
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.

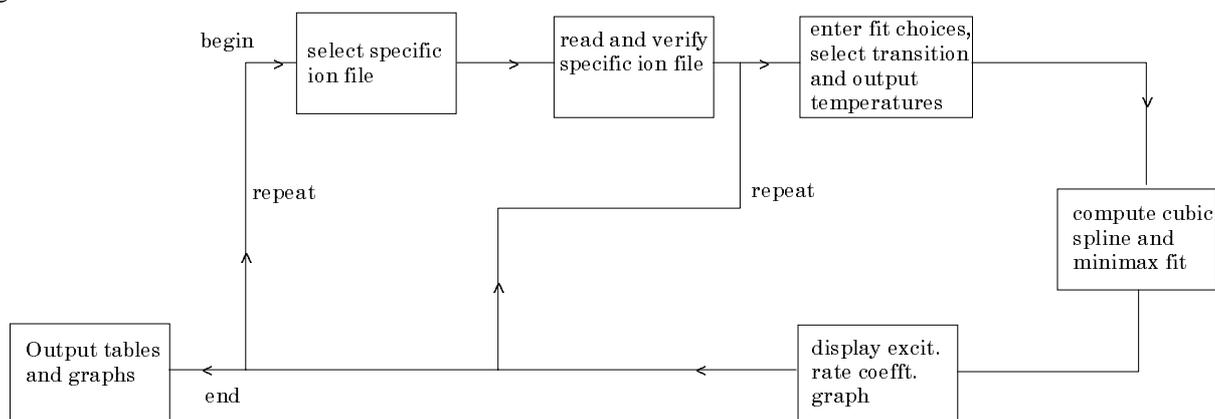
Background theory:

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:

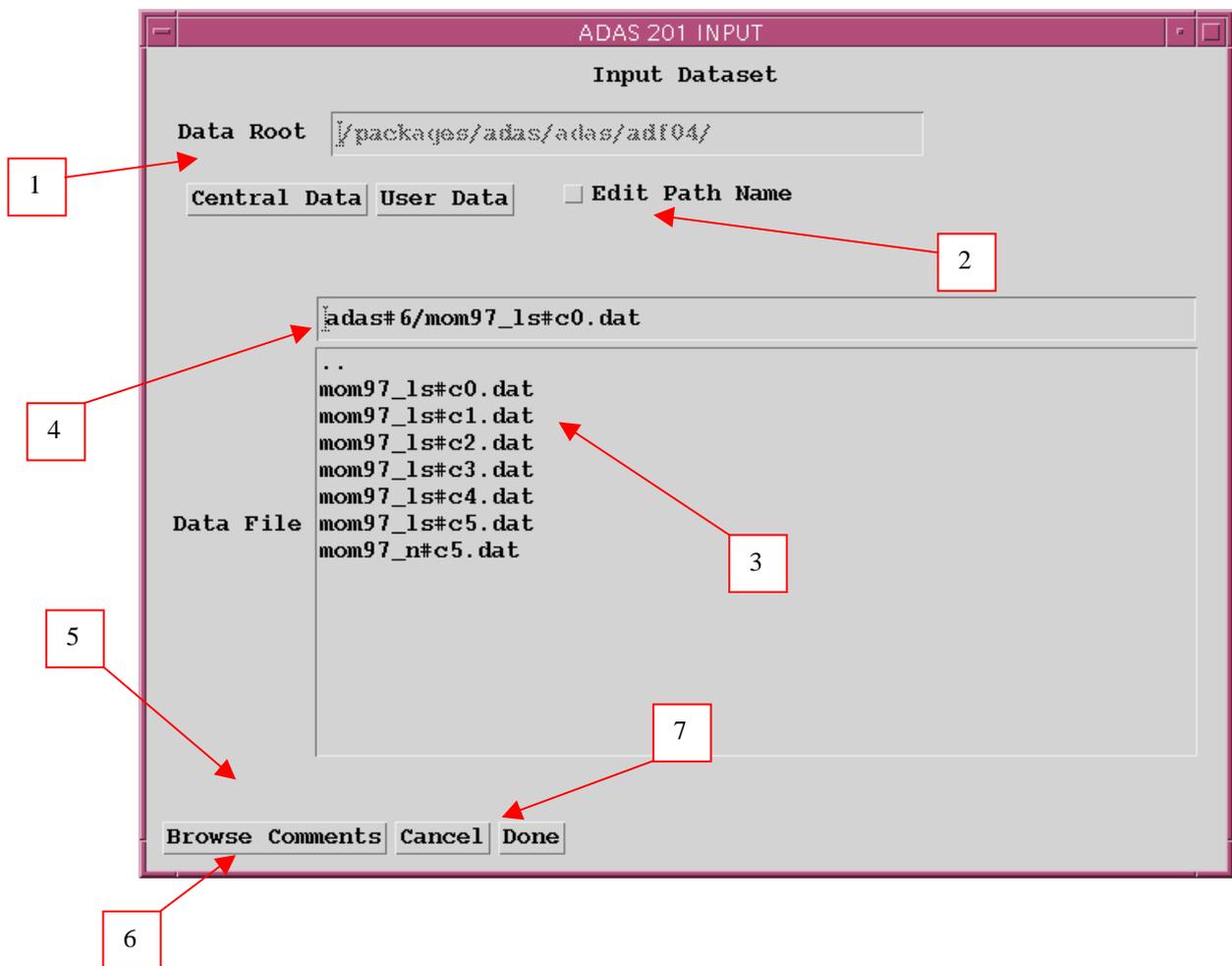
ADAS201, which make use of data from archived ADAS datasets, initiates an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output.

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

1. Data root 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 – ADF04 in this case. 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.
3. Available sub-directories are shown in the large file display window. 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).

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 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. 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, 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

3. 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 just above the line list display window.
4. Your settings of electron temperatures (output) are shown in the temperature display window. 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 program

ADAS201 PROCESSING OPTIONS

Title for Run

Data File Name: /packages/adas/adas/adf04/adas#6/mom97_ls#c0.dat

Number of Electron Impact Transitions : 992
Number of Index Energy levels : 64

Polynomial Fitting

Fit Polynomial value % :

Select Specific Electron Impact Transition

TRANSITION INDEX	LOWER LEVEL			UPPER LEVEL			
	INDEX	DESIGNATION		INDEX	DESIGNATION		
541	1	2S2 2P2	(3)P(4.0)	17	2S2 2P1 3D1	(3)D(7.0)	
1	1	2S2 2P2	(3)P(4.0)	2	2S2 2P2	(1)D(2.0)	
2	1	2S2 2P2	(3)P(4.0)	3	2S2 2P2	(1)S(0.0)	
3	1	2S2 2P2	(3)P(4.0)	9	2S2 2P1 3P1	(3)D(7.0)	
4	1	2S2 2P2	(3)P(4.0)	11	2S2 2P1 3P1	(3)P(4.0)	
5	1	2S2 2P2	(3)P(4.0)	12	2S2 2P1 3P1	(1)D(2.0)	

Select Temperatures for output file

Output Electron Temperatures

INDEX	Output	Input
1	1.000E+00	8.617E-01
2	1.500E+00	1.077E+00
3	2.500E+00	2.154E+00
4	4.000E+00	3.231E+00

Temperature Units: eV

Edit the processing options data and press Done to proceed

5. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures
6. 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.
7. 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

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.

ADAS201 OUTPUT OPTIONS

Data File Name: /packages/adas/adas/adf04/adas#6/mom97_ls#c0.dat

Browse Comments

Graphical Output

Graph Title: User manual example

Explicit Scaling

X-min : [] X-max : []

Y-min : [] Y-max : []

Enable Hard Copy Replace

File Name : adas201_graph.ps

Select Device

Post-Script

Post-Script HP-PCL

HP-GL

Text Output Append Replace Default File Name

File Name : adas201_paper.txt

Cancel Done

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.
5. 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.

- 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

- Printing of the currently displayed graph is activated by the *Print* button.

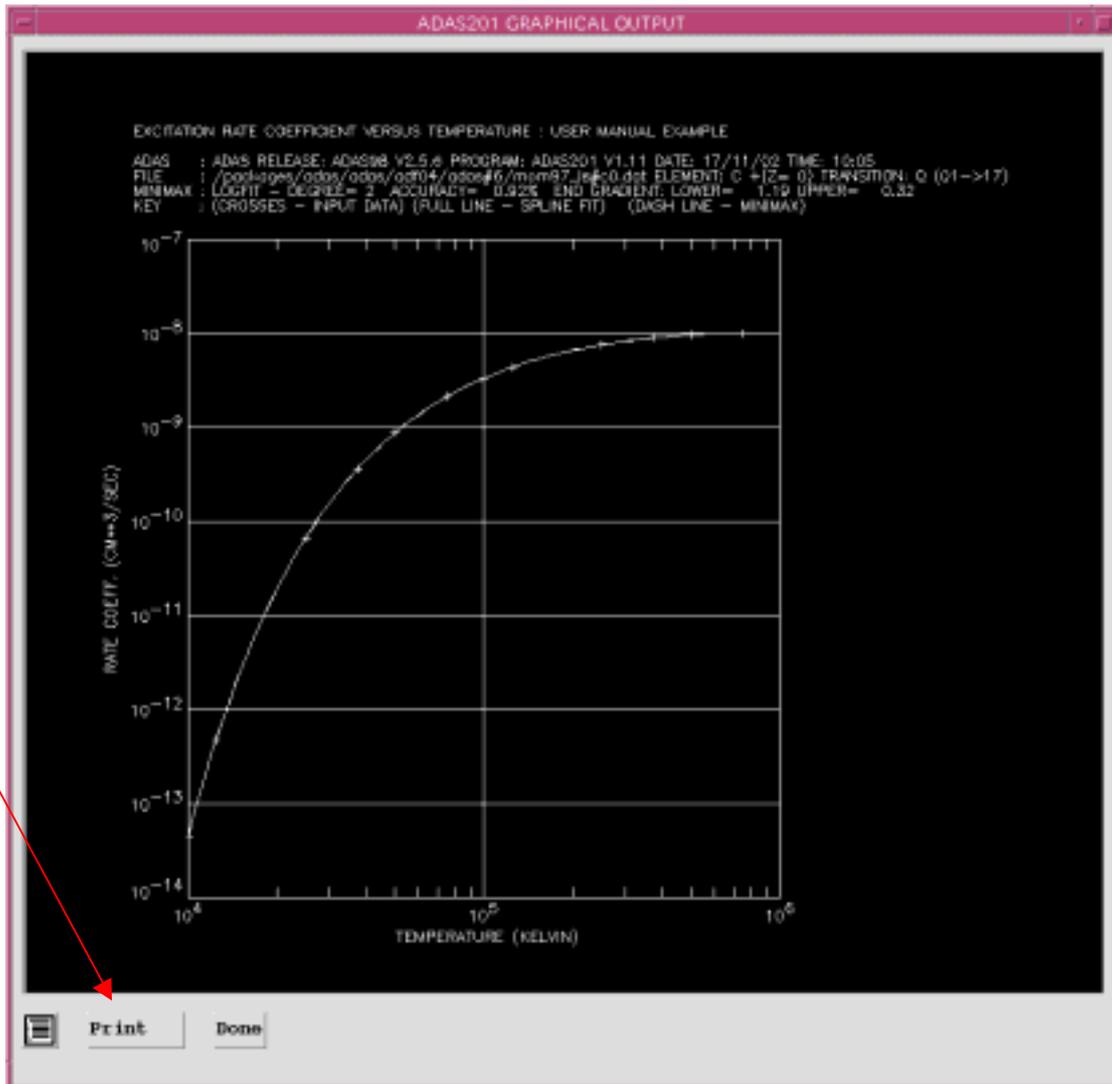
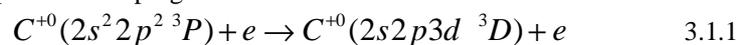


Illustration:

The output from the program is illustrated for the transition



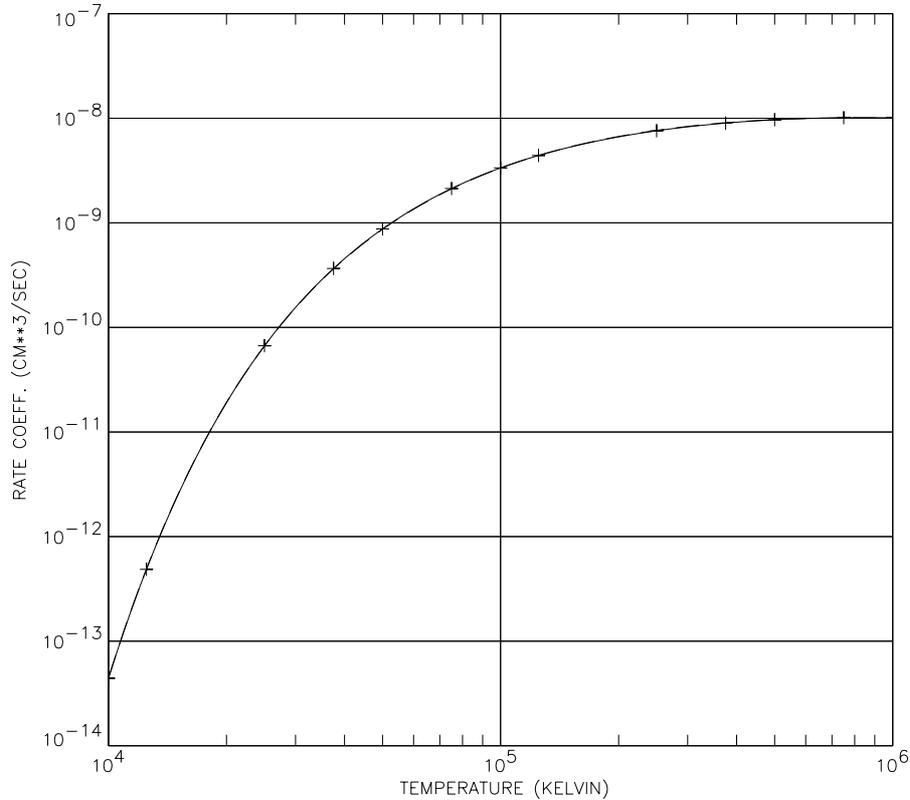
extracted from the specific ion file `../adas/adas/adf04/adas#6/mom97_1s#c0.dat`.

Figure 3.1a shows the Maxwell averaged excitation rate coefficient (cm³ s⁻¹) for the transition. The solid line is the interpolating cubic spline. The dashed line is the mimmax polynomial fit to the data. Input values are shown as crosses.

Figure 3.1a

EXCITATION RATE COEFFICIENT VERSUS TEMPERATURE : USER MANUAL EXAMPLE

ADAS : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS201 V1.11 DATE: 17/11/02 TIME: 10:13
 FILE : /packages/adas/adas/adf04/adas#6/mom97_ls#c0.dat ELEMENT: C +(Z= 0) TRANSITION: Q (01->17)
 MINIMAX : LOGFIT - DEGREE= 2 ACCURACY= 0.92% END GRADIENT: LOWER= 1.19 UPPER= 0.32
 KEY : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT) (DASH LINE - MINIMAX)



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.

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ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS201 V1.11 DATE: 17/11/02 TIME: 10:13
***** TABULAR OUTPUT FROM SPECIFIC Z EXCITATION FILES INTERROGATION PROGRAM: ADAS201 - DATE: 17/11/02 *****
-----
EXCITATION RATE COEFFICIENTS AS A FUNCTION OF TEMPERATURE
-----
DATA GENERATED USING PROGRAM: ADAS201
-----
FILE : /packages/adas/adas/adf04/adas#6/mom97_ls#c0.dat ELEMENT: C +(Z= 0) TRANSITION: Q (01->17)

NUCLEAR CHARGE (Z0) = 6
RECOMBINING ION CHARGE (Z1) = 1
RECOMBINED ION CHARGE (Z) = 0

IONISATION POTENTIAL = 9.08204D+04 (cm-1) = 8.27618D-01 (rydberg)

LEVEL      CONFIGURATION      QUANTUM NUMBERS      ENERGY RELATIVE TO LEVEL 1
-----
2S+1  L  (WI-1)/2      (cm-1)              (rydberg)
-----
17 - UPPER  2S2 2P1 3D1          3  2  7.0             7.82801D+04         7.13342D-01
1 - LOWER  2S2 2P2              3  1  4.0             0.00000D+00         0.00000D+00

TRANSITION A-VALUE = 2.15D+08 (sec-1)
TRANSITION ENERGY = 7.82801D+04 (cm-1) = 7.13342D-01 (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 4.26D-01 2.275D-09 2.313D-13
1.74D+04 1.50D+00 1.74D+04 6.74D-01 2.941D-09 7.593D-12
2.90D+04 2.50D+00 2.90D+04 1.16D+00 3.917D-09 1.345D-10
4.64D+04 4.00D+00 4.64D+04 1.82D+00 4.847D-09 7.139D-10
5.80D+04 5.00D+00 5.80D+04 2.21D+00 5.273D-09 1.262D-09
1.16D+05 1.00D+01 1.16D+05 3.80D+00 6.413D-09 4.049D-09
1.74D+05 1.50D+01 1.74D+05 4.99D+00 6.873D-09 5.998D-09
2.32D+05 2.00D+01 2.32D+05 5.95D+00 7.101D-09 7.285D-09
-----

MINIMAX POLYNOMIAL - TAYLOR COEFFICIENTS: LOG10(GAMMA) vs. LOG10(TEMP<kelvin>)
-----
A( 1) = -8.711868110D+00 A( 2) = 2.941697854D+00
A( 3) = -2.186226028D-01

LOGFIT - DEGREE= 2 ACCURACY= 0.92% END GRADIENT: LOWER= 1.19 UPPER= 0.32
-----

```

Notes:

