

# ADAS503: PEC - graph and fit photon emissivity coefficients

The program interrogates photon emissivity (PEC) files of type ADF15. The coefficient is extracted for a selected radiative transition of an ion. The data may be interpolated using cubic splines at selected electron temperature/electron density pairs. A minimax polynomial approximation is made to the interpolated data. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the polynomial approximation.

## Background theory:

The emissivity in a transition  $j \rightarrow k$  of an ion may be written (see equation 3.8.7) as

$$\begin{aligned} \varepsilon_{j \rightarrow k} = & A_{j \rightarrow k} \left( \sum_{\sigma=1}^{M_z} \mathcal{F}_{j\sigma}^{(exc)} N_e N_{\sigma} + \sum_{v'=1}^{M_{z+1}} \mathcal{F}_{jv'}^{(rec)} N_e N_{v'} + \right. \\ & \left. \sum_{v'=1}^{M_{z+1}} \mathcal{F}_{jv'}^{(CX)} N_H N_{v'} + \sum_{\mu'=1}^{M_{z+1}} \mathcal{F}_{j\mu'}^{(ion)} N_e N_{\mu'} \right) \end{aligned} \quad 6.3.1$$

where  $N_{\sigma}$  denotes the population density of the specified ion in the metastable state  $\sigma$ ,  $N_{v'}^+$  denotes the population density of ions in the metastable state  $v'$  of the adjacent higher ionisation stage and  $N_{\mu'}^-$  denotes the population density of ions in the metastable state  $\mu'$  of the adjacent lower ionisation stage. The  $\mathcal{F}_{j\sigma}^{(exc)}$ ,  $\mathcal{F}_{jv'}^{(rec)}$ ,  $\mathcal{F}_{jv'}^{(CX)}$  and  $\mathcal{F}_{j\mu'}^{(ion)}$  are the effective contributions to the population of the upper excited level  $j$  of the transition from excitation from the metastables, from free electron capture, from charge exchange recombination from neutral hydrogen and from ionisation respectively. All these coefficients depend on density as well as temperature.  $N_e$  is the electron density and  $N_H$  the neutral hydrogen density.

This allows specification of the *excitation* photon emissivity coefficient

$$\mathcal{PEC}_{\sigma, j \rightarrow k}^{(exc)} = A_{j \rightarrow k} \mathcal{F}_{j\sigma}^{(exc)} \quad 6.3.2$$

the *recombination* photon emissivity coefficient

$$\mathcal{PEC}_{v', j \rightarrow k}^{(rec)} = A_{j \rightarrow k} \mathcal{F}_{jv'}^{(rec)} \quad 6.3.3$$

the *charge exchange* photon emissivity coefficient

$$\mathcal{PEC}_{v', j \rightarrow k}^{(CX)} = A_{j \rightarrow k} \mathcal{F}_{jv'}^{(CX)} \quad 6.3.4$$

and the *inner shell ionisation* photon emissivity coefficient

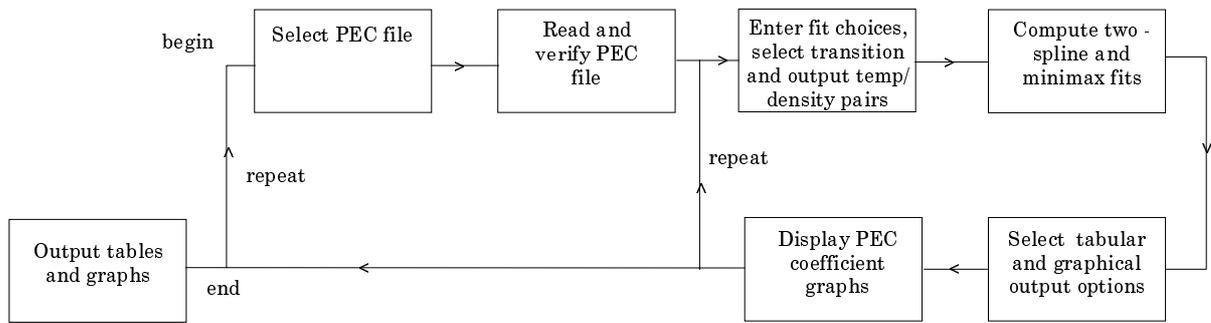
$$\mathcal{PEC}_{\mu', j \rightarrow k}^{(ion)} = A_{j \rightarrow k} \mathcal{F}_{j\mu'}^{(ion)} \quad 6.3.5$$

PEC data are extracted from archived files of type ADF15. They are interpolated by cubic splines in electron temperature and density to provide results at an arbitrary set of temperature/density pairs. The interpolated data are approximated by a minimax polynomial and a graph produced. A tabulation of the the interpolated spline data and the minimax approximation is prepared.

## Program steps:

These are summarised in figure 6.3.

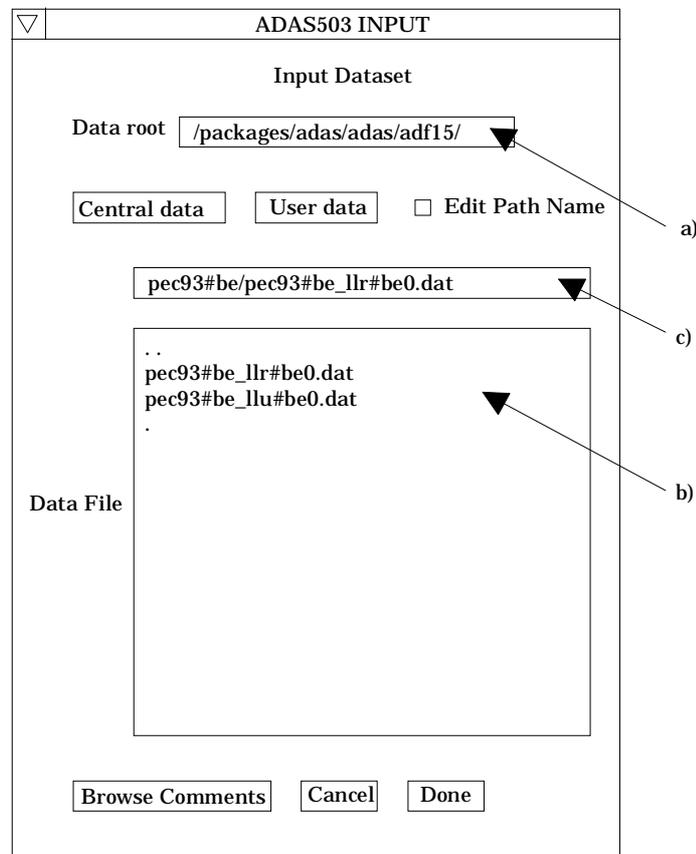
Figure 6.3



## Interactive parameter comments:

Programs of this series (ADAS5) which make use of data from archived ADAS datasets initiate an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output.

The **file selection window** has the appearance shown below



1. Data root a) 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). 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.

**N. B. Under the IDL Graphical User Interface which controls the window**

**operations, you must remember to press the *return* key on the keyboard for any change to be recorded.**

3. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.
4. Click on a name to select it. The selected name appears in the smaller selection window c) 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 a). 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, in the case of ADAS503, an 'emissivity coefficient', may be fitted with a polynomial. This is as a function of temperature. Clicking the *Fit polynomial* button b) 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. **Remember to press the *return* key on the keyboard to record the value.**
3. Spectrum lines for which emissivity coefficients are available in the data set are displayed in the line 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 line to select it. The selected line appears in the selection window c) just above the line list display window.
4. Your settings of electron temperature/electron density pairs (outputs) are shown in the temperature/density display window d). The temperature and density values at which the emissivity coefficients are stored in the datafile (inputs) are also shown for information. **Note that you must give temperature/density pairs, ie. the same number of each as for a model.** The underlying datafile has a two-dimensional storage as a function of temperature and density.
5. The program recovers the output temperature/density pairs you used when last executing the program. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures, all at the same density. A choice of density from the input density set is allowed on a 'pop-up' window.
6. The Temperature & Density 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, appears as shown below:

▽
**ADAS503 PROCESSING OPTIONS**

Title for run

Data file name : /packages/adas/adas/adf15/pec93#be/pec93#be\_lhr#be0.dat

Polynomial Fitting

◊ Fit Polynomial value % :

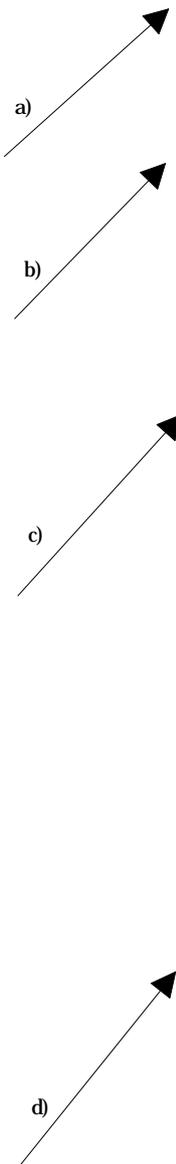
Select data block

Index	Wavelength	Ion Source	Processing Code	Metastable Index
3	3321.1A	WJD91#BE	ADAS208	1
1	2349.3A	WJD91#BE	ADAS208	1
2	1661.5A	WJD91#BE	ADAS208	1
3	3321.1A	WJD91#BE	ADAS208	1
4	2651.4A	WJD91#BE	ADAS208	1
5	2495.4A	WJD91#BE	ADAS208	1

Temperature & Density Values

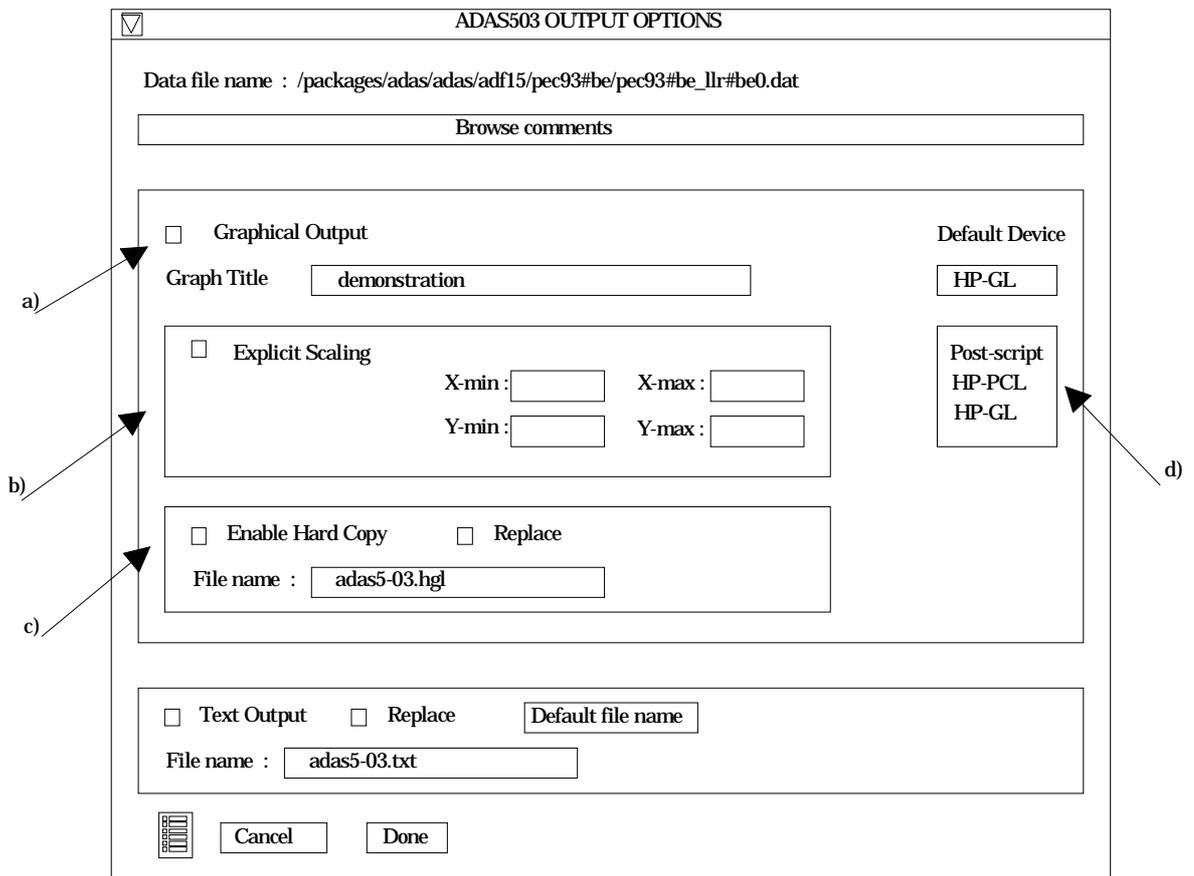
Index	Temperature		Density	
	Output	Input	Output	Input
1	1.000E+00	1.000E+00	1.000E+12	1.000E+11
2	2.000E+00	2.000E+00	1.000E+12	2.000E+11
3	5.000E+00	5.000E+00	1.000E+12	5.000E+11
4	1.000E+01	1.000E+01	1.000E+12	1.000E+12
5	2.000E+01	2.000E+01	1.000E+12	2.000E+12
6	5.000E+01	5.000E+01	1.000E+12	5.000E+12
7	1.000E+02	1.000E+02	1.000E+12	1.000E+13
8	2.000E+02	2.000E+02	1.000E+12	2.000E+13

Temperature units : eV      Density units : cm-3



The **output options window** appearance 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 a). 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. Press the *Explicit Scaling* button b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.



3. Hard copy is activated by the *Enable Hard Copy* button c). 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.
4. A choice of output graph plotting devices is given in the Device list window d). 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.
6. The graph is displayed in a following **Graphical Output** window.

### Illustration:

Figure 6.3a shows a PEC coefficient of excitation type, associated with the ground state (metastable 1) for the spectrum line BeI ( $2s2p\ ^1P - 2s^2\ ^1S$ ) of neutral beryllium. The solid line connects the spline fit points obtained in the main interpolation and the dashed curve is the minimax fit.

Figure 6.3a

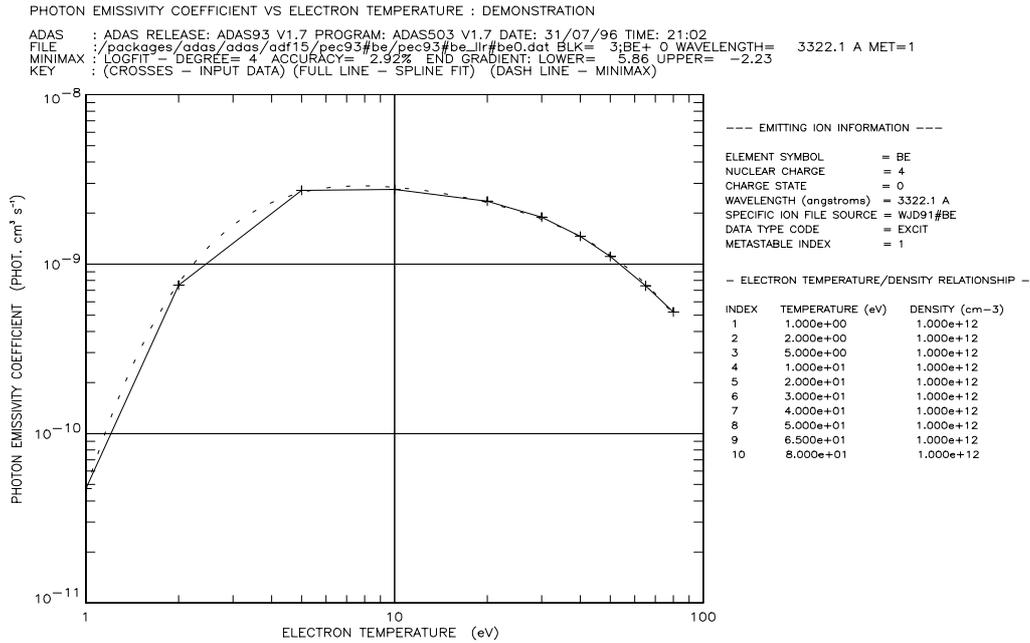


Table 6.3a

ADAS RELEASE: ADAS93 V1.7 PROGRAM: ADAS503 V1.7 DATE: 31/07/96 TIME: 21:02  
 \*\*\*\*\* TABULAR OUTPUT FROM PHOTON EMISSIVITY INTERROGATION PROGRAM: ADAS503 - DATE: 31/07/96 \*\*\*\*\*

----- demonstration -----  
 PHOTON EMISSIVITIES AS A FUNCTION OF ELECTRON TEMPERATURE AND DENSITY  
 -----  
 DATA GENERATED USING PROGRAM: ADAS503  
 -----  
 FILE : /packages/adas/adas/adf15/pec93#be/pec93#be\_llr#be0.dat - DATA-BLOCK: 3  
 EMITTING ION INFORMATION:  
 -----  
 ELEMENT NAME = BERYLLIUM  
 ELEMENT SYMBOL = BE  
 NUCLEAR CHARGE (Z0) = 4  
 CHARGE STATE (Z) = 0  
 WAVELENGTH (angstroms) = 3322.1 A  
 SPECIFIC ION FILE SOURCE = WJD91#BE  
 DATA TYPE CODE = EXCIT  
 METASTABLE INDEX = 1

--- ELECTRON TEMPERATURE ---		ELECTRON DENSITY		PHOT. EMISS.
kelvin	eV	cm-3	cm-3	cm**3 s-1
1.161D+04	1.000D+00	1.000D+12		4.730D-11
6.321D+04	2.000D+00	1.000D+12		7.500D-10
5.803D+04	5.000D+00	1.000D+12		2.720D-09
1.161D+05	1.000D+01	1.000D+12		2.760D-09
5.803D+05	5.000D+01	1.000D+12	1.110D-09	
	7.544D+05	6.500D+01	1.000D+12	7.420D-10
	9.284D+05	8.000D+01	1.000D+12	5.210D-10

NOTE: \* => PHOTON EMISSIVITIES EXTRAPOLATED FOR TEMPERATURE/DENSITY VALUE

-----  
 MINIMAX POLYNOMIAL FIT TO ELECTRON TEMPERATURES - TAYLOR COEFFICIENTS:  
 -----  
 - LOG10(PHOTON EMISSIVITIES) VERSUS LOG10(ELECTRON TEMPERATURE<eV>) -  
 -----  
 A( 1) = -1.033763749D+01      A( 2) = 5.858733940D+00  
 A( 3) = -6.987389839D+00      A( 4) = 3.710939472D+00  
 A( 5) = -7.912383706D-01  
 LOGFIT - DEGREE= 4 ACCURACY= 2.92% END GRADIENT: LOWER= 5.86 UPPER= -2.23  
 -----

Notes: