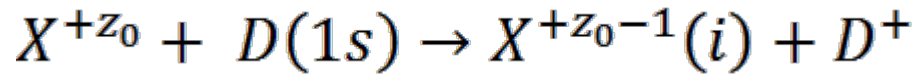


Charge exchange spectroscopy

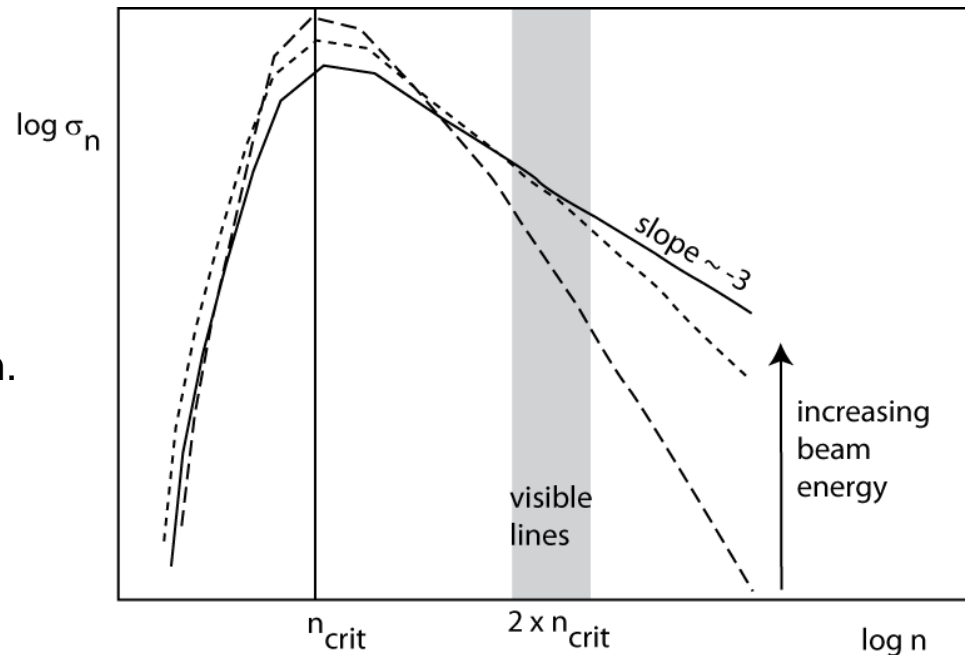
- Preliminaries
- ADAS series 5/series2 - thermal charge transfer
- ADAS series 3 - charge transfer with neutral beams

Preliminaries

- We are concerned with the charge exchange reaction



- 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

Title for Run

Data File Name: /home/hps/adas_central/adas/adf24/scx#h0/scx#h0_cfm#c3.dat

Polynomial Fitting

Fit Polynomial value % :

Select data Block

INDEX	Donor Ion	Recvr Ion	Final State	Type
1	H + 0 (1)	C + 3 (1)	Total	1
1	H + 0 (1)	C + 3 (1)	Total	1
2	H + 0 (1)	C + 3 (1)	2p2	1
3	H + 0 (1)	C + 3 (1)	2p2	1
4	H + 0 (1)	C + 3 (1)	2s3s(1S)	1
5	H + 0 (1)	C + 3 (1)	2s3p(1P)	1

Please enter the reactant mass numbers Donor: Recvr:

Select Energies for output file

Output Collision Energies

INDEX	Output	Input
1	2.840E-02	3.757E-04
2	3.449E-02	6.163E-04
3	4.016E-02	8.683E-04
4	4.490E-02	1.157E-03
5	5.313E-02	2.008E-03

Energy Units: at. un.

Select Temperatures for TCX file

Output Temperatures

INDEX	Output	Input
1	4.000E+01	7.000E-03
2	5.900E+01	1.884E-02
3	8.000E+01	3.740E-02
4	1.000E+02	6.640E-02
5	1.400E+02	2.000E-01

Temperature Units: eV(don.)

Edit the processing options data and press Done to proceed

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

Title for Run

Data File Name: /home/hps/adas_dev/adas/adf04/adas#6/mom97_ls#c3.dat

Nuclear Charge: 6 Ion Charge: 3

INDEX	Electron	Ion	Neutral Hydrogen	Input Value
1	5.000E+02	5.000E+02	5.000E+02	5.000E+02
2	1.000E+03	1.000E+03	1.000E+03	1.000E+03
3	2.000E+03	2.000E+03	2.000E+03	2.000E+03
4	5.000E+03	5.000E+03	5.000E+03	5.000E+03
5	1.000E+04	1.000E+04	1.000E+04	1.000E+04

INDEX	Electron Densities	Ion Densities	NH/NE Ratio	N(Z1)/N(Z)
1	1.000E-03	0.0000	0.0000	0.0000
2	1.000E+00	0.0000	0.0000	0.0000
3	1.000E+03	0.0000	0.0000	0.0000
4	1.000E+06	0.0000	0.0000	0.0000
5	1.000E+09	0.0000	0.0000	0.0000

Temperature Units: Reduced

Density Units: Reduced

<input type="checkbox"/>	1S2 2S1	(2)S(0.5)
<input type="checkbox"/>	1S2 2P1	(2)P(2.5)
<input type="checkbox"/>	1S2 3S1	(2)S(0.5)
<input type="checkbox"/>	1S2 3P1	(2)P(2.5)

<input type="checkbox"/>	Proton Impact Collisions
<input type="checkbox"/>	Scale Proton Impact for Zeff
Enter Z-Effective for Collisions <input type="text"/>	
<input type="checkbox"/>	Ionisation Rates
<input checked="" type="checkbox"/>	Neutral H Charge Exchange
<input type="checkbox"/>	Free Electron Recombination

Activate thermal CX

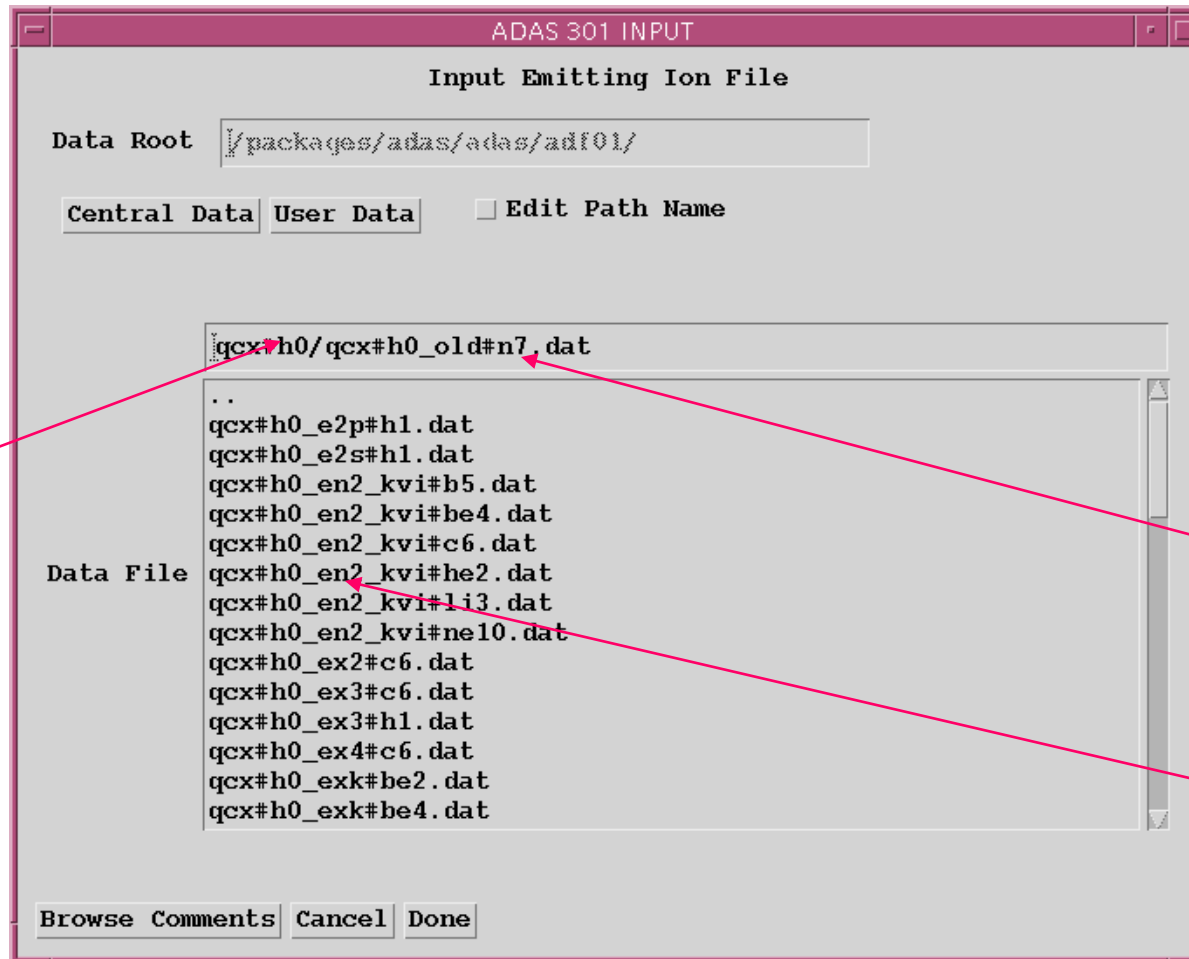
Charge transfer with neutral beams

- 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.

ADAS301 input



Hydrogen donor data

N bare nucleus receiver

excited donors

ADAS302 Processing

ADAS301 PROCESSING OPTIONS

Title for Run

Data File Name:

Polynomial Fitting

Fit Polynomial value % :

Select Velocities/Energies for output file

Select quantum numbers for processing

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:

Principal quantum no. N Range: (4 - 9) Total: [7] [0]

Orbital quantum no. L Range: (0 - N-1) Total: [3] [-1]

Azimuthal quantum no. M Range: (0 - L) Total: [0] [-1]

Data is N and L resolved.

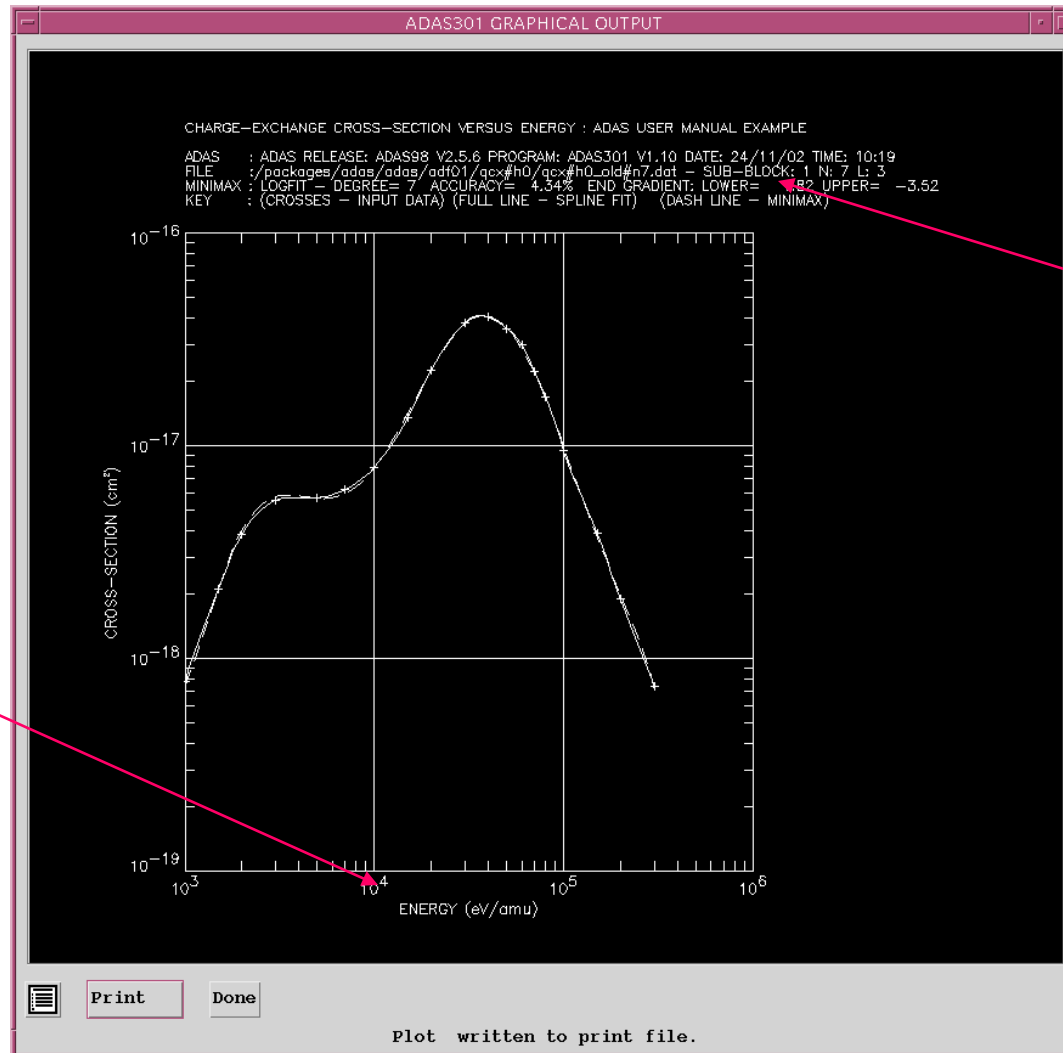
Edit the processing options data and press Done to proceed

Polynomial fit

select partial xsect

Specify energies & units

ADAS301 graph



graph is a
function of
energy

specification
of
extracted
xsect.

Charge exchange effective emission

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

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

Interrogating CXS effective emission coefficients

- Datasets of class ADF12 contain CXS effective emission (q_{ef}) data as a function of beam and plasma parameters.
- These coefficients include the effect of collisional redistribution of n -substate populations of the receiver ion in the plasma.
- The individual components of the $n \rightarrow n'$ 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.

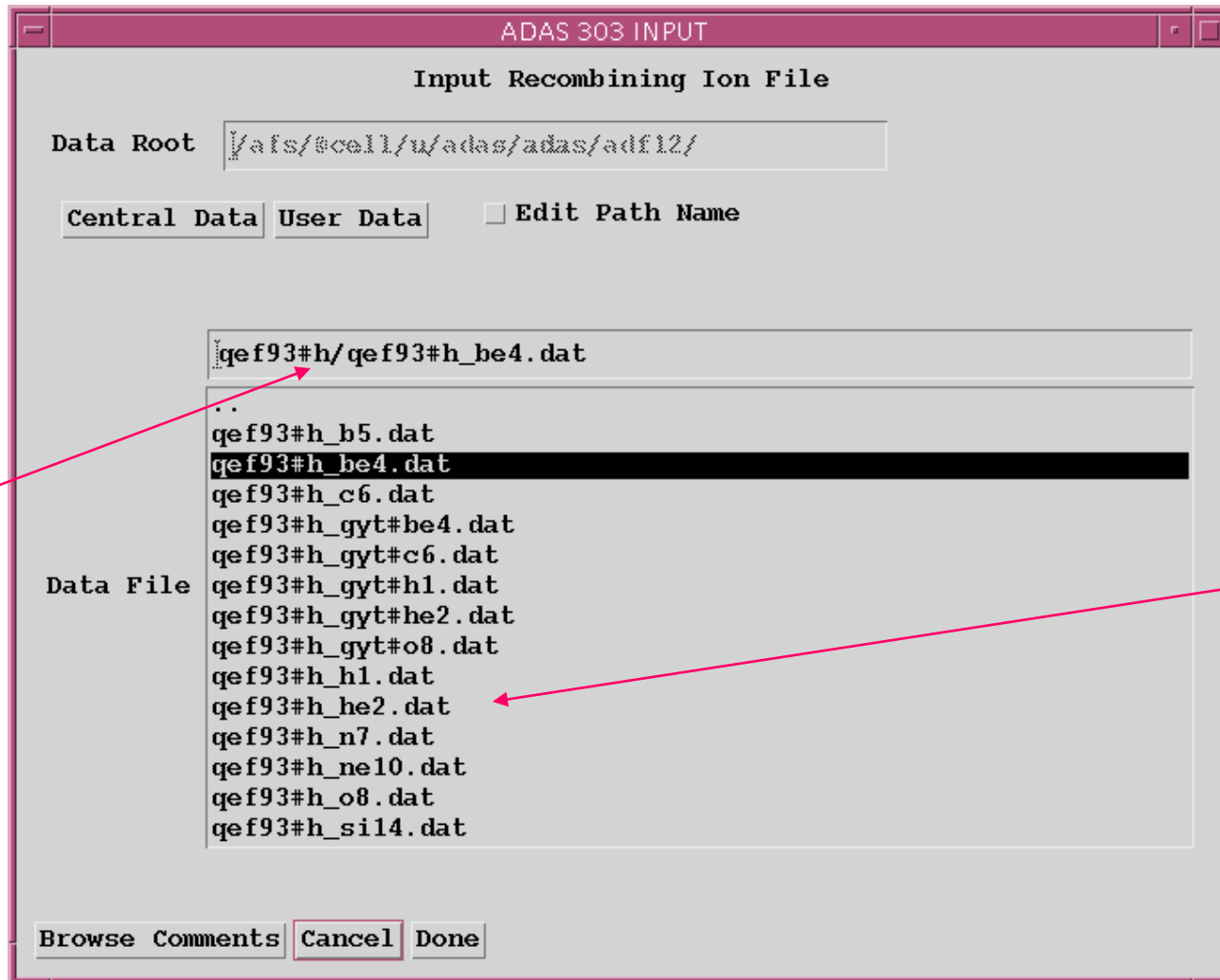
ADF12 charge exchange cross-sections

The diagram illustrates the structure of the ADF12 charge exchange cross-sections table. Red callout boxes identify key components: 'reference rate coefft' points to the first column; 'receiver' points to the second column; 'transition' points to the third column; 'reference parameter values' points to the rightmost columns (ISEL, QEFREF, PARMREF, NPARMSC, ENER, QENER, TIEV, QTIEV, BMAG, QBMAG); '1-D scans from ref.' points to the first six columns; and 'energy scan' points to the last two columns.

reference rate coefft	receiver	transition	reference parameter values							
33	SPSCLMS	ON	HE+2	6-4	H(1S)	DONOR	10/7/90	HE2NEW1(4)	LMS	ISEL=8
6.52D-10	4.00D+04	5.00D+03	2.50D+13	2.00D+00	3.00D+00					QEFREF
	19	12	17	6	1					PARMREF
	1.00D+03	1.50D+03	2.00D+03	3.00D+03	5.50D+03	7.00D+03				NPARMSC
	1.00D+04	1.50D+04	2.00D+04	3.00D+04	4.00D+04	5.00D+04				ENER
	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				
	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 EFFECTIVE COEFFICIENT LIST:										
C	ISEL	TYPE	ION	INFORMATION						
C	----	----	----	-----						
C	8.	CX.EMIS.	HE+ 1	N = 6 - 4	6559.4	10/7/90	J2460			

ADAS303 input



Hydrogen donor data

Bare nucleus receivers

ADAS303 Processing

ADAS303 PROCESSING OPTIONS

Title for Run []

Data File Name: /afs/@cell/u/adas/adas/adf12/qef93#h/qef93#h_be4.dat

Browse Comments

Polynomial Fitting

Fit Polynomial value % : 5

Select data Block

INDEX N - N'	Transition	Donor	Receiver	QCX File Source	Processing Code	Emission Type
3	5-4	H(1S)	BE+4	OLD#BE4	ADAS309	CX
2	4-3	H(1S)	BE+4	OLD#BE4	ADAS309	CX
3	5-4	H(1S)	BE+4	OLD#BE4	ADAS309	CX
4	6-5	H(1S)	BE+4	OLD#BE4	ADAS309	CX
5	7-6	H(1S)	BE+4	OLD#BE4	ADAS309	CX

Neutral Beam Donor Energy Values

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

Energy/Velocity Units: eV/amu

Edit Table

Default Energy/Velocity Values

Select supplementary plasma parameters

	Output Value:	Reference Value:	--- Scan Range --- Minimum Maximum	
Ion Density (cm ⁻³)	2.500E+13	2.500E+13	1.000E+11	1.000E+14
Ion Temperature (eV)	5.000E+03	5.000E+03	1.000E+03	3.000E+04
Z Effective	2.000E+00	2.000E+00	1.000E+00	6.000E+00
B Magnetic (T)	3.000E+00	3.000E+00	3.000E+00	3.000E+00

Cancel Done

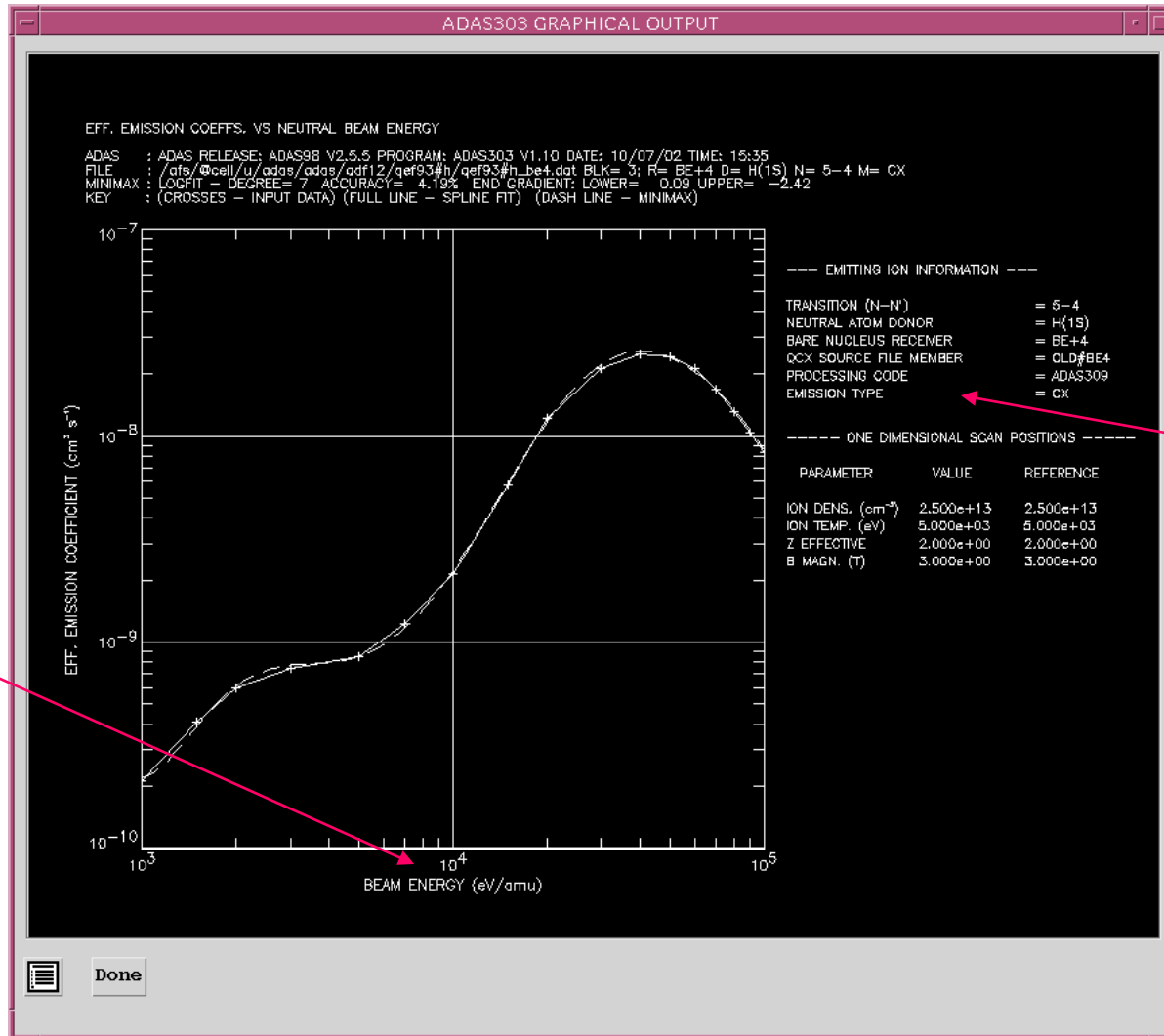
Select transition

Scan range and reference

Specify donor energies

Select plasma conditions

ADAS303 graph



graph is a function of beam energy

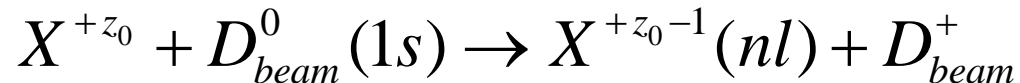
plasma and beam conditions for graph

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



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

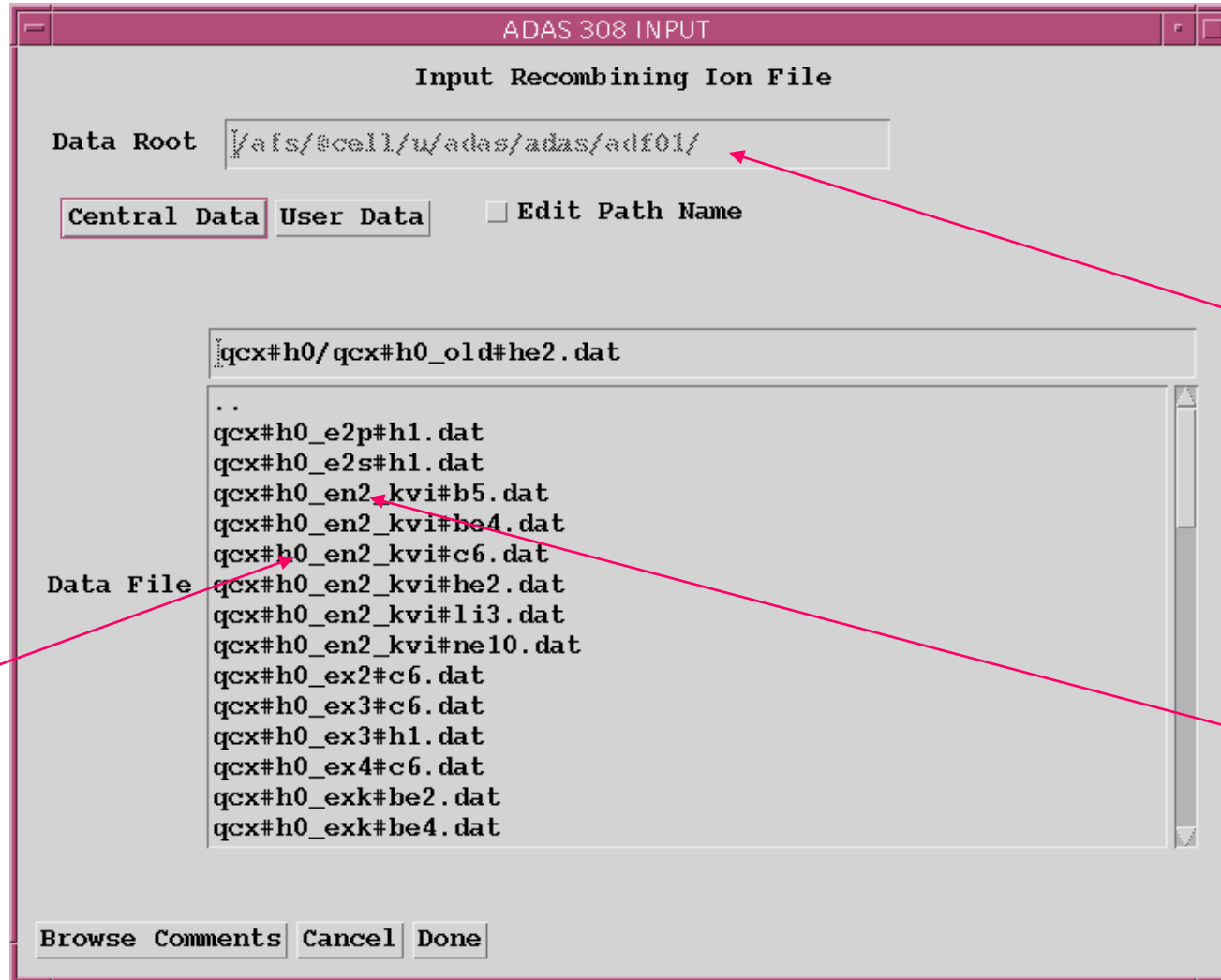
$$q_{n \rightarrow n'}^{(eff)} = \sum_{l, l'} A_{nl \rightarrow n'l'} (N_{nl}^{(z_0-1)} / N_D N^{(z_0)})$$

- 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



hydrogen
beam donor
data

fundamental
state selective
CX x-sects.

excited (n=2)
beam donor
data

Calculating CXS effective emission (contd.)

- ADAS308 is designed to do more than solve for the effective emission coefficients, q_{ef} .
- The program computes the q_{ef} and solves for the emission measure given the line of sight intensity in a charge exchange line as

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

- 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 q_{ef} and its components alone.

ADAS308 processing

ADAS308 PROCESSING OPTIONS

Title for Run []

Data File Name: /afs/@cell/u/adas/adas/adf01/qcx#h0/qcx#h0_old#he2.dat

Receiver			- Neutral donor -	
Nuclear Symbol	Initial charge	Final ion charge	Nuclear Symbol	charge
HE	2	1	H	1

Please input following receiver information:-
Atomic mass number of receiver [4.0]

Input beam and spectrum line information:-
 Beam parameter information
 Observed spectrum lines
 Required emissivity predictions

Input plasma parameter information:-
Ion temp. (eV) : [5.0e+03] Elec temp. (eV) : [5.0e+03]
Ion dens. (cm-3) : [2.5e+13] Elec dens. (cm-3) : [5.0e+13]
Z effective : [2.00] B Magn. (T) : [3.00]

Select charge exchange theory :
Select donor state :
Select emission measure model :
Is rate table printing required?

Required emissivity predictions

INDEX	Upper level N	Lower level N	Key
1	4	3	1
2			
3			
4			

Note: maximum allowed N quantum no. : 20
minimum allowed N quantum no. : 1

Key: 1 = Graphical and tabular output (max. 2)
2 = Tabular output only (max. 5 non-blank entries)
Blank = Summary only

Edit the processing options data and press Done to proceed

information from data set

masses required for ion collisions

various data required - appropriate is table displayed

model choice - usually input data and CX

key determines tables and graphs

ADAS308 output

two plots -
stick and
broadened

ADAS308 OUTPUT OPTIONS

Data File Name: /afs/cell/u/adas/adas/adf01/qcx#h0/qcx#h0_old#he2.dat [Browse Comments](#)

Graphical Output

Graph Title:

Explicit Scaling

Plot A: X-min: X-max:
Y-min: Y-max:

Plot B: X-min: X-max:
Y-min: Y-max:

Select Device

Post-Script


Post-Script
HP-PCL
HP-GL

Enable Hard Copy Replace

File Name:

Text Output Replace

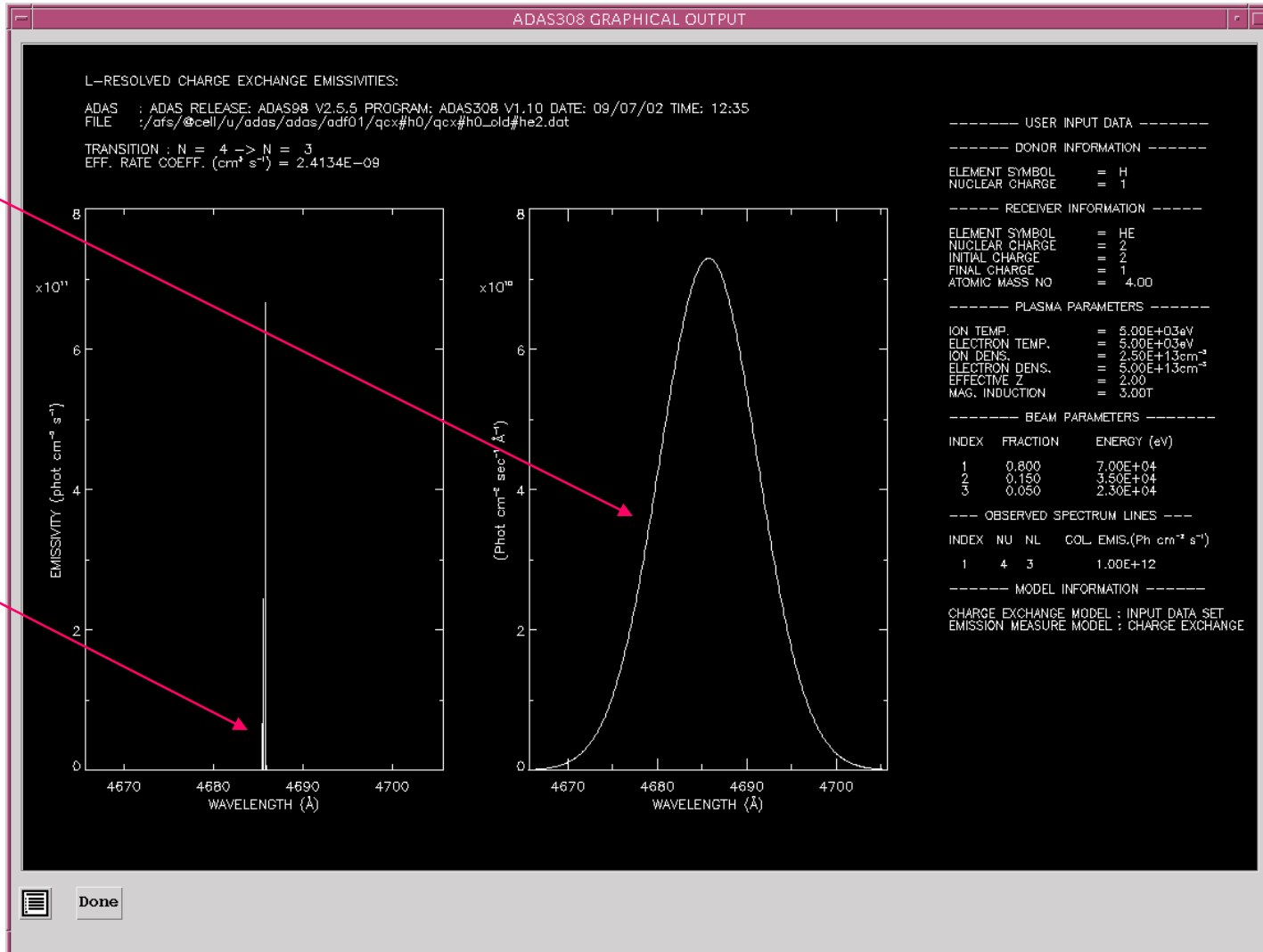
File Name:



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.