

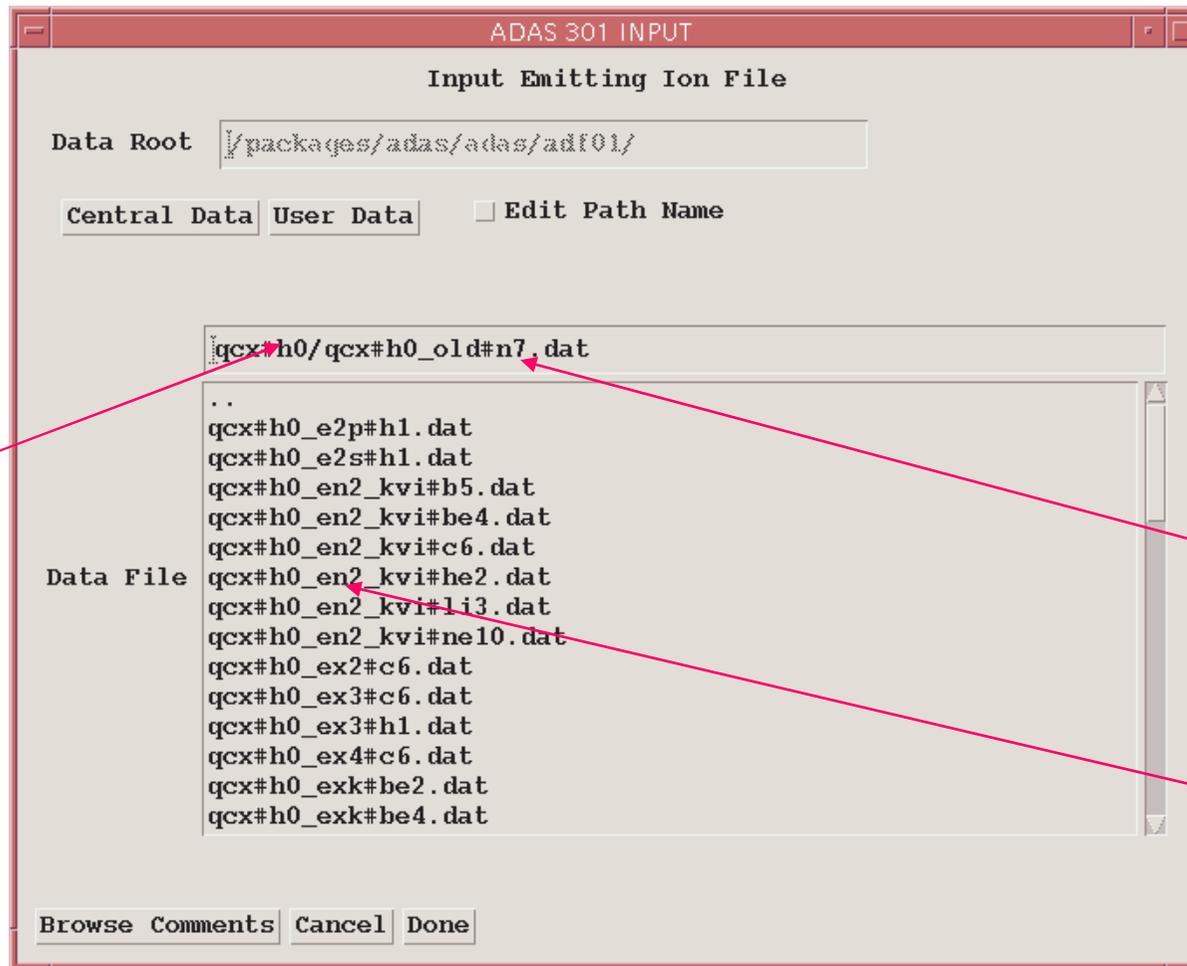
Part I : Charge exchange spectroscopy

- 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: 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

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: eV/amu

Edit Table

Default Velocity/Energy Values

	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

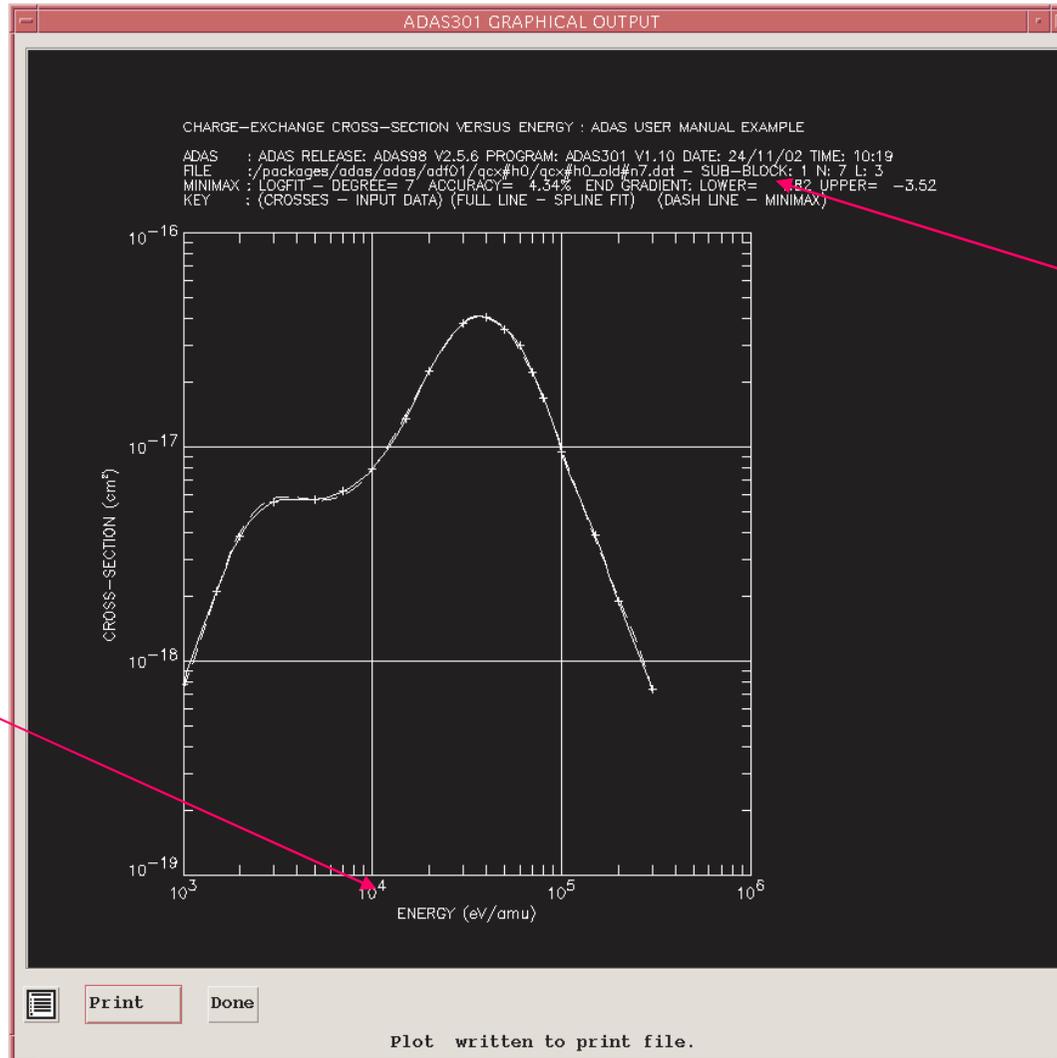
Cancel Done

Polynomial fit

select partial xsect

Specify energies & units

ADAS301 graph



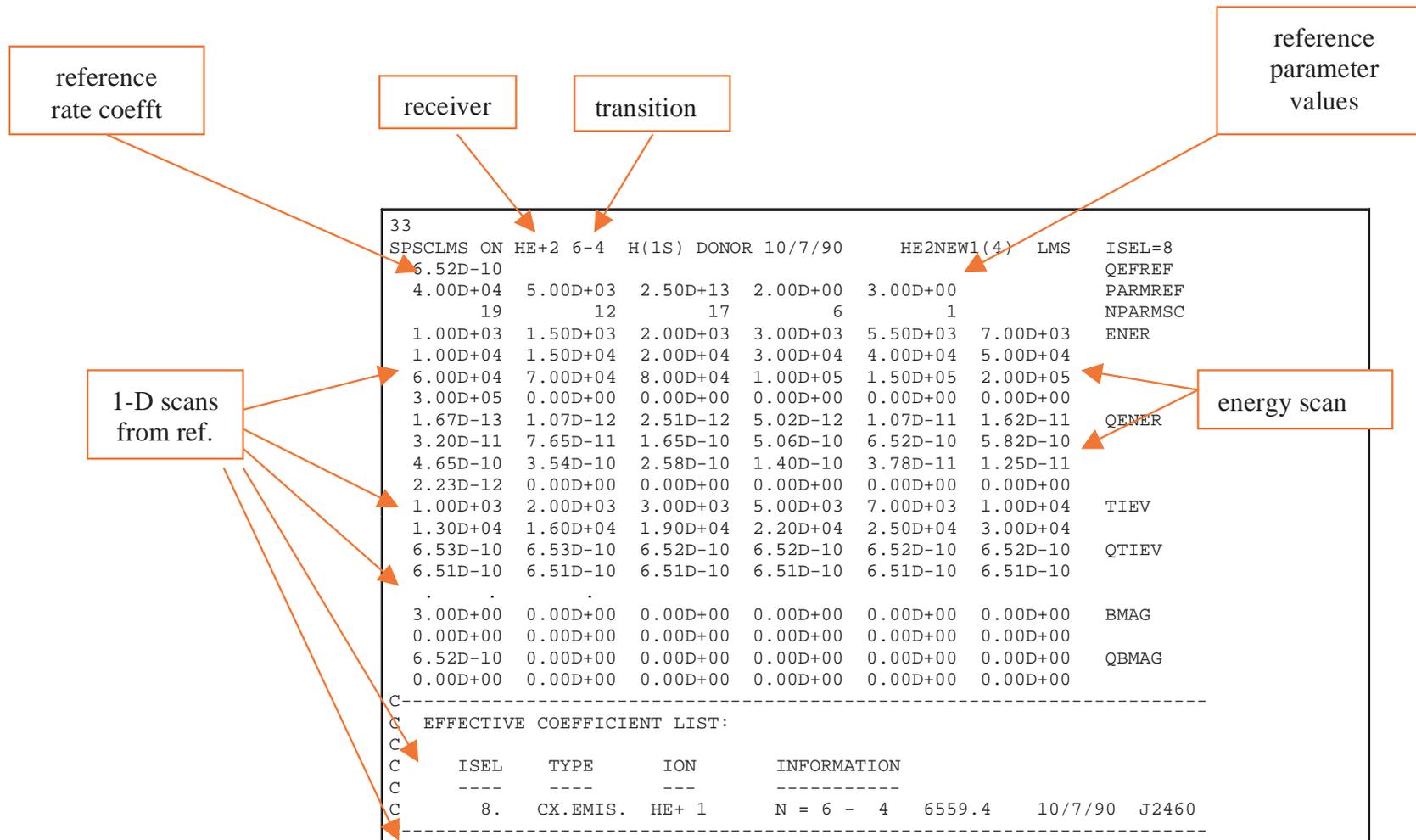
graph is a
function of
energy

specification
of
extracted
xsect.

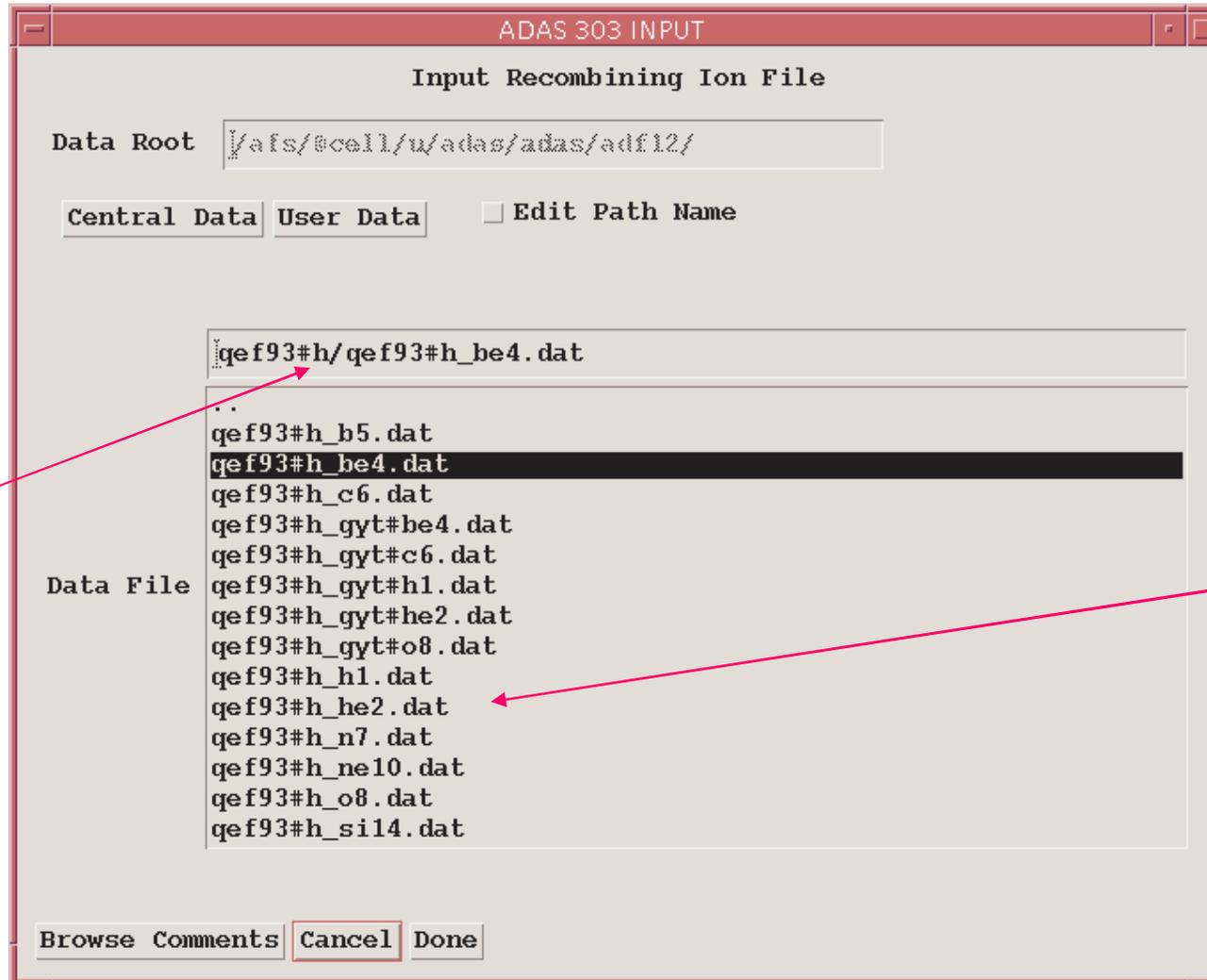
Interrogating CXS effective emission coefficients

- 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



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

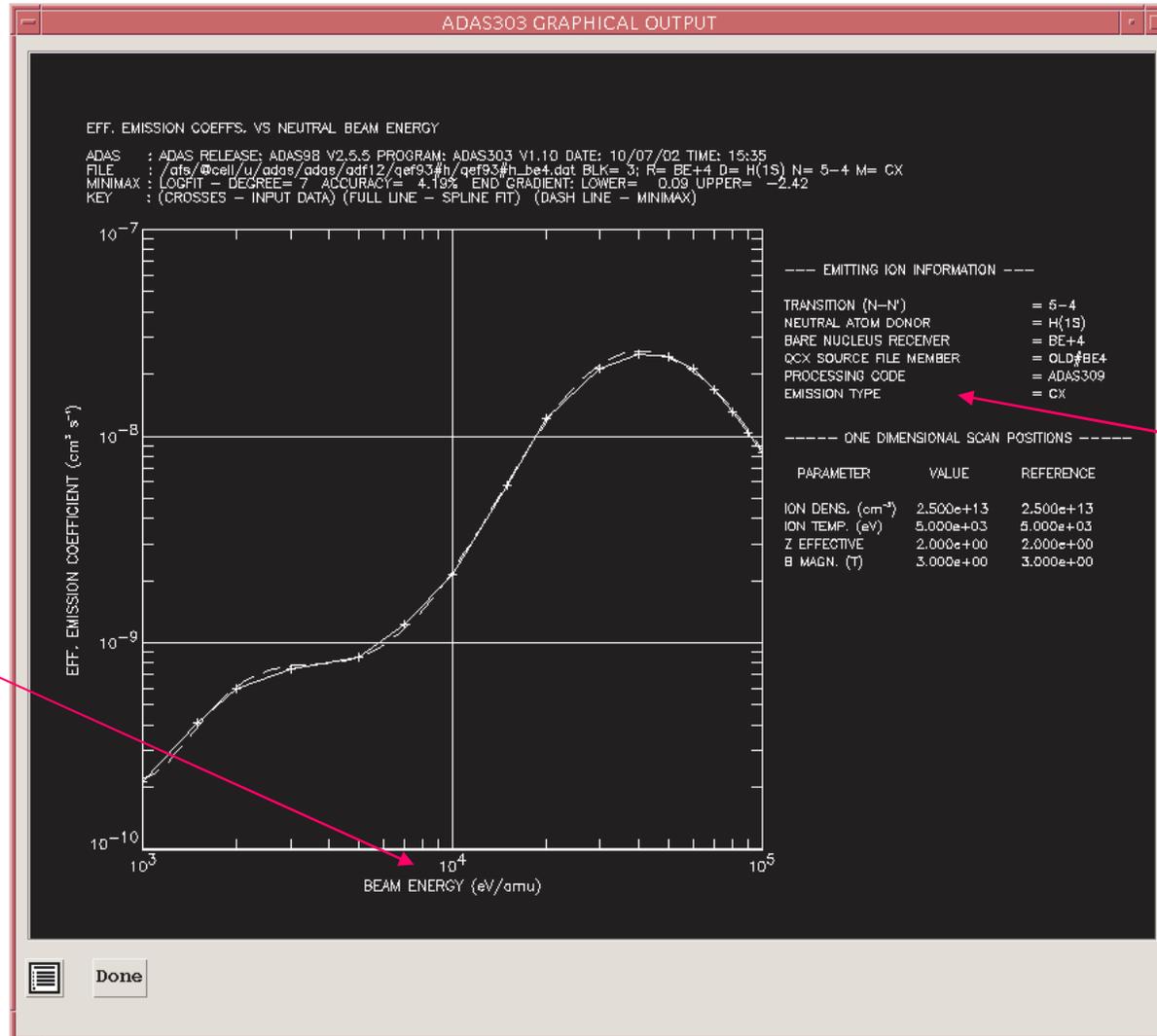
Select transition

Scan range and reference

Specify donor energies

Select plasma conditions

ADAS303 graph



graph is a function of beam energy

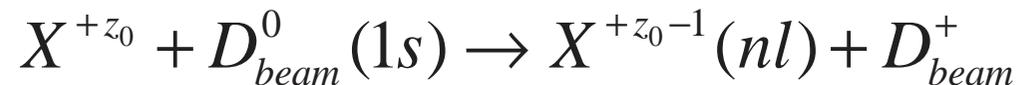
plasma and beam conditions for graph

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

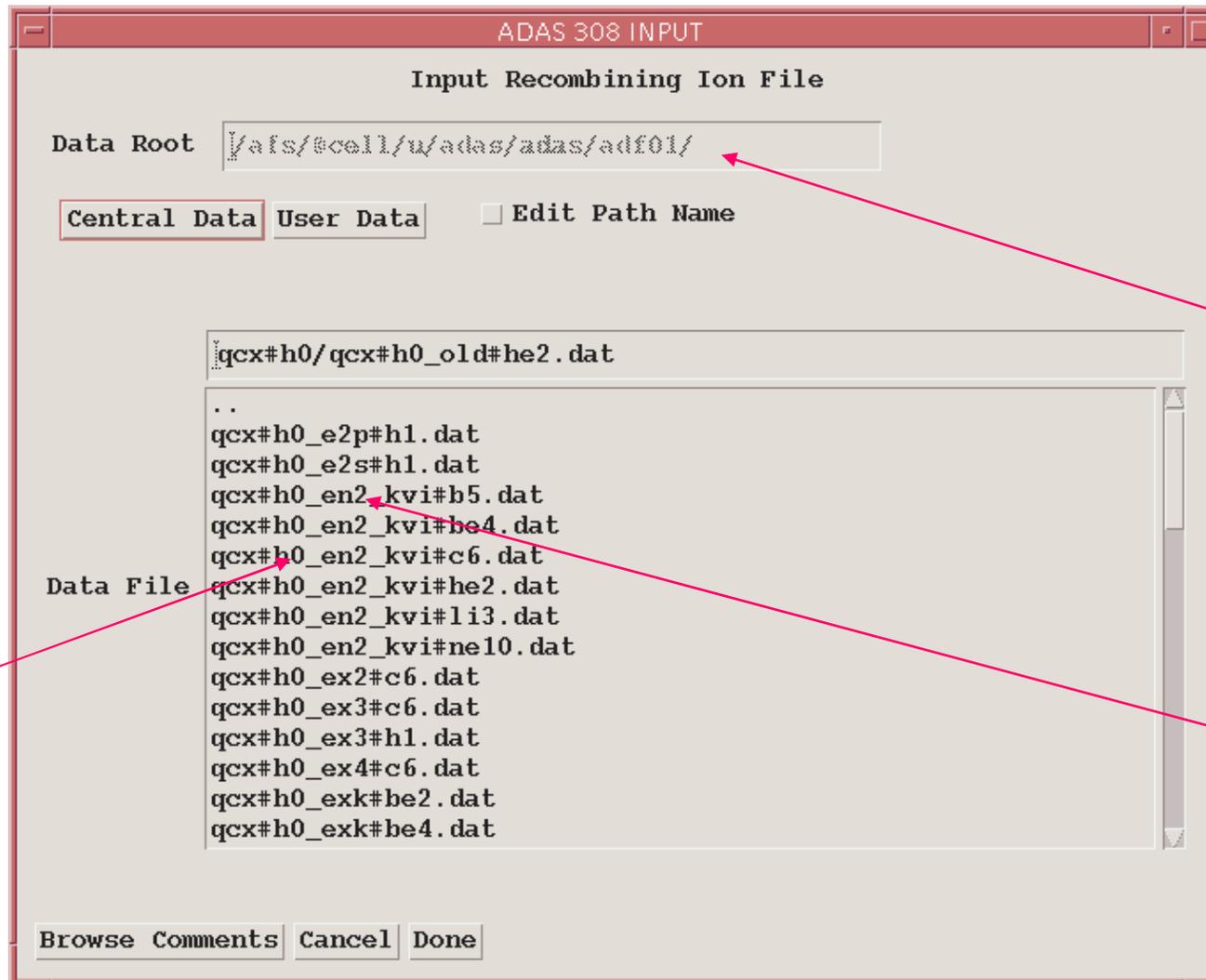
$$q_{n \rightarrow n'}^{(eff)} = \sum_{l, l'} A_{nl \rightarrow n'l'} (N_{nl}^{(z_0-1)} / N_D N^{(z_0)})$$

- 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

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

- 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 [Browse](#) [Comments](#)

Receiver			Neutral donor	
Nuclear Symbol	Initial charge	Final ion charge	Symbol	Nuclear charge
HE	2	2	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 : [Use input data set]
 Select donor state : [H (IS)]
 Select emission measure model : [Charge exchange]

Is rate table printing required? [No]

Required emissivity predictions

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

Edit Table

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

Cancel Done

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 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 :

Enable Hard Copy Replace

File Name :

Text Output Replace [Default File Name](#)

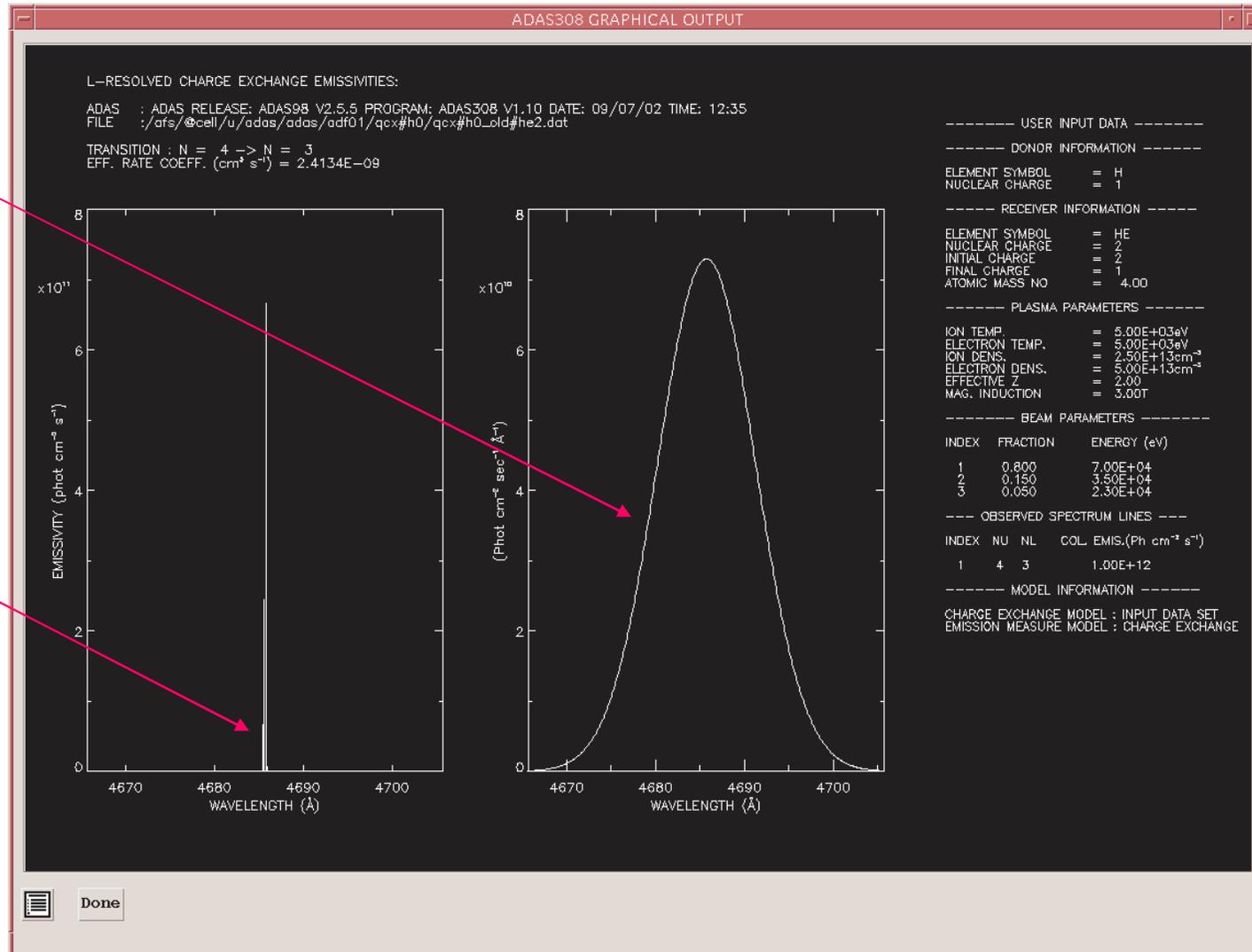
File Name :

 [Cancel](#) [Done](#)

Select Device
[Post-Script](#)
[HP-PCL](#)
[HP-GL](#)

two plots -
stick and
broadened

ADAS308 graph



doppler
broadened
n->n' line

exact
component
wavelengths
and relative
emissivities

Mass production of CX effective emission coeffs.

- 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.

Extension of the CXS capabilities to heavier species

- Motivated by the need to cope with heavier receiver ions beyond argon, which may be partially ionized.
- There are two new codes ADAS315 and ADAS316. ADAS315 works on a scaleable universal dataset of format ADF49 to produce an ADF01 data set.
- ADAS316 is a bundle-n population model. It 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.
- 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 than ADF12.

Part II: Beam stopping and beam emission spectroscopy

- Extracting effective beam stopping coefficients or beam emission coefficients using ADAS304.
- Calculating the beam population structure using ADAS310
- Details of beam emission with `adas305_get_stark.pro`

Interrogating effective beam stopping coefficients

- Datasets of class ADF21 contain effective stopping data as a function of beam and plasma parameters for different plasma species.
- Datasets of class ADF22 contain effective beam emission data as a function of beam and plasma parameters for different plasma species.
- Code ADAS304 interrogates ADF21 or ADF22 data sets to provide coefficients at beam and plasma conditions of your choice.

ADAS304 Input

The image displays the ADAS304 INPUT software interface. The main window, titled "ADAS 304 INPUT", shows the "Input Stopping Ion File Details:-" section. The "Data Root" is set to `/afs/cell1/u/adas/adas/adf21/`. There are three tabs: "Central Data" (selected), "User Data", and "Edit Path Name". The "Group name for input files" is `bms97#h` (usually `bms97#<beam>`). The "Class prefix for input member" is blank (up to 3 characters - Blank=none). The "Stopping Ion List" is `Be4 C6 H1` (maximum of 10). At the bottom, there are buttons for "Browse Comments", "Reselect Ion List", "Cancel", and "Done".

A secondary window, titled "Select Stopping Ions", is open, showing a list of beam species with checkboxes. The list includes: B5, Be4, C6, F9, H1, He2, Li3, N7, Ne10, and O8. Below the list, it says "Make a Maximum of 10 selections" and has "Cancel" and "Done" buttons.

Annotations include a red circle around the "Central Data" tab with the text "sub-library of data for beam species" and an arrow pointing to the "Reselect Ion List" button with the text "click to choose stopping elements".

ADAS304 Processing

ADAS304 PROCESSING OPTIONS

Title for run:

Stopping ion list: Be4 C6 H1

Polynomial Fitting

Fit Polynomial value % :

Select co-ordinate type for output graph:-

Energy

Density

Temperature

Output values:

INDEX	Output Beam Energies (Units : eV)	Input Beam Energies (Units : eV)	Output Electron Densities (Units : cm ⁻³)	Input Elect Densi
1	5.000E+03		6.000E+13	
2	1.000E+04	MIN RANGE	6.000E+13	MIN
3	1.500E+04	-----	6.000E+13	----

Stopping ion fractions:

INDEX	Ion Symbol	Ion Charge	Fraction
1	Be	4	0.100
2	C	6	0.100
3	H	1	0.800
4			

Note: Total fraction should = 1.00 (Otherwise values will be renormalised)

select type of graph display

specify beam and plasma conditions

set fractions for each stopping species

Obtaining effective beam stopping or emission coefficients (contd.)

- The composite stopping for a mixed composition plasma is assembled as

$$N_e S_{CR}^{(A)}(E_B, N_I, T_I) \approx \sum_{i=1}^I N_{e,i} [S_{CR}^{(i,e)}(E_B, N_I, T_I) + (1/z_{0i}) S_{CR}^{(i,z_0)}(E_B, N_I, T_I)]$$

ADAS304 output

ADAS304 OUTPUT OPTIONS

Graphical output

Graph Title _____

Beam energy plot:-

Explicit scaling

X-min: _____ X-max: _____

Y-min: _____ Y-max: _____

Enable Hard Copy Replace

File Name :

Select Device

Post-Script

Post-Script

HP-PCL

HP-GL

Text Output Replace

File Name : _____

beam
energy
plot
selected

ADAS304 graph



Each contribution to stopping and total

specified conditions

Computing effective beam coefficients

- The first step is the calculation of the full collisional-radiative population structure of the hydrogen beam atoms.
- Code ADAS310 performs these calculations in the bundle-n model.
- It executes these repeatedly for the sets of plasma parameters required to construct tables containing the excited population structure and beam stopping.

Computing effective beam coefficients (contd.)

- The full population structures are archived in ADF26 according to (single) impurity.
- Code ADAS312 post-processes the ADF25 files to extract the beam stopping and beam emission coefficients of choice.
- The output is structured according to the ADF21 (beam stopping) and ADF22 (beam emission) specifications.

Computing effective beam coefficients (contd.)

- File selection
 - » Two input files may be selected.
 - » The first, called the expansion file, gives the pathway for storing condensed collisional-radiative matrices.
 - » The second, charge exchange file, is not important for the beam case. ADAS310 can compute hydrogen populations in the plasma (including CX) as well as beams

ADAS310 Input

ADAS 310 INPUT

Please enter beam species details:-

Beam species element symbol : Beam species ion charge :

Expansion File Details:-

Data Root

Central Data User Data Edit Path Name

Data File

-
-

Charge Exchange File Details:-

Data Root

Central Data User Data Edit Path Name

Data File

-
-
-
-

Browse Comments Cancel Done

beam species

expansion file for high n-shell handling

advanced usage not applicable to simple stopping

Computing effective beam coefficients (contd.)

- Processing options
 - » There are many parameters to specify but most are set with defaults.
 - » The main user data are the impurity specifications and the plasma parameter scans.
 - » ADAS310 can work with mixed impurities but main tabulations are for single impurities which are linearly combined for mixtures at the spectral analysis stage

ADAS310 Processing

ADAS310 PROCESSING OPTIONS

Select which parameters to display : General Switches (I) Switches(II)

Please enter the following parameters:-

Radiation field temperature (eV) : [Blank for default]

General radiation field dilution : [Blank for default]

Multiplier for ionisation cross-sections : [Blank for default]

Multiplier for Regemorter cross-sections : [Blank for default]

Ionising radiation field dilution : [Blank for default]

Beam species isotope mass : [Blank for default]

Select table for display:-

Impurity information

Representative N-shells

Enter limits on N-shells:

Minimum N-shell:

Maximum N-shell:

Note:
The first representative N-shell is set equal to the minimum N-shell

INDEX	N Shell
1	1
2	2
3	3

Edit Table

Clear Table

Select table for display:-

Electron/proton density scan

Electron/proton temperature scan

Beam energy scan

Electron/proton densities (units: cm⁻³)

INDEX	Electron density	Proton density
1	5.000E+12	5.000E+12
2	7.000E+12	7.000E+12

Edit Table

Clear Table

Enter index of reference densities :

Cancel Done

three sets of switches - defaults are set

general parameters controlling x-sect. use

specify details of bundle-n model for hydrogen

specify scans in key parameters

note use of reference conditions

ADAS310 Processing (contd.)

third
switch
set

ADAS310 PROCESSING OPTIONS

Select which parameters to display : General Switches (I) Switches(II)

Please enter the following parameter switches:-

Activate ion impact cross-sections : YES

Delta N range for ion impact cross-sections : 2

Use Lodge ion impact cross-sections : YES [NO defaults to Vainshtein X-sections]

Use beam energy in forming ion cross-sections : YES

Select table for display:-

Impurity information

Representative N-shells

Select mode of operation: Multiple impurities

Multiple impurities (total fraction must be <= 1.0)

INDEX	Symbol	Atomic Mass no.	Fraction
1			
2			
3			

Edit Table

Select table for display:-

Electron/proton density scan

Electron/proton temperature scan

Beam energy scan

Electron/proton densities (units: cm-3)

INDEX	Electron density	Proton density
1	5.000E+12	5.000E+12
2	7.000E+12	7.000E+12

Edit Table

Clear Table

Enter index of reference densities : 8

Cancel Done

Computing effective beam coefficients (contd.)

- Output options
 - » There is no graphical display from ADAS310.
 - » Several pass files are created
 - » The fourth passing file is the population structure (ADF26)
 - » Execution time is longer than most interactive codes.

ADAS310 Output

extended
set of
passing
files for
post-
processing

ADAS310 OUTPUT OPTIONS

Title for run: |

Run Summary Output Replace

File Name : | paper.txt

First Passing File Replace

File Name : |

Second Passing File Replace

File Name : |

Third Passing File Replace

File Name : |

Fourth Passing File Replace

File Name : |

Cancel Run Now

Beam emission and the Balmer alpha Stark multiplet structure

- The calculation of local Stark/Zeeman emission feature from H (D/T) beams is accessed via an IDL procedure call *adas305_get_stark.pro* or within FORTRAN by calling the *stark.for* routine in the adas3xx library.
- The beam, plasma, E and B fields and observation orientation must be specified. General geometry specification is defined by direction cosines. The polarisation can be specified by multipliers on the π and σ components.
- The feature is returned as either a collection of component wavelengths and emissivities or a Doppler broadened feature over a specified wavelength range (specify minimum and maximum wavelengths and number of pixels).

adas305_get_stark.pro

```
PRO stark_fig

beam   = {mass : 2.0, energy : 40.0e3, te : 10.0, density : 4.27e9, $
          dc_x : 0.0, dc_y : 0.0, dc_z : 1.0}
plasma = {mass : 2.0, te : 8e3, density : 5.0e13, zeff : 2.0}
bfield = {value : 3.3915, dc_x : 0.788, dc_y : 0.0053, dc_z : 0.6152}
efield = {value : 0.0000, dc_x : 1.000, dc_y : 0.0000, dc_z : 0.0000}
obs     = {dc_x : 0.8701, dc_y : -0.047, dc_z : 0.4905, sigma : 0.00, pi : 1.0}

wave_min = 6510
wave_max = 6550
npix     = 500

adas305_get_stark, beam           = beam,           $
                    plasma        = plasma,        $$$
                    bfield        = bfield,        $$$
                    efield        = efield,        $$$
                    obs            = obs,           $$$
                    n_lower       = 2,             $$$
                    n_upper       = 3,             $$$
                    wave_comp      = wave_comp,     $$$
                    emiss_comp    = emiss_comp,    $$$
                    wave_min      = wave_min,     $$$
                    wave_max      = wave_max,     $$$
                    npix          = npix,         $$$
                    emiss_doppler = demiss , /doppler ; , /nocheck

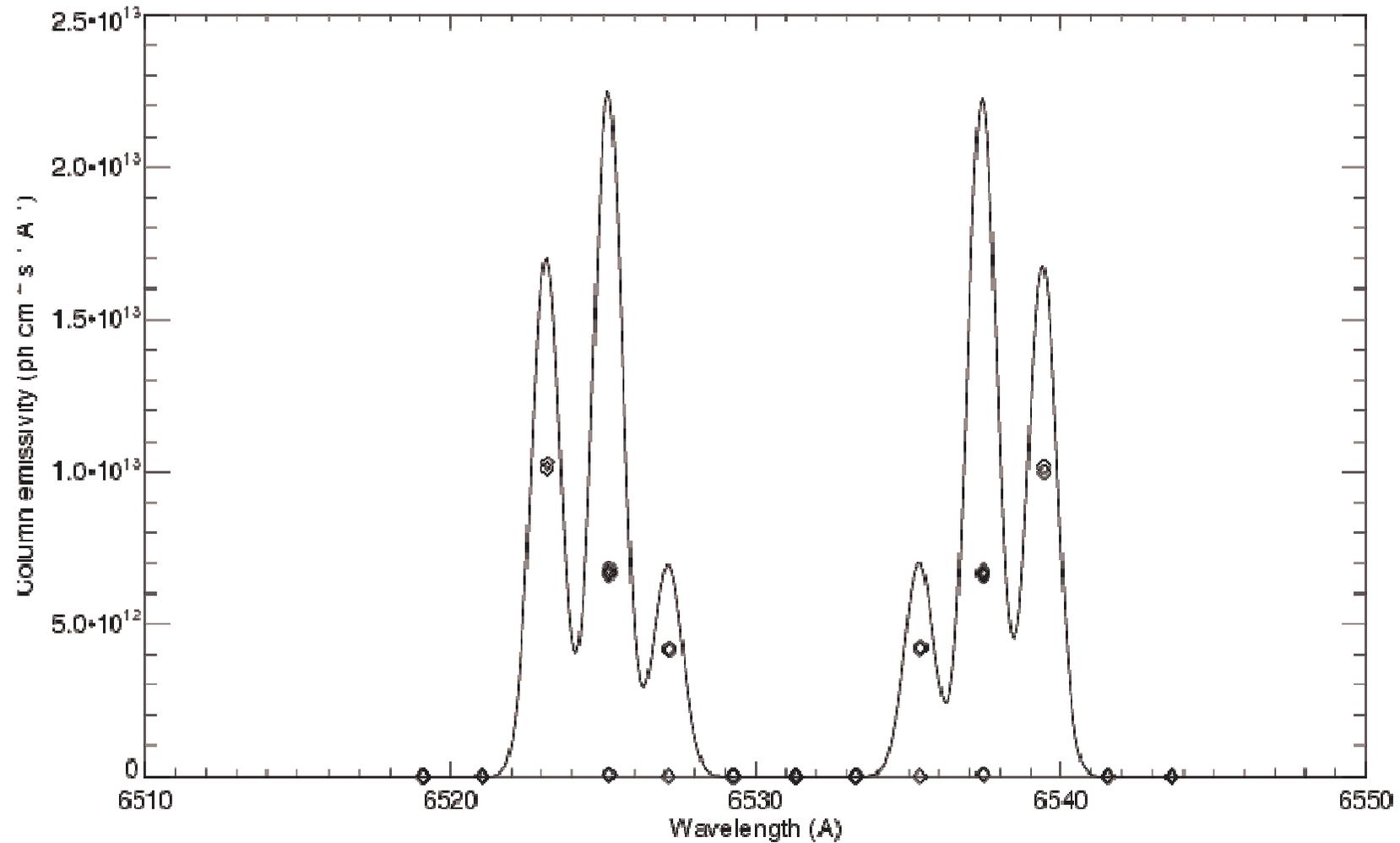
wave = adas_vector(low=wave_min,high=wave_max,num=npix, /linear)
dwave = wave[1]-wave[0]

plot, wave, demiss/dwave, $
      xtitle = 'Wavelength (A)', $
      ytitle = 'Column emissivity (ph cm!u-2!n s!u-1!n A!u-1!n)'

plots, wave_comp, emiss_comp, psym=4[

END
```

Balmer alpha Stark multiplet



Feature variation

B: 1.4T – 50 T

E: 0.5Mev/amu – 100eV/amu

