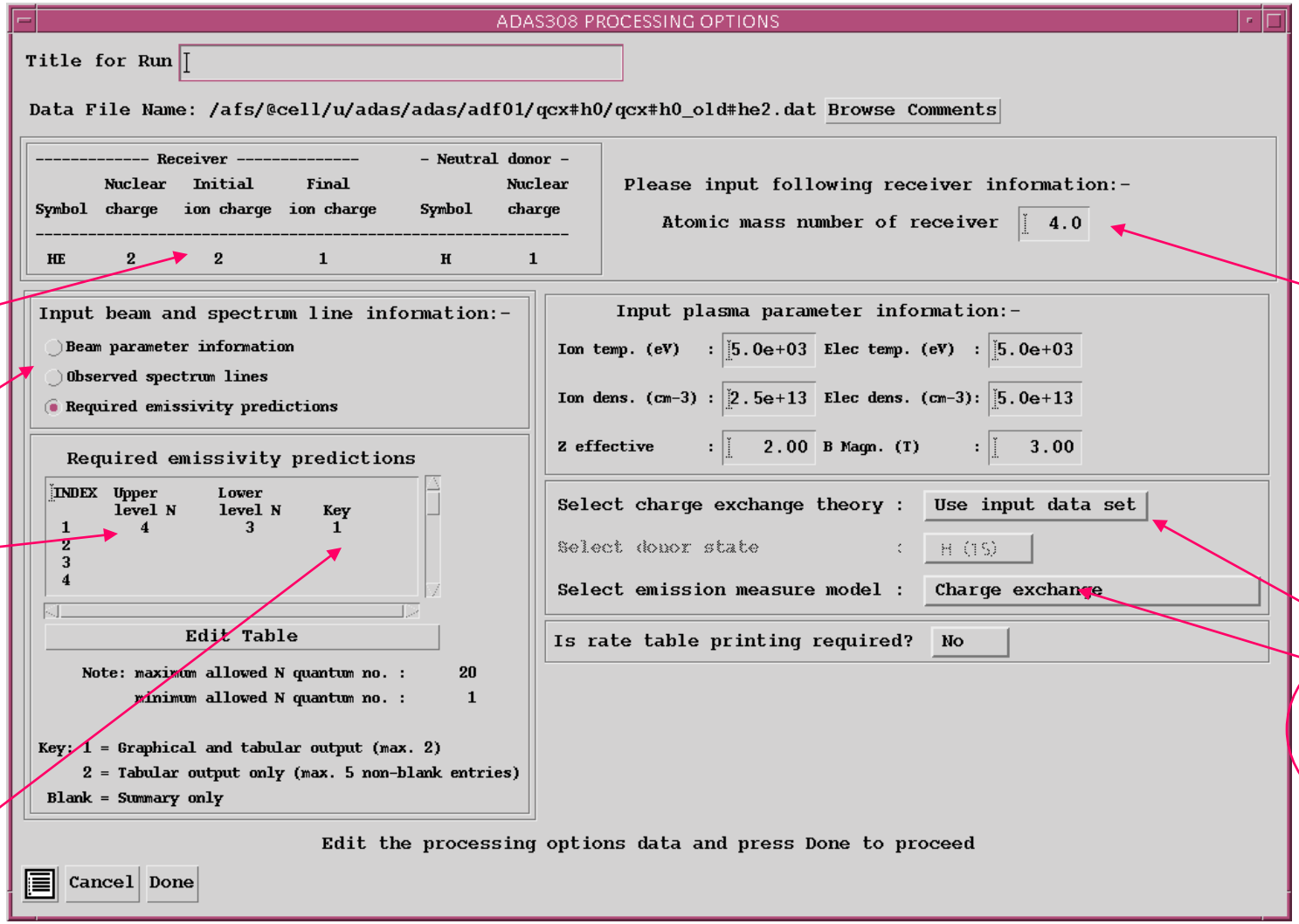
- ADAS308 is designed to do more than solve for the effective emission coefficients, qef.

- The program computes the qef and solves for the emission measure given the line of sight intensity in a charge exchange line as

$$I_{n\to n'}^{(z_0-1)} \approx q_{n\to n'}^{(eff)} \int_s N_D N^{(z_0)} ds$$

- If more than one charge exchange line intensity, with different upper levels, the code can assess the consistency between experimental and theoretical data. ADAS308 casts this onto the consistency of the ADF01 total n-shell capture with observation.
- Most use of ADAS308 has been directed at qef and its components alone.

ADAS308 processing



information from data set

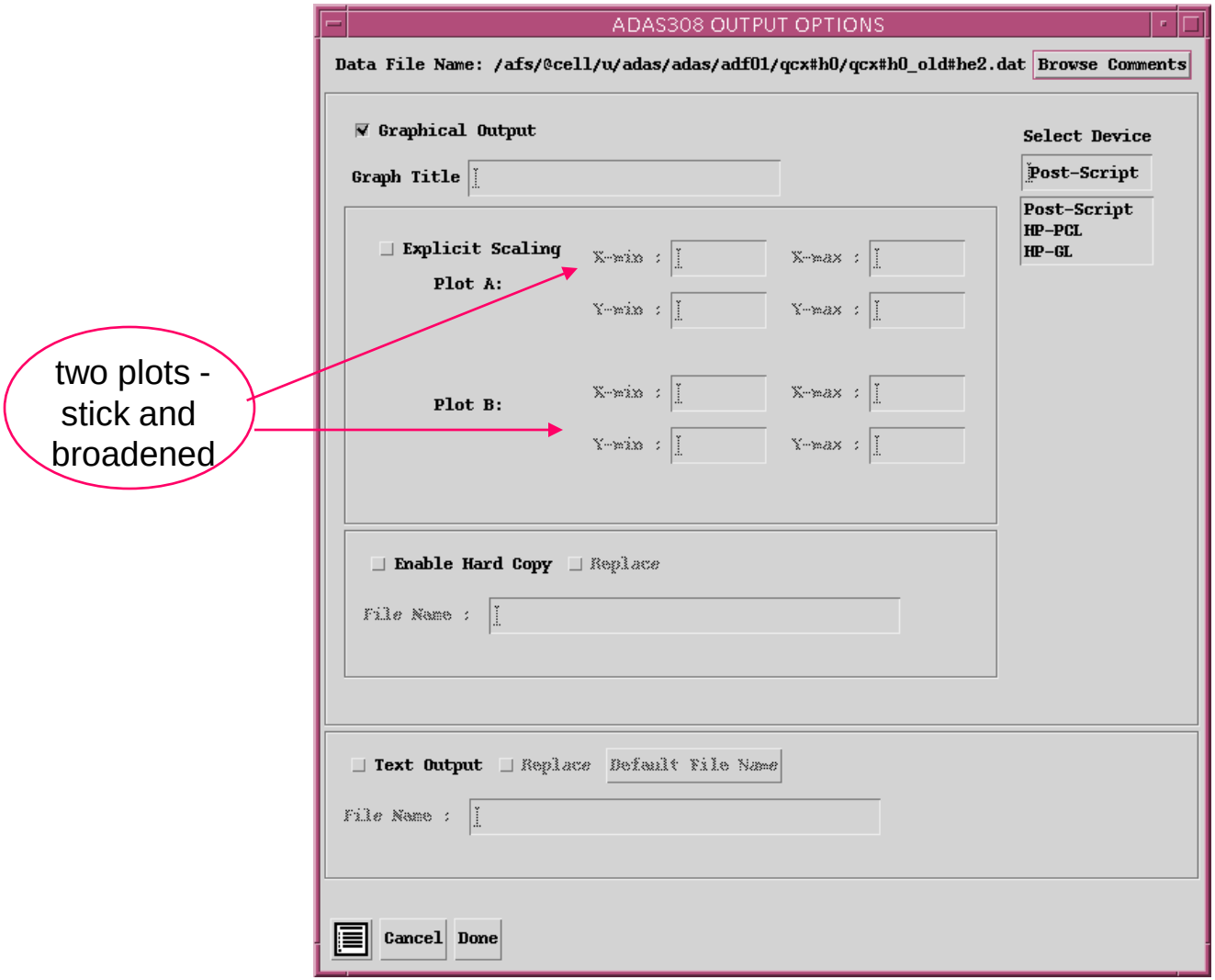
various data required - appropriate is table displayed

key determines tables and graphs

masses required for ion collisions

model choice - usually input data and CX

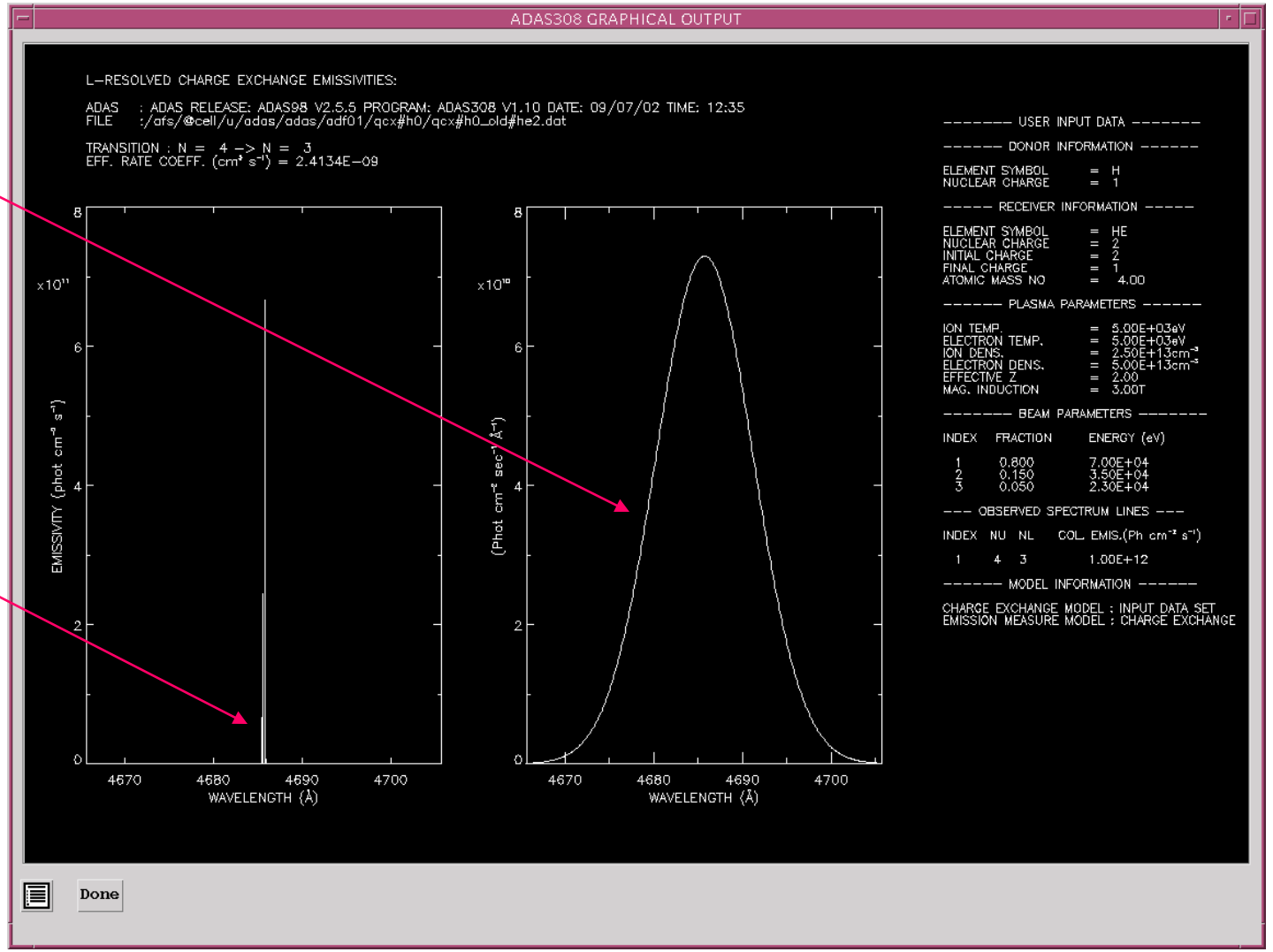
ADAS308 output



ADAS308 graph

doppler broadened n->n' line

exact component wavelengths and relative emissivities



Mass production of CX effective emission coeffts.

- ADAS309 is the mass production code for the effective emission coefficients for charge exchange lines.
- The user input is similar to that for ADAS308 but there is no graphical output, nor does it attempt the inversion solution.
- Many transitions can be entered at the one time. An output file of effective emission coefficients is delivered fully formatted to the ADF12 specification.