

# ADAS502: SZD - graph and fit zero-density ionisation rate coefficients

The program interrogates zero-density electron impact ionisation rate coefficient (SZD) files of type ADF07. The data may be interpolated using cubic splines at selected electron temperatures. 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:

Consider the ionisation reaction



where the ion  $X^{+z}$  in initial state  $\gamma$  is ionised leaving the residual ion  $X^{+z+1}$  in the state  $p_{\rho}$ .

Often ionisation from the ground state of the ion  $X^{+z}$  only is present in sources of atomic data. Also the particular final state of the ion  $X^{+z+1}$  is not specified, but rather a sum over final states is given. For more detailed studies, 'metastable resolved' ionisation data is required, that is where the states  $\gamma$  and  $p_{\rho}$  are distinguished. If the ionisation cross-section is  $Q_{\gamma \rightarrow p_{\rho}}^{(z \rightarrow z+1)}(\epsilon)$ , then the program accesses Maxwell averaged rate coefficients of the form

$$S_{\gamma \rightarrow p_{\rho}}^{(z \rightarrow z+1)}(T_e) = 2\sqrt{\pi} \alpha c a_o^2 (kT_e / I_H)^{1/2} \int_{I_{\gamma, p_{\rho}} / kT_e}^{\infty} \frac{Q_{\gamma \rightarrow p_{\rho}}^{(z \rightarrow z+1)}(\epsilon)}{\pi a_o^2} (\epsilon / kT_e) \exp(-\epsilon / kT_e) d(\epsilon / kT_e) \quad 6.2.2$$

where  $2\sqrt{\pi} \alpha c a_o^2 = 2.1716 \times 10^{-8} \text{ cm}^3 \text{ s}^{-1}$ .

In a plasma of zero density where there is no stepwise ionisation through excited states, the above ionisation rate coefficient is the effective ionisation rate coefficient from  $\gamma$  to  $p_{\rho}$ . It is called the zero density ionisation rate coefficient. Collections of such coefficients are held in 'SZD' archived files of ADAS data format type ADF07. Each file is for an element and contains metastable resolved ionisation coefficients  $S_{\gamma \rightarrow p_{\rho}}^{(z \rightarrow z+1)}(T_e)$  and the summed ionisation coefficients

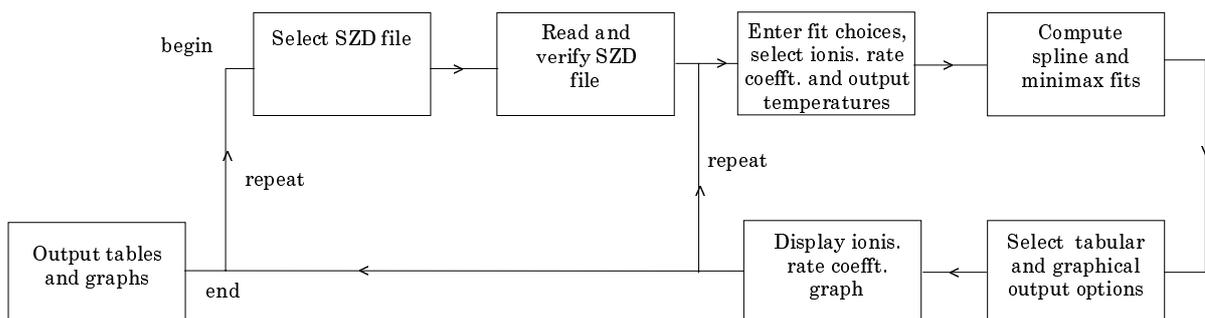
$$S_{\gamma}^{(z \rightarrow z+1)}(T_e) = \sum_{p_{\rho}} S_{\gamma \rightarrow p_{\rho}}^{(z \rightarrow z+1)}(T_e) \quad 6.2.3$$

for each adjacent ion pair of the element.

## Program steps:

These are summarised in figure 6.2.

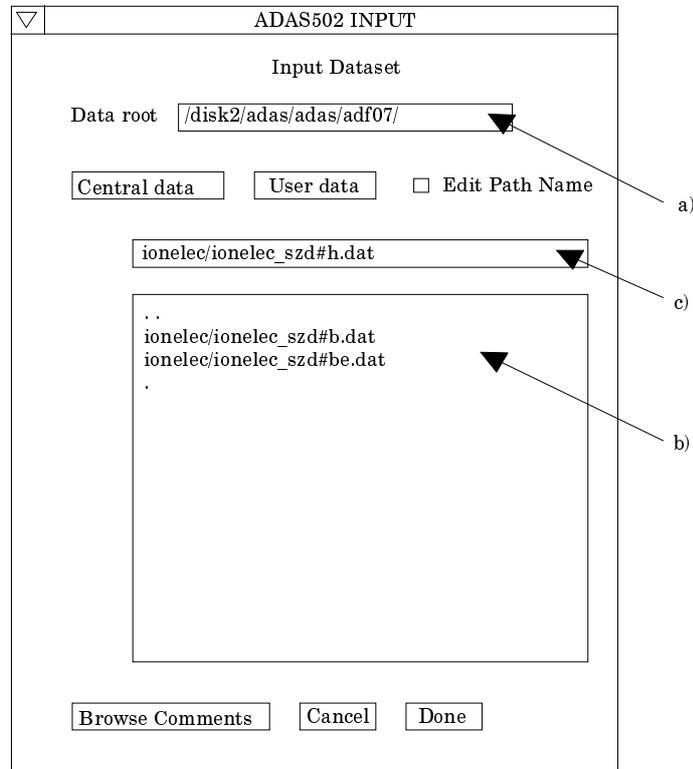
Figure 6.2



## 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.
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.

ADAS502 PROCESSING OPTIONS

Title for run

Data file name : /disk2/adas/adas/adf07/ionelec/ionelec\_szd#h.dat

Polynomial fitting

value % :

Select data block

| Index | Initial ion | Metstable index | Final ion | Metastable index |
|-------|-------------|-----------------|-----------|------------------|
| 2     | H + 0       | 1               | H + 1     | 1                |
| 1     | H + 0       | 1               | H + 1     | 1                |
| 2     | H + 0       | 1               | H + 1     | 1                |

Select Temperatures for output file

Output Electron Temperature

| Index | Output    | Input     |
|-------|-----------|-----------|
| 1     | 1.000E+00 | 1.000E+00 |
| 2     | 2.000E+00 | 2.000E+00 |
| 3     | 5.000E+00 | 5.000E+00 |
| 4     | 1.000E+01 | 1.000E+01 |
| 5     | 2.000E+01 | 2.000E+01 |
| 6     | 5.000E+01 | 5.000E+01 |
| 7     | 1.000E+02 | 1.000E+02 |
| 8     | 2.000E+02 | 2.000E+02 |

Temperature units : eV

Edit the processing options data and press Done to proceed

2. The output data extracted from the datafile, in the case of ADAS502, an 'ionisation 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.**
3. Available rate coefficients in the data set are displayed in the coefficient 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 coefficient to select it. The selected rate appears in the selection window c) just above the coefficient list display window.

- Your settings of electron temperatures (output) are shown in the temperature display window d). The temperature values at which the ionisation rate coefficients are stored in the datafile (input) are also shown for information.
- The program recovers the output temperatures you used when last executing the program. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures.
- 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, appears as shown below:

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

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

ADAS502 OUTPUT OPTIONS

Data file name : /disk2/adas/adas/adf07/ionelec/ionelec\_szd#h.dat

Browse comments

Graphical Output

Graph Title : Figure 1

Explicit Scaling

X-min :  X-max :

Y-min :  Y-max :

Enable Hard Copy  Replace

File name : graph.ps

Text Output  Replace

File name : graph.ps

Default Device

Post-script

Post-script  
HP-PCL  
HP-GL

Cancel Done

- 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.
- 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.
- 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**.

### Illustration:

Figure 6.2a shows the zero density ionisation rate coefficient for the reaction  $N^{+1}(2s^2 2p^2 \ ^3P) + e \rightarrow N^{+2}(2s^2 2p \ ^2P) + e + e$ . The solid line is the spline fit used for the main interpolation and the dashed curve is the minimax fit.

Figure 6.2a

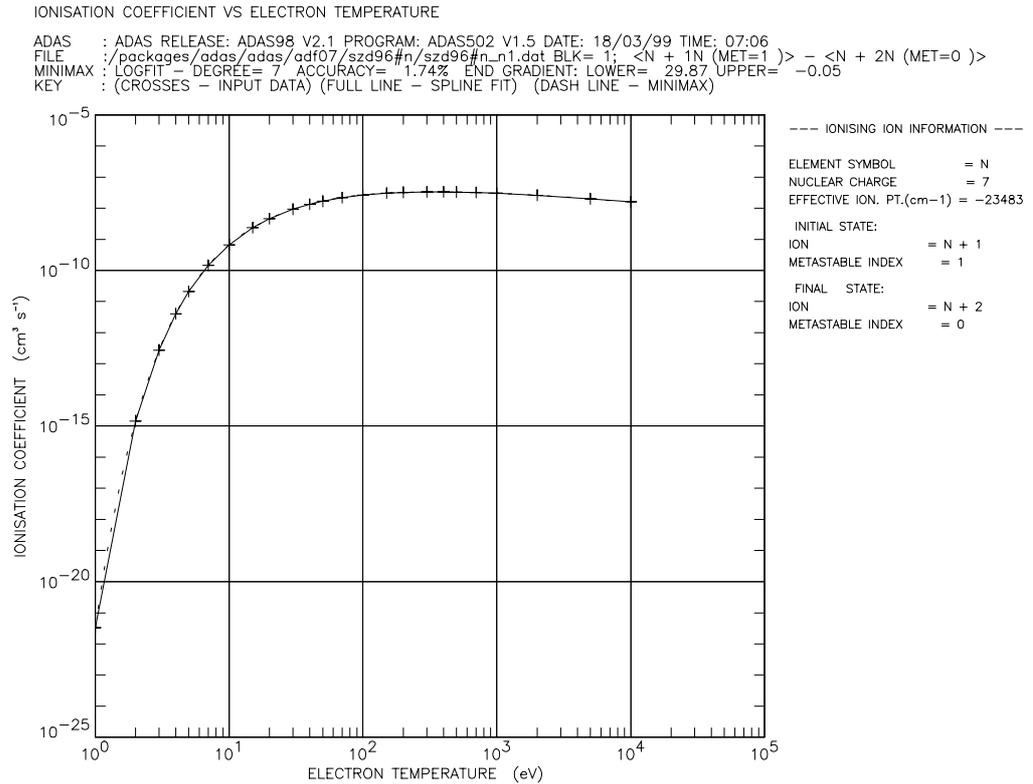


Table 6.2a

```

ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS502 V1.5 DATE: 18/03/99 TIME: 07:06
TABULAR OUTPUT FROM ZERO DENSITY IONIZATION RATE-COEFFICIENT INTERROG. PROGRAM: ADAS502 - DATE: 18/03/99

-----
ZERO-DENSITY IONIZATION RATE-COEFFICIENT AS A FUNCTION OF ELECTRON TEMPERATURE
-----
DATA GENERATED USING PROGRAM: ADAS502
-----
                                     /packages/adas/adas/adf07/szd96#n/szd96#n_n1.dat - DATA-BLOCK: 1
IONISING ION INFORMATION:
-----
ELEMENT NAME           = NITROGEN
ELEMENT SYMBOL         = N
NUCLEAR CHARGE        (Z0) = 7

EFFECTIVE IONIZATION POTENTIAL = 238661.6 cm-1

INITIAL STATE:
  ION                   = N + 1
  ION CHARGE            (Z) = 1
  METASTABLE INDEX     = 1
FINAL STATE:
  
```

ION = N + 2  
 ION CHARGE (Z1) = 2  
 METASTABLE INDEX = 0

| ----- ELECTRON TEMPERATURE ----- |             |             | IONIZATION RATE-COEFFT. |
|----------------------------------|-------------|-------------|-------------------------|
| kelvin                           | eV          | K/Z1**2     | cm**3/sec.              |
| 1.161D+04                        | 1.000D+00   | 2.902D+03   | 3.339D-22               |
| 2.321D+04                        | 2.000D+00   | 5.802D+03   | 1.451D-15               |
| 3.482D+04                        | 3.000D+00   | 8.705D+03   | 2.738D-13               |
| 4.642D+04                        | 4.000D+00   | 1.160D+04   | 4.014D-12               |
| 5.803D+04                        | 5.000D+00   | 1.451D+04   | 2.092D-11               |
| 8.124D+04                        | 7.000D+00   | 2.031D+04   | 1.461D-10               |
| 1.161D+05                        | 1.000D+01   | 2.902D+04   | 6.719D-10               |
| 1.741D+05                        | 1.500D+01   | 4.352D+04   | 2.353D-09               |
| 2.321D+05                        | 2.000D+01   | 5.802D+04   | 4.565D-09               |
| 3.482D+05                        | 3.000D+01   | 8.705D+04   | 9.191D-09               |
| 4.642D+05                        | 4.000D+01   | 1.160D+05   | 1.327D-08               |
| 5.803D+05                        | 5.000D+01   | 1.451D+05   | 1.665D-08               |
| 8.124D+05                        | 7.000D+01   | 2.031D+05   | 2.166D-08               |
| 1.161D+06                        | 1.000D+02   | 2.902D+05   | 2.632D-08               |
| 1.741D+06                        | 1.500D+02   | 4.352D+05   | 3.028D-08               |
| 2.321D+06                        | 2.000D+02   | 5.802D+05   | 3.209D-08               |
| 3.482D+06                        | 3.000D+02   | 8.705D+05   | 3.321D-08               |
| 4.642D+06                        | 4.000D+02   | 1.160D+06   | 3.318D-08               |
| 5.803D+06                        | 5.000D+02   | 1.451D+06   | 3.276D-08               |
| 8.124D+06                        | 7.000D+02   | 2.031D+06   | 3.161D-08               |
| 1.161D+07                        | 1.000D+03   | 2.902D+06   | 2.989D-08               |
| 2.321D+07                        | 2.000D+03   | 5.802D+06   | 2.573D-08               |
| 5.803D+07                        | 5.000D+03   | 1.451D+07   | 1.988D-08               |
| 1.161D+08                        | * 1.000D+04 | * 2.902D+07 | 1.588D-08               |

NOTE: \* => IONIZATION RATE-COEFFTS. EXTRAPOLATED FOR ELECTRON TEMPERATURE VALUE

MINIMAX POLYNOMIAL FIT - TAYLOR COEFFICIENTS:

- LOG10(RATE-COEFFICIENT<cm\*\*3/sec>) versus LOG10(ELECTRON TEMPERATURE<eV>) -

|                          |                         |
|--------------------------|-------------------------|
| A( 1) = -2.147398963D+01 | A( 2) = 2.987121158D+01 |
| A( 3) = -3.162762881D+01 | A( 4) = 2.085044745D+01 |
| A( 5) = -8.724145845D+00 | A( 6) = 2.217767830D+00 |
| A( 7) = -3.101252796D-01 | A( 8) = 1.821723254D-02 |

LOGFIT - DEGREE= 7 ACCURACY= 1.74% END GRADIENT: LOWER= 29.87 UPPER= -0.05

**Notes:**