

ADAS303: Effective charge exchange spectroscopy emission data - graph and fit coefficient

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.

Background theory:

Data from files of type ADF12 contain charge exchange effective emission coefficients for principal quantum shell transitions of hydrogen-like impurity ions, $q_{n \rightarrow n'}^{(eff)}$, 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 $q_{n \rightarrow n'}^{(eff)}$ 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 $q_{n \rightarrow n'}^{(eff)}$ sets at the following parameter sets:

$$\{E_{u,i} : i = 1, I_E\}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, zeff^{(ref)}, B^{(ref)} \quad \text{with}$$

$$E_u^{(ref)} \in \{E_{u,i} : i = 1, I_E\},$$

$$E_u^{(zeff)}, \{N_{zeff} : i = 1, I_N\}, T_{zeff}^{(ref)}, zeff^{(ref)}, B^{(ref)} \quad \text{with}$$

$$N_{zeff}^{(ref)} \in \{N_{zeff} : i = 1, I_N\},$$

$$E_u^{(ref)}, N_{zeff}^{(ref)}, \{T_{zeff,i} : i = 1, I_T\}, zeff^{(ref)}, B^{(ref)} \quad \text{with}$$

$$T_{zeff}^{(ref)} \in \{T_{zeff,i} : i = 1, I_T\},$$

$$E_u^{(ref)}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, \{zeff_i : i = 1, I_{zeff}\}, B^{(ref)} \quad \text{with}$$

$$zeff^{(ref)} \in \{zeff_i : i = 1, I_{zeff}\},$$

$$E_u^{(ref)}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, zeff^{(ref)}, \{B_i : i = 1, I_B\} \quad \text{with } B^{(ref)} \in \{B_i : i = 1, I_B\}.$$

The code uses cubic spline interpolation to obtain the $q_{n \rightarrow n'}^{(eff)}$ at specified N_{zeff} , T_{zeff} , $zeff$ and B_{mag} for the set $\{E_{u,i} : i = 1, I_E\}$. Finally, cubic spline interpolation is performed in energy to provide the effective emission coefficients at set of energies of the user's choice. These data are also fitted with a minimax polynomial.

The interactive code provides basic interrogation and display of mono-energetic effective emission coefficients only. However, in general application, it is the emission coefficients for a receiving plasma ion of thermal distribution function in collision with a monoenergetic beam atom which is required. The interrogation code has at its core a subroutine which both extracts mono-energetic effective emission coefficients and forms first integrals over the equivalent cross-sections. This routine is available in the ADAS subroutine library for use in applications. For completeness the detail of the averaging over the receiver ion velocity distribution function is below.

For particles of masses m_1 and m_2 with speeds v_1 and v_2 , since the collision cross-section depends only on the relative velocity of the collision partners, it is convenient to orientate the direction of the first particle (the beam particle) along the z-axis and

measure the direction of the second particle (the thermal particle) relative to this. Since $v_{rel} = \sqrt{v_1^2 + v_2^2 - 2v_1v_2 \cos \theta_{12}}$, the integral over the angle θ_{12} is performed first as

$$q_{rel}(v_1, v_2) = \int_0^\pi |v_{rel}| Q(|v_{rel}|) \sin \theta_{12} d\theta_{12} \quad 4.3.1$$

$$= \frac{1}{v_1 v_2} \int_{|v_1-v_2|}^{v_1+v_2} |v_{rel}|^2 Q(|v_{rel}|) dv_{rel}$$

followed by the integral over the speed of the second particle v_2 as

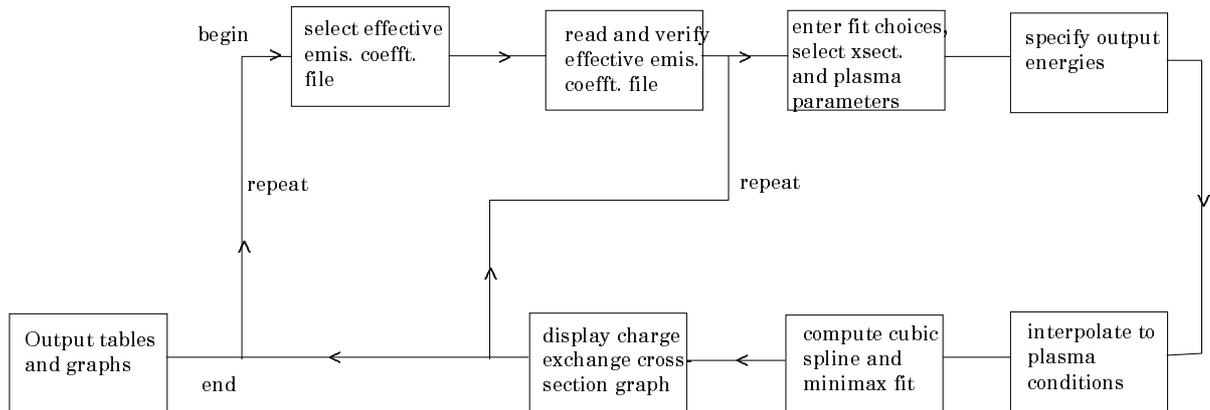
$$q(v_1, T_2) = 2\pi \left(\frac{m_2}{2\pi k T_2} \right)^{3/2} \int_0^\infty v_2^2 e^{-\frac{1}{2} m_2 v_2^2 / k T_2} q_{rel}(v_1, v_2) dv_2 \quad 4.3.2$$

where T_2 is the thermal temperature of the second particle. This integral is relevant to beam plasma reactions and is used extensively in the ADAS3 series codes. Other angular weighted integrals are important for emission line profiles in charge exchange spectroscopy.

Program steps:

These are summarised in figure 4.3.

Figure 4.3



Interactive parameter comments:

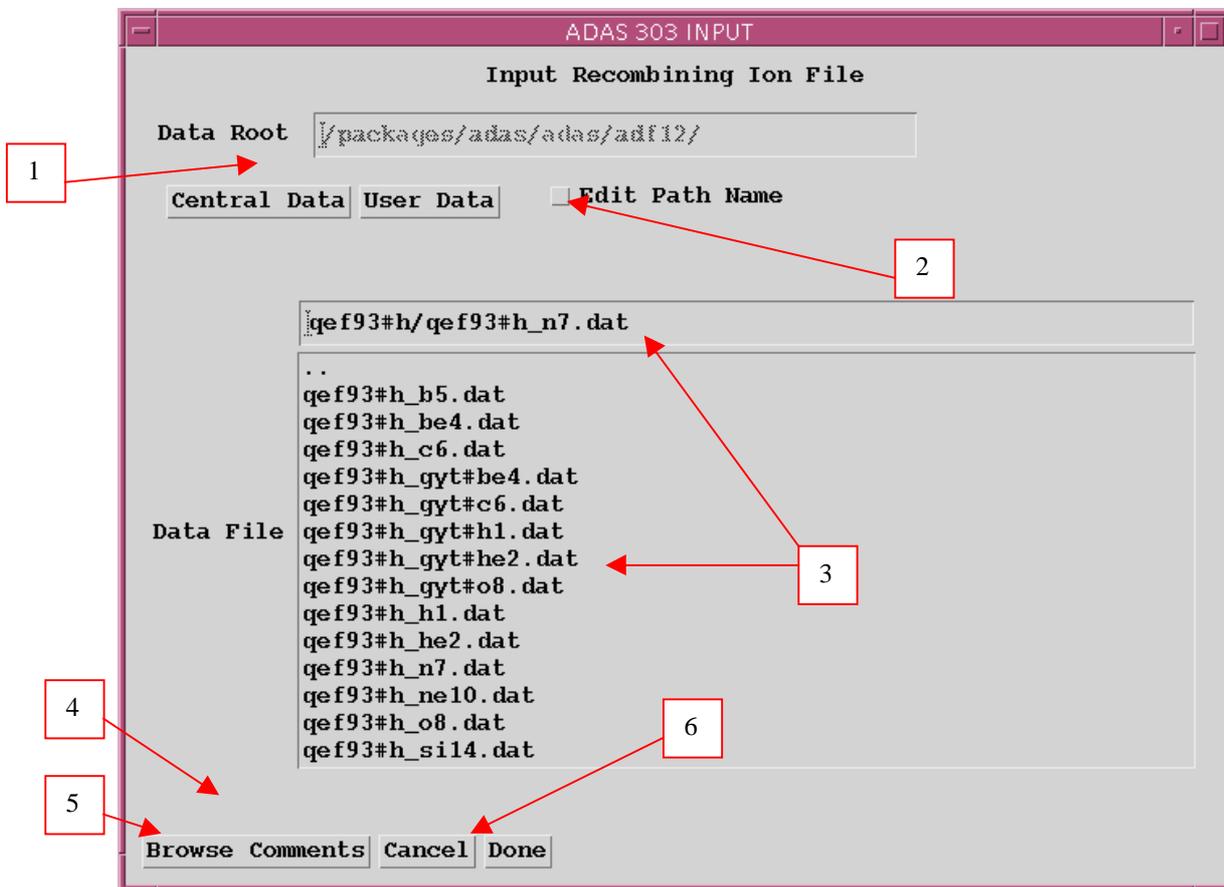
Most ADAS interactive routines have three tasks, namely, file selection, user data processing and output. This is achieved in three sequential windows.

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*.

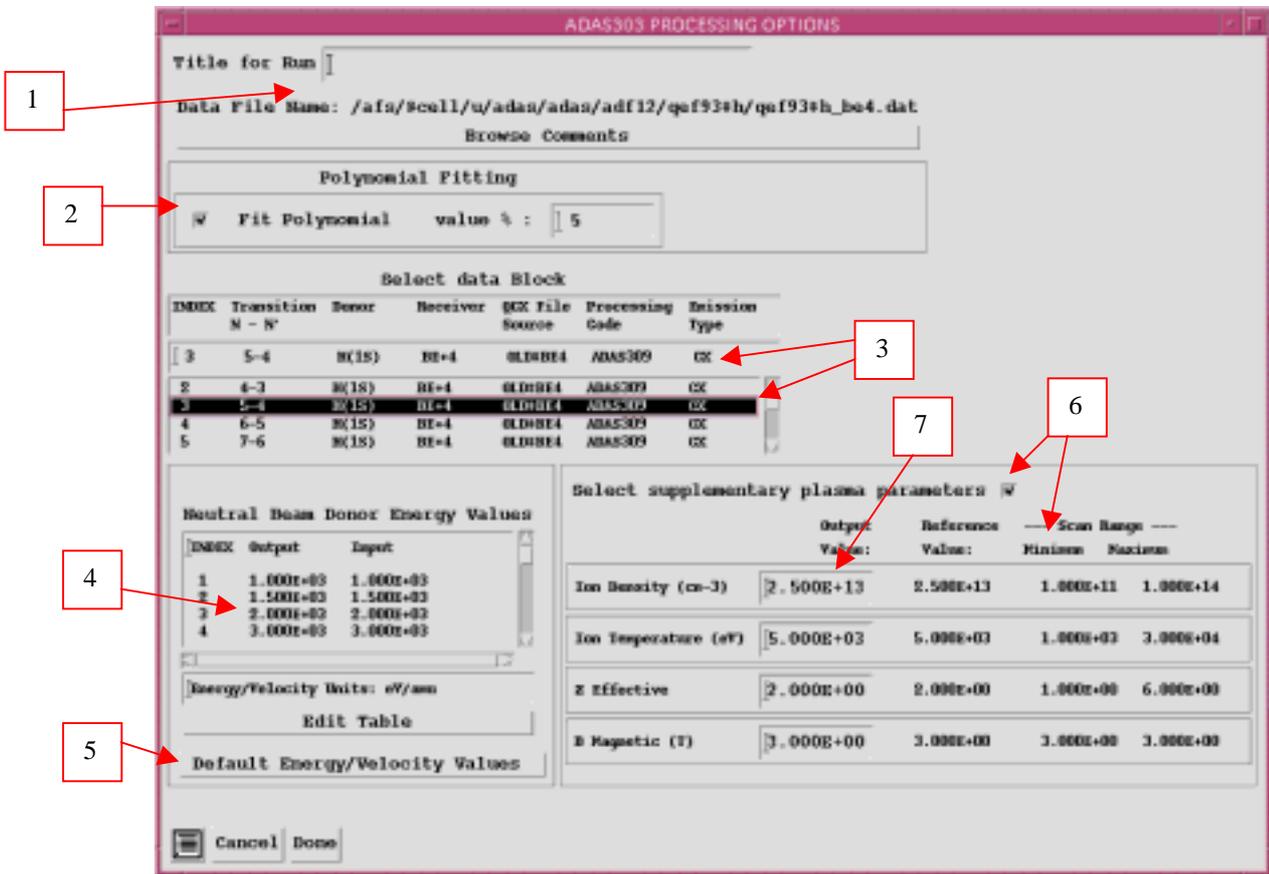
4. Once a data file is selected, the set of buttons at the bottom of the main window become active.
5. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility 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:

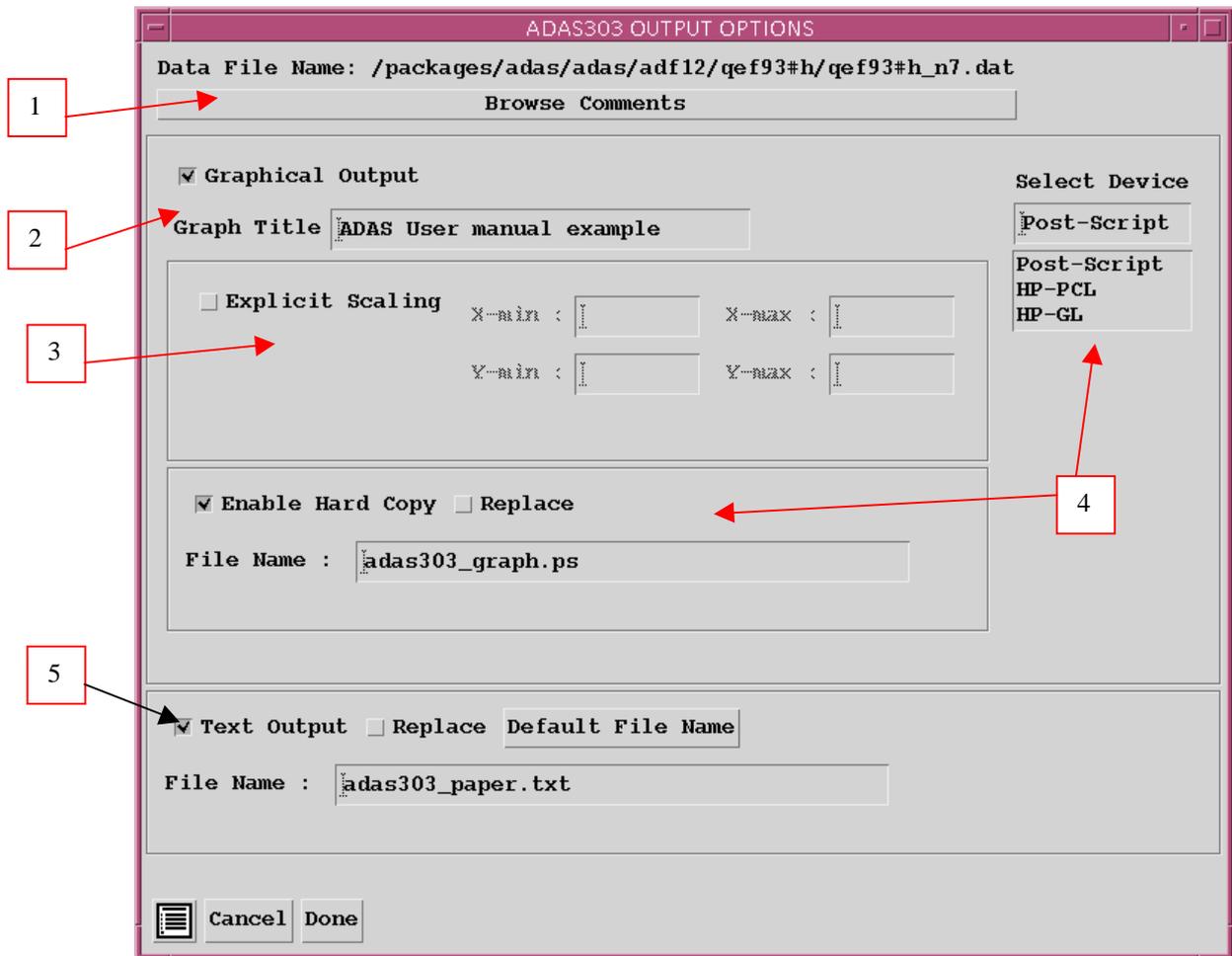
1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
2. The output data extracted 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.

- 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.



- 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).
- 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
- 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.
- 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.

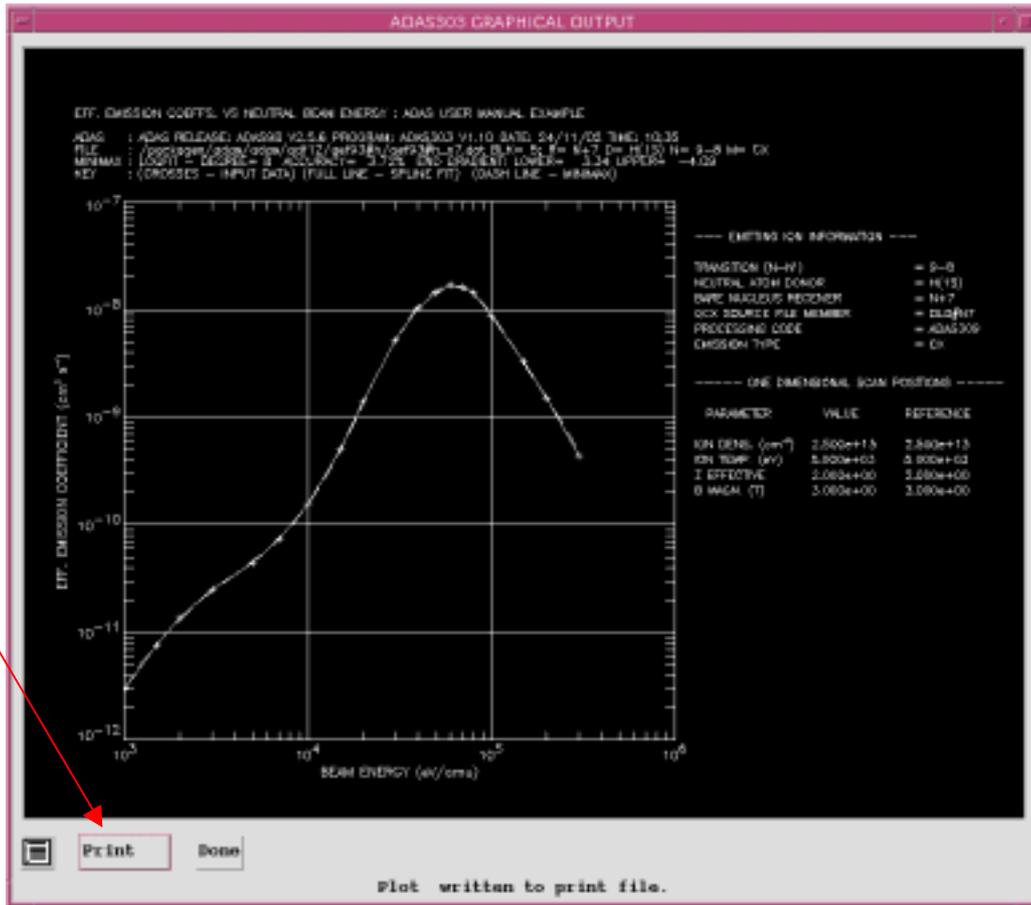
The **output options window** is shown below



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 exists 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.
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*. 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.



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Illustration:

Figure 4.3

EFF. EMISSION COEFFS. VS NEUTRAL BEAM ENERGY : ADAS USER MANUAL EXAMPLE

ADAS : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS303 V1.10 DATE: 24/11/02 TIME: 10:35
 FILE : /pockages/adass/adass/old12/gef93#h/gef93#h_n7.dot BLK= 5: R= N+7 D= H(1S) N= 9-8 M= CX
 MINIMAX : LOOFIT - DEGREE= 8 ACCURACY= 3.72% END GRADIENT: LOWER= 3.34 UPPER= -4.09
 KEY : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT) (DASH LINE - MINIMAX)

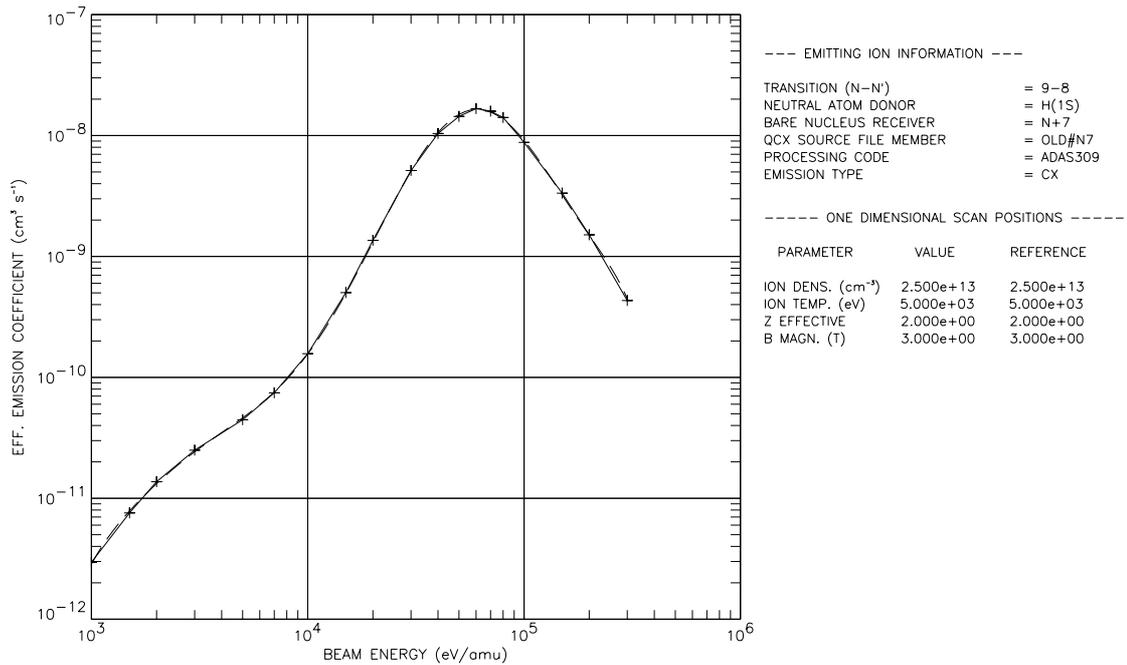


Table 4.3

ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS303 V1.10 DATE: 24/11/02 TIME: 10:35
 ***** TABULAR OUTPUT FROM EFF. EMISSION COEFFTS. INTERROGATION PROGRAM: ADAS303 - DATE: 24/11/02 *****

----- ADAS User manual example -----
 EFFECTIVE EMISSION COEFFICIENTS AS A FUNCTION OF NEUTRAL BEAM ENERGY

 DATA GENERATED USING PROGRAM: ADAS303

/packages/adas/adas/adf12/qef93#h/q - DATA-BLOCK: 5
 EMITTING ION INFORMATION:

 TRANSITION (N-N') = 9-8
 NEUTRAL ATOM DONOR = H(1S)
 BARE NUCLEUS RECEIVER = N+7
 QCX SOURCE FILE MEMBER = OLD#N7
 PROCESSING CODE = ADAS309
 EMISSION TYPE = CX

ONE DIMENSIONAL SCAN POSITIONS:

PARAMETER	INTERPOLATED VALUES	REFERENCE VALUES
ION DENSITY (cm-3)	= 2.500D+13	2.500D+13
ION TEMPERATURE (eV)	= 5.000D+03	5.000D+03
Z-EFFECTIVE	= 2.000D+00	2.000D+00
MAGNETIC FIELD (T)	= 3.000D+00	3.000D+00

----- BEAM ENERGY -----			EFFECTIVE
EV/AMU	AT. V0	CM/SEC	EMIS. COEF. (CM3/SEC)
1.000D+03	2.001D-01	4.377D+07	2.960D-12
1.500D+03	2.450D-01	5.361D+07	7.570D-12
2.000D+03	2.829D-01	6.190D+07	1.370D-11
3.000D+03	3.465D-01	7.581D+07	2.500D-11
5.000D+03	4.474D-01	9.787D+07	4.460D-11
7.000D+03	5.293D-01	1.158D+08	7.450D-11
1.000D+04	6.327D-01	1.384D+08	1.570D-10
1.500D+04	7.749D-01	1.695D+08	5.020D-10
2.000D+04	8.947D-01	1.957D+08	1.360D-09
3.000D+04	1.096D+00	2.397D+08	5.140D-09
4.000D+04	1.265D+00	2.768D+08	1.040D-08
5.000D+04	1.415D+00	3.095D+08	1.440D-08
6.000D+04	1.550D+00	3.390D+08	1.670D-08
7.000D+04	1.674D+00	3.662D+08	1.590D-08
8.000D+04	1.789D+00	3.915D+08	1.410D-08
1.000D+05	2.001D+00	4.377D+08	8.780D-09
1.500D+05	2.450D+00	5.361D+08	3.340D-09
2.000D+05	2.829D+00	6.190D+08	1.510D-09
3.000D+05	3.465D+00	7.581D+08	4.320D-10

 NOTE: * => EFF. EMISSION COEFFTS. EXTRAPOLATED FOR BEAM ENERGY VALUE

ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS303 V1.10 DATE: 24/11/02 TIME: 10:35

MINIMAX POLYNOMIAL FIT TO BEAM ENERGIES - TAYLOR COEFFICIENTS:

 - LOG10(EFF. EMISSION COEFFT.) versus LOG10(BEAM ENERGY<EV/AMU>) -

A(1) = -5.380300525D+04	A(2) = 1.096882509D+05
A(3) = -9.720797664D+04	A(4) = 4.887682803D+04
A(5) = -1.524382089D+04	A(6) = 3.018703409D+03
A(7) = -3.705648601D+02	A(8) = 2.577690218D+01
A(9) = -7.778688441D-01	

LOGFIT - DEGREE= 8 ACCURACY= 3.72% END GRADIENT: LOWER= 3.34 UPPER= -4.09

Notes: