ADAS201: Specific z excitation - graph and fit coefficient

The program interrogates specific ion files of type ADF04. It extracts electron impact rate coefficient data for selected transitions. The data may be interpolated using cubic splines to provide excitation rate coefficients at arbitrarily chosen electron temperatures. A minimax polynomial approximation is also made to the source data. The source and interpolated excitation rate coefficient data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the minimax polynomial approximation.

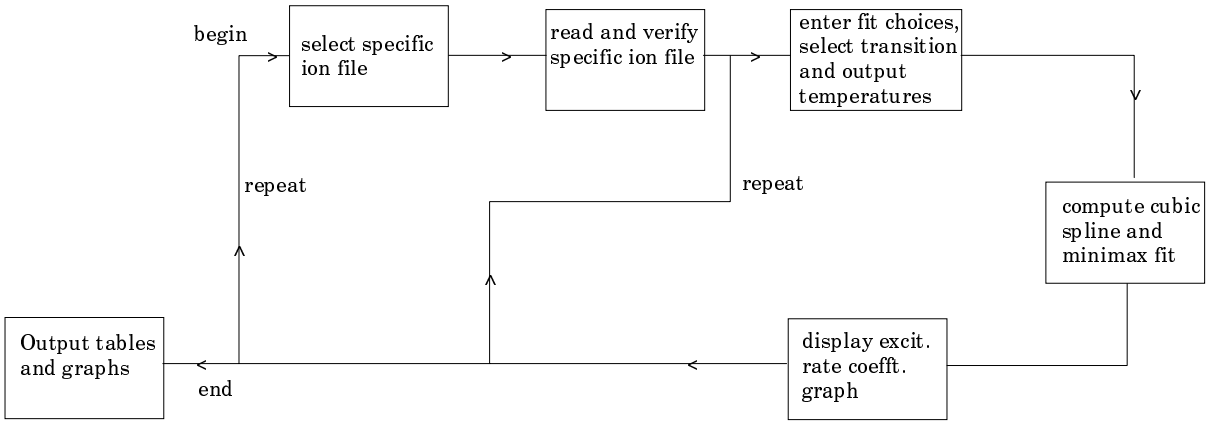
Background theory:

Maxwell averaged rate coefficient data are extracted for specific ion files of type ADF04. This is presented as excitation rate coefficients and de-excitation coefficients. Relevant theory is given in ADAS101.

Program steps:

These are summarised in figure 3.1.

Figure 3.1



Interactive parameter comments:

Remember to ensure you have a defaults directory allocated. This should have the pathway

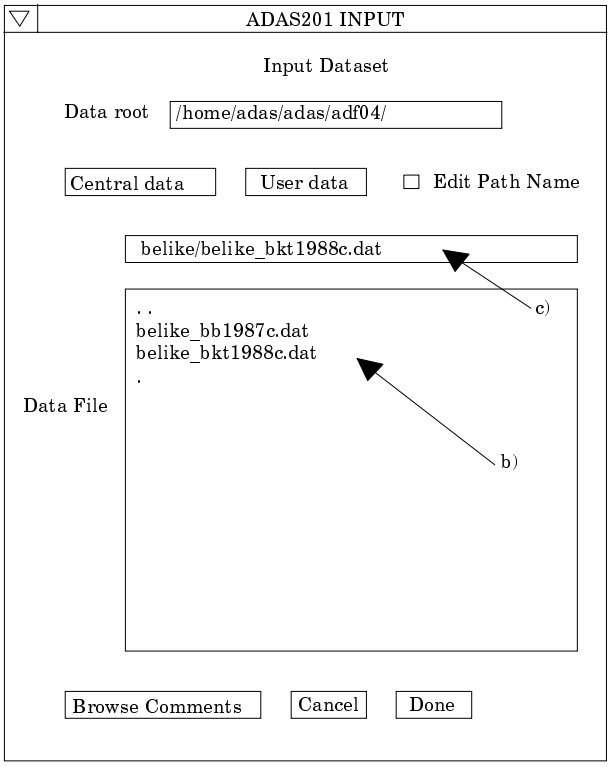
/..../uid/adas/defaults

where *uid* is your user identifier. The defaults directory records the parameters you set the last time you ran each ADAS code. Move to the directory in which you wish any ADAS created files to appear. These include the output text file produced after executing any ADAS program (*paper.txt* is the default) and the graphic file if saved (e.g. *graph.ps* if a postscript file). Initiate ADAS, move to the series 2 menu and click on the first button to activate ADAS201.

The **file selection window** is as shown below

1. Note that each type of data is stored according to its ADAS data format (*adf* number). *adf04* is the appropriate format for use by the program ADAS201. Your personal data of this type should be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas.*

2. 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. There are a large number of these, named (a) by iso-electronic sequence (eg. *belike*) (b) by isoelectronic sequence associated with a particular source (eg. *copsm#be*) (c) by iso-nuclear sequence associated with a particular source (eg. *copmm#16* , where the 16 is the nuclear charge)



3. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then 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 has gone into the dataset and the attribution of 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** has the appearance shown below:

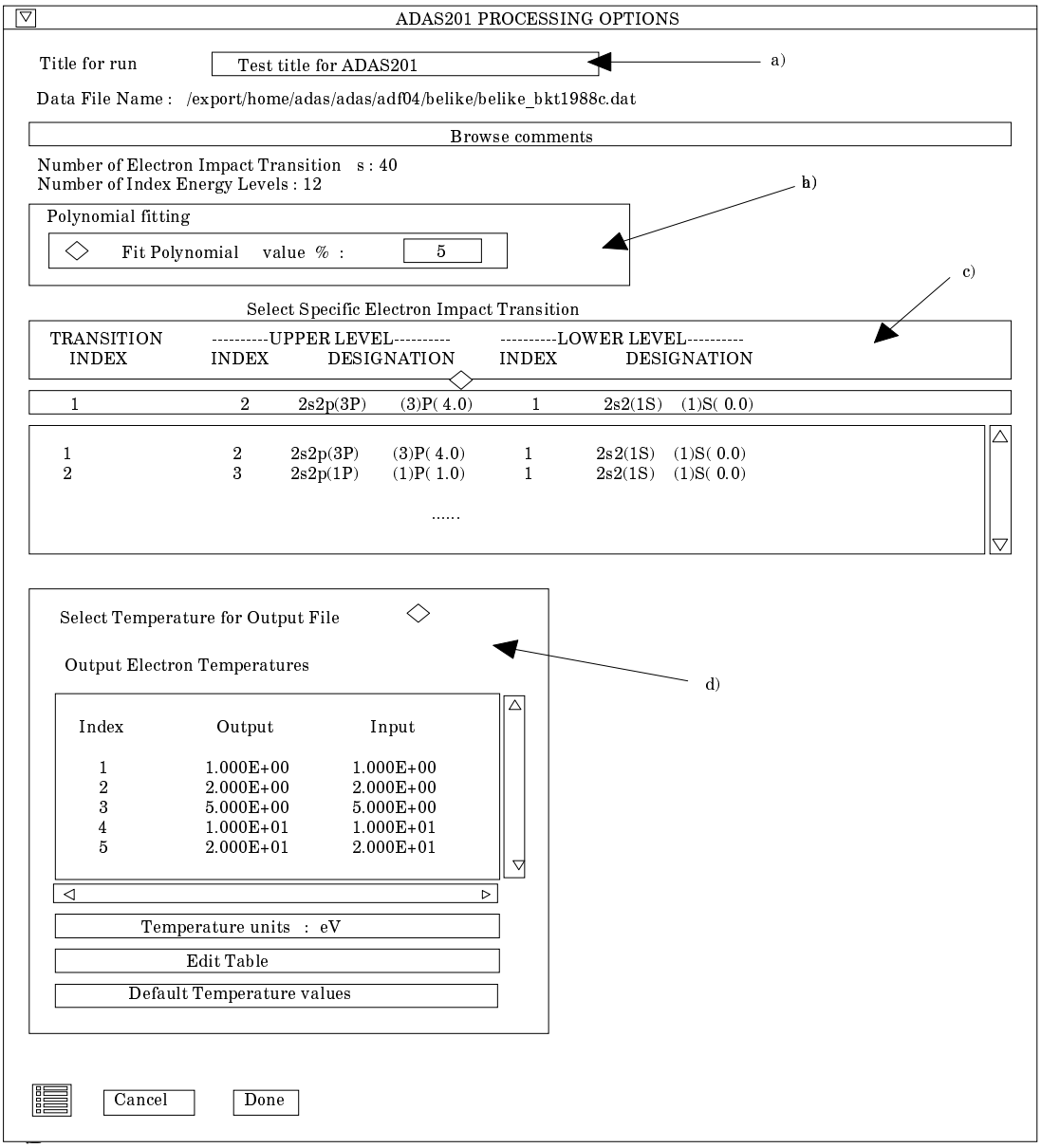
7. An arbitrary title may be given for the case being processed a). For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.

8. The output data extracted from the datafile, an ‘excitation rate 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**.

9. Transitions for which electron impact excitation data 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 transition appears in the selection window c) just above the line list display window.

10. Your settings of electron temperatures (output) are shown in the temperature display window d). The temperature values at which the excitation rate coefficients (in fact ‘upsilons’) are stored in the datafile (input) are also shown for information.

The program recovers the output temperatures you used when last executing the



12. program. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures

13. The Temperature 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: It follows the same pattern of operation as described in bulletin.

14. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **output options window** is as shown below

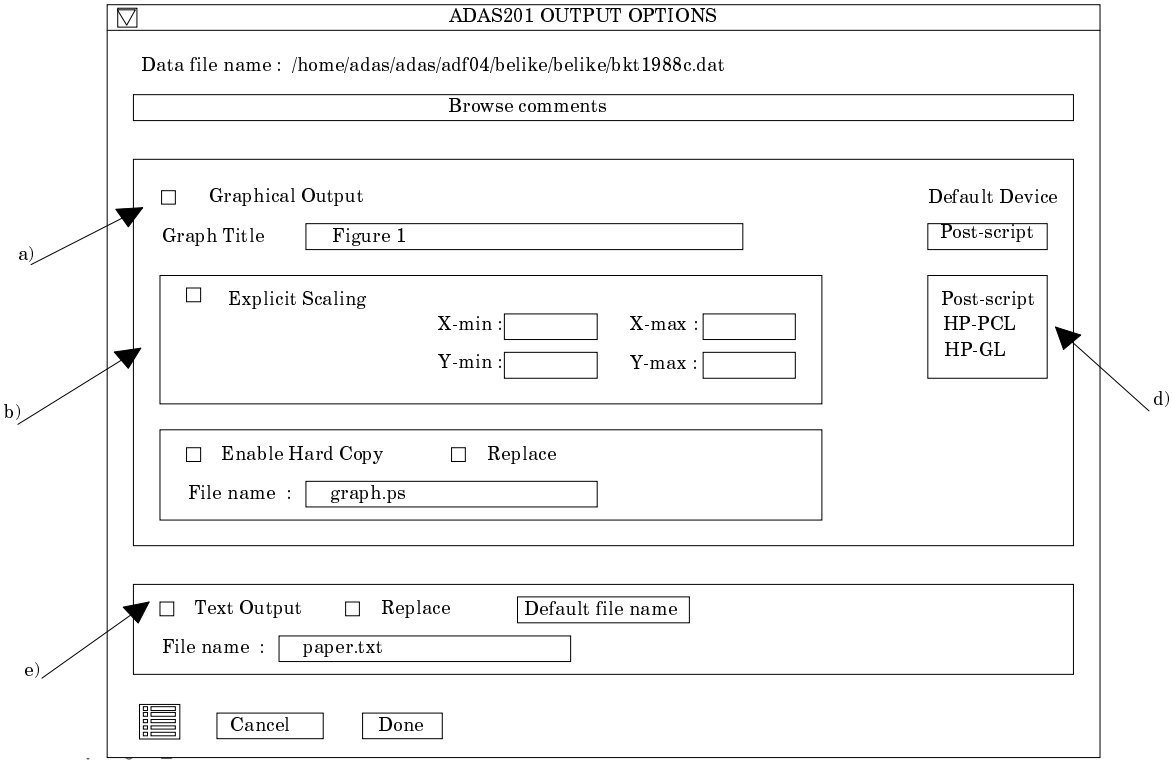
15. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.

16. 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.

17. Hard copy is activated by the *Enable Hard Copy* button c). The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a 'pop-up' window issues a warning.

18. 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.

19. 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.



21. The graph is displayed in a following **Graphical Output** window.

Illustration:

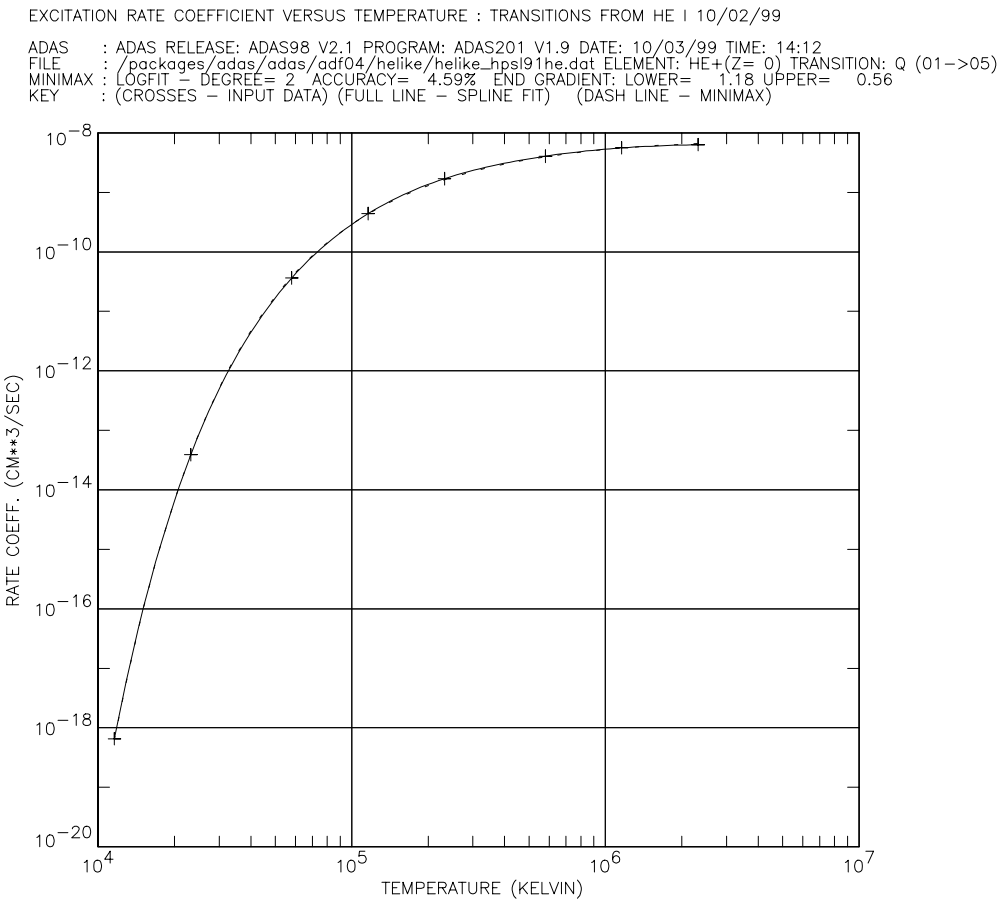
The output from the program is illustrated for the transition

$$He^{+0}(1s^2\ {}^1S) + e \rightarrow He^{+0}(1s2p\ \ {}^1P) + e \qquad 3.1.1$$

extracted from the specific ion file /…/adas/adas/adf04/helike/helike_hpsl91he.dat.

Figure 3.1a shows the Maxwell averaged excitation rate coefficient ($cm^3\ s^{-1}$) for the transition. The solid line is the interpolating cubic spline. The dashed line is the miminax polynomial fit to the data. Input values are shown as crosses.

Figure 3.1a



The tabular output is shown in table 3.1. It includes full specification of the levels of the transition. Output data which required extrapolation beyond the range of the original data in the source specific ion file are indicated by *.

Table3.1.

```
ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS201 V1.9 DATE: 10/03/99 TIME: 14:12
**** TABULAR OUTPUT FROM  SPECIFIC Z EXCITATION FILES INTERROGATION PROGRAM: ADAS201 - DATE: 10/03/99 ****

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          EXCITATION RATE COEFFICIENTS AS A FUNCTION OF TEMPERATURE
          ---------------------------------------------------------
                    DATA GENERATED USING PROGRAM: ADAS201
                    -------------------------------------

FILE :  /packages/adas/adas/adf04/helike/helike_hpsl91he.dat  ELEMENT: HE+(Z= 0)  TRANSITION: Q (01->05)

NUCLEAR CHARGE         (Z0) =   2
RECOMBINING ION CHARGE (Z1) =   1
RECOMBINED ION CHARGE  (Z)  =   0

IONISATION POTENTIAL        =  1.98305D+05 (cm-1)  =  1.80709D+00 (rydberg)
```

```
   LEVEL      CONFIGURATION      QUANTUM NUMBERS    ENERGY RELATIVE TO LEVEL 1
                                2S+1  L  (WI-1)/2     (cm-1)         (rydberg)
-------------------------------------------------------------------------------
 5 - UPPER    1S2P                1    1    1.0     1.71129D+05     1.55945D+00
 1 - LOWER    1S1S                1    0    0.0     0.00000D+00     0.00000D+00

TRANSITION A-VALUE =  1.80D+09 (sec-1)

TRANSITION ENERGY  =  1.71129D+05 (cm-1)  =  1.55945D+00 (rydberg)
```

```
------------- TEMPERATURE -------------   GAMMA   RATE COEFFICIENTS  (cm**3/s)
    kelvin         eV      kelvin/Z1**2            DE-EXCITATION   EXCITATION
-------------------------------------------------------------------------------
  1.16D+04     1.00D+00     1.16D+04     1.35D-02     3.605D-10     6.543D-19
  2.32D+04     2.00D+00     2.32D+04     2.80D-02     5.288D-10     3.901D-14
  5.80D+04     5.00D+00     5.80D+04     7.10D-02     8.480D-10     3.646D-11
  1.16D+05     1.00D+01     1.16D+05     1.46D-01     1.233D-09     4.428D-10
  2.32D+05     2.00D+01     2.32D+05     2.75D-01     1.642D-09     1.705D-09
  5.80D+05     5.00D+01     5.80D+05     5.50D-01     2.077D-09     4.076D-09
  1.16D+06     1.00D+02     1.16D+06     8.70D-01     2.323D-09     5.637D-09
  2.32D+06     2.00D+02     2.32D+06     1.25D+00     2.360D-09     6.368D-09
-------------------------------------------------------------------------------

MINIMAX POLYNOMIAL - TAYLOR COEFFICIENTS: LOG10(GAMMA) vs. LOG10(TEMP<kelvin>)
-------------------------------------------------------------------------------
           A( 1) =  -8.912700123D+00            A( 2) =   2.274910203D+00
           A( 3) =  -1.345485026D-01

LOGFIT - DEGREE= 2  ACCURACY=  4.59%  END GRADIENT: LOWER=   1.18 UPPER=   0.56
-------------------------------------------------------------------------------
```

Notes: