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# ADAS203: General z excitation - extraction from general z file

The program prepares a fully specified specific ion file of type *adf04* for an unknown ion of an isoelectronic sequence from a general z excitation file of type *adf05* for the sequence. The general z excitation file contains ionisation potentials, energy levels and transition probabilities in addition to rate parameter (Upsilon) data for a set of members of the isoelectronic sequence. As part of its operation ADAS203, which is essentially a z-interpolation code, also allows display of individual reaction rates for the selected ion and improvement 'visually' of the fitting parameters beyond those present in the general z excitation file.

## Background theory:

In many cases, theoretical electron impact cross-section data are available for a number of members of an iso-electronic sequence. Also, often these data are consistent in that they are generated by a particular theoretical method and span the same set of transitions. In these circumstances, regularities of cross-section data along the iso-electronic sequence are apparent. ADAS203 in association with the data type ADF05, called a 'general z excitation file', seeks to take advantage of this by interpolation to intermediate ions of the sequence. Since the primary starting point of population calculation in ADAS2 series is the specific ion file, the organisation of the ADF05 data type and ADAS203 is such that a fully specified specific ion file can be generated from the general z file. Thus the general z file contains ionisation potentials, energy levels and transition probabilities in addition to rate parameter (Upsilon) data of a set of members of the isoelectronic sequence, all of which are interpolable.

### Ionisation potentials

Consider a set of members of an isoelectronic sequence of ion charges  $\{z_i: i = 1, \dots, I_s\}$ . If the nuclear charge of the neutral member of the sequence is  $z_s$ , then the member nuclear charges are  $\{z_{0,i} = z_i + z_s: i = 1, \dots, I_s\}$ . The ion charges  $+1$  are of principal importance for interpolation in z, namely,  $\{z_{1,i} = z_i + 1: i = 1, \dots, I_s\}$ .

Let the ionisation potentials of the sequence members be  $\{BW_i: i = 1, \dots, I_s\}$ , where the  $BW_i$  are expressed in wave number units. The *reduced ionisation potentials* are defined by

$$bw_i = BW_i / (109737.3 z_{1,i}) - z_{1,i} / n_{0,i}^2 \quad 3.3.1$$

where  $n_{0,i}$  is the principal quantum number of the ground level of the ion  $i$ . A cubic spline, with independent variable  $z_1$  is fitted to the  $bw_i$  for interpolation to intermediate z. Zero curvature end conditions are set for the spline.

### Energy levels

Let the energy levels be  $\{EW_{k,i}: k = 1, \dots, L; i = 1, \dots, I_s\}$  where the  $EW_{k,i}$  are expressed in wave number units relative to the lowest level and  $L$  is the number of energy levels. The *reduced energy levels* are defined by

$$ew_{k,i} = EW_{k,i} / (109737.3 z_{1,i}) - z_{1,i} (1/n_{0,i}^2 - 1/n_{k,i}^2) \quad 3.3.2$$

where  $n_{0,i}$  is the principal quantum number of the ground level of the ion  $i$  and  $n_{k,i}$  is the principal quantum number of the excited level  $k$  of the valence electron. A cubic spline, with independent variable  $z_1$  is fitted to the  $ew_i$  for interpolation to intermediate z. Zero curvature end conditions are set for the spline.

### Transition probabilities

Let the transition probabilities be  $\{A_{t,i}: t = 1, \dots, T; i = 1, \dots, I_s\}$  where the  $A_{t,i}$  are expressed in  $s^{-1}$  and  $T$  is the number of number of transitions given in the general z file. The *reduced transition probabilities* are defined by

$$a_{t,i} = A_{t,i} / z_{1,i}^{\alpha_t} \quad 3.3.3$$

where  $\alpha_t$  is chosen for the particular transition. The general z file contains a default value for the parameter  $\alpha_t$  for each transition deduced from inspection of reduced transition probability curves. The value is a compromise, especially between high and low z regions and some improvement is possible when interpolation is sought in a particular region of z. The ADAS203 code permits such adjustment. A cubic spline, with independent variable either  $z_1$  or  $1/z_1$  is fitted to the  $a_{t,i}$  for interpolation to intermediate z. The independent variable choice is influenced in practise by observing the smoothness and flatness of the  $a_t$  reduced graph. Zero curvature end conditions are set for the spline.

#### Rate parameters (upsilons)

Let the rate parameters be  $\{Y_{t,j,i} : t = 1, \dots, T ; j = 1, \dots, M ; i = 1, \dots, I_s\}$  where the  $Y_{t,j,i}$  are given for *reduced temperatures*  $\{\theta_j = T_{e,j} / z_1^2 : j = 1, M\}$ . The same set of reduced temperatures applies to the data for each ion of the sequence and transition, but different sets may be present in the general z file for different transitions.  $T$  is the number of number of transitions given in the general z file. The *reduced rate parameters* are defined by

$$\gamma_{t,i} = Y_{t,i} / z_{1,i}^{\beta_t} \quad 3.3.4$$

where  $\beta_t$  is chosen for the particular transition. The general z file contains a default value for the parameter  $\beta_t$  for each transition deduced from inspection of the closeness of the superposition of reduced rate parameter curves for each sequence member as a function of reduced temperature. The value is a compromise, especially between high and low z regions and some improvement is possible when interpolation is sought in a particular region of z. The ADAS203 code permits such adjustment.

The first interpolation is in z at each reduced temperature. A cubic spline, with independent variable either  $z_1$  or  $1/z_1$  is fitted to the  $\gamma_{t,i}$  for interpolation to intermediate z. Zero curvature end conditions are set for the spline. The result is a set of reduced rate parameters for the transition for the selected intermediate ion at the set of reduced temperatures.

The second interpolation is in temperature to obtain rate parameters at the output temperatures required for the specific ion file. This interpolation uses the methods of ADAS102. Three distinct types of rate coefficient are recognised, namely, dipole, non-dipole and spin change. Each has an expected approximate form, namely,

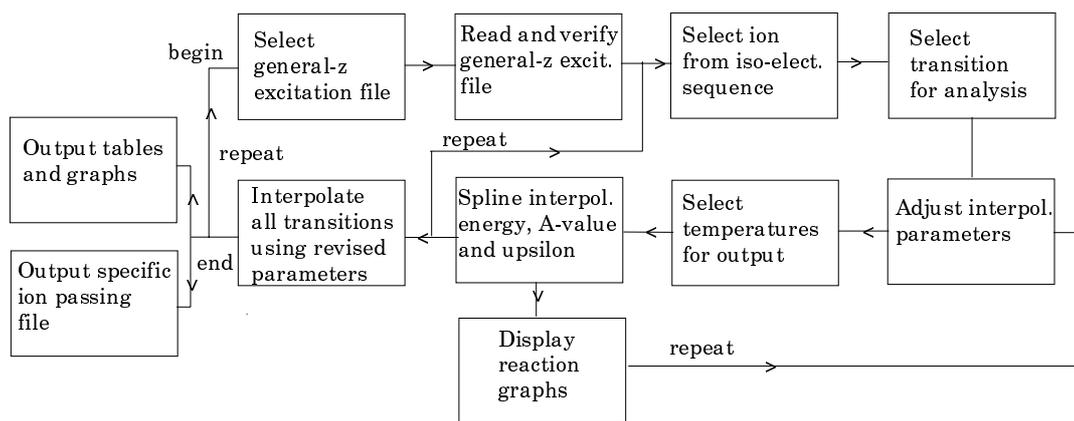
$$\begin{aligned} \text{dipole:} \quad Y_{ij} &\approx F_3 S_{ij} \left[ \log(1 + F_2) + EEI((1 + F_2) \Delta E_{ij} / kT_e) \right] \\ \text{non-dipole:} \quad Y_{ij} &\approx [*** update in progress ***] \\ \text{spin change:} \quad Y_{ij} &\approx \frac{F_3 (\Delta E_{ij} / kT_e)}{1 + F_2} EE2((1 + F_2) \Delta E_{ij} / kT_e) \end{aligned} \quad 3.3.5$$

where  $EEI(x) = \exp(x)E_1(x)$  and  $EE2(x) = \exp(x)E_2(x)$  with  $E_1$  and  $E_2$  the first and second exponential integrals. A ratio is formed of the actual to approximate form. This ratio is interpolated by cubic spline. The end conditions are of zero gradient. The final interpolated rate parameters are obtained by multiplying the interpolant by the approximate form. For completeness, a fourth approximate form is available which is a simple constant. In the event of oscillatory behaviour of the spline or of expected poor first interpolation an option to use linear interpolations is available.

## Program steps:

These are summarised in figure 3.3.

Figure 3.3

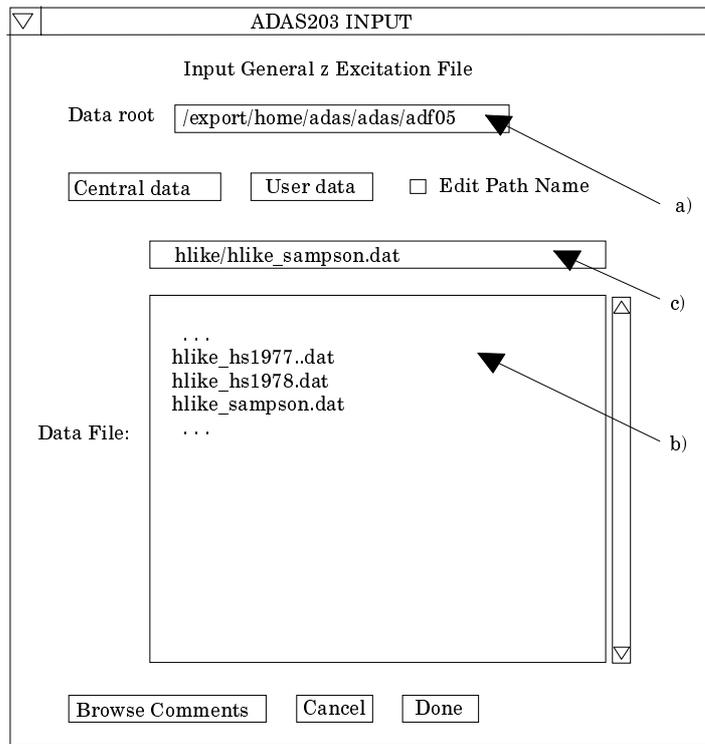


### Interactive parameter comments:

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 and move to the series 2 menu. Select ADAS203.

The **file selection window** appears first and is illustrated below. Its operation follows the usual pattern.

1. *adf05* is the appropriate format for use by the program ADAS203. 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. A Data root path to the correct data type *adf05* appears automatically a). 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.
3. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
4. 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.
5. 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*.
6. Clicking on the *Browse Comments* button displays any information stored in the selected charge exchange 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

8. An arbitrary title may be given for the case being processed a). For information the full pathway to the general z 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.
9. Enter at b) your selection of the ion for analysis and for which a specific ion file is sought. For guidance, some details of the content of the source general z file are displayed. The isoelectronic sequence is shown first. We call this the 'recombined ion' isoelectronic sequence. Then the nuclear charge, recombined ion charge and element symbol, for each member of the isoelectronic sequence explicitly present in the general z file, are shown in the scrollable display window. The object of the code is to interpolate to an intermediate ion of the sequence within the span of the members. Enter the nuclear charge of the ion for which you wish output.
10. At c) a summary of the number of energy levels and number of electron impact transitions present in the general z file is given and then an actual list of these transitions in the display window. You can choose to examine (or modify) the z-interpolation for a particular transition by clicking on that transition in the list. The selected transition is shown in the transition selection window above.
11. The general z file has predefined settings and scaling parameters for each transition within it, designed as far as possible to give acceptable interpolation. The settings are divided into two classes namely those for obtaining the transition energy and transition probability (I) and those for obtaining the upsilons (II). Activate the appropriate button at d) and the corresponding settings and scalings are shown in the sub-window. These choices may be changed by the user. The usual practise is to choose values which make the graphs of the transition energy, transition probability and upilon look as flat as possible (in fact reduced quantities are displayed on the graphs). This is done by visual inspection of the displayed graphs and iteration back to this window.
12. Your settings of electron temperatures for the output specific ion file are shown in the temperature display window f). The temperature values present in the source general z file are also shown for reference. Note that the general z file has the upilon data for all the member ions at the same set of z-scaled temperatures. Thus the actual input temperatures change as you select different ions for output.

13. The program recovers the output temperatures you used when last executing the program. The output temperatures may be edited in the usual manner. Click on the *Edit Table* button if you wish to change the values. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures. For convenience a *Clear Table* button has been added.

ADAS203 PROCESSING OPTIONS

Title for Run

General-z file : /export/home/adas/adas/adf05/hlike/hlike\_sampson.dat

Select Ion For Analysis

Recombined ion iso-electronic sequence = H  
----- members -----

Index	Nuclear Charge	Recombined Ion Charge	Element Symbol
1	14	13	Si
2	18	17	Ar
3	26	25	Fe
4	42	41	Mo

Specify nuclear charge of member required

Select Specific Electron Impact Transition :-  
No. of electron impact transitions = 11  
No. of index energy levels = 6  
----- Transitions -----

Transition Index	Upper Level Index	Upper Level Designation	Lower Level Index	Lower Level Designation
1	2	2s (2)S( 0.5)	1	1s (2)S( 0.5)
2	3	2p (2)P( 2.5)	1	1s (2)S( 0.5)
3	4	3s (2)S( 0.5)	1	1s (2)S( 0.5)

Select option for display :  Settings/scalings (I)  
 Settings/scalings (II)

Transition energy - z-zpline independent variable

Einstein coefficient - z-spline independent variable

Einstein coefficient - Transition type

Einstein coefficient - z1 power for scaling factor

Output Electron Temperatures

INDEX	Output values	Input values
1		
2		
3		
4		

Temperature Units : Kelvin

Edit the processing options data and press Done to proceed

14. The *Exit to Menu* icon is present in ADAS203. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **Output options window** is shown below. Broadly it follows the pattern of other ADAS interrogation codes. However since a number of graphs and text outputs are possible, the window has been designed to avoid too much complexity on screen.

15. As usual, the input general z file under analysis is shown at a) and can be browsed. Two buttons have been added at a), namely, *Graphics* and *Text*. Activate *Graphics* and the standard graphical output sub-window appears. Activate *Text* and the standard text file output sub-windows appears instead.
16. In the *Graphics* case, on screen graphical display is enabled by clicking on the *Graphical output* button. There are three choices of graph, namely, transition wave number, A-value and rate parameter. Click the appropriate button at b). Default scaling of the chosen graph may be over-riden by appropriate selections. Labelling of the separate curves on the rate parameter plot may be switched on by the choices at c). Below this the usual hard copy may be enabled and a choice of type of output device made.

17. In the Text case, two output files are permitted (arrowed at e)), namely, the standard line printer text output file summarising the interrogation and the output specific ion file of type *adf04*. For historic and nostalgic reasons we call this the COPASE passing file. It is put in your */pass* directory as *copase.pass* by default. The usual *Replace* and *Default File Name* buttons are present for both output files.
18. Various completion buttons are available at d). Click the *View Graph* button to show the graph. *Back to Processing* returns you to the previous window for choice of another transition for analysis. Note that the settings from analyses carried out by you are accumulated. Click the *Output and Exit* to write the COPASE passing file and then exit. Note that the COPASE file contains all the transitions in the general z file with the default settings for the transition interpolations except where you have conducted an analysis. In these latter cases, your adjusted settings are used and suitably documented in the comments section at the foot of the COPASE passing file. There is an alternative button, *Output and Return Here* which similarly creates the COPASE file but instead of exiting returns you to this window. The *Exit to Menu* icon takes you directly to the ADAS2 series menu.

The screenshot shows the 'ADAS203 OUTPUT OPTIONS' dialog box. At the top, it displays the script file path and a 'Browse Comments' button. Below this, there are radio buttons for 'Graphics' and 'Text'. The 'Graphics' section includes a 'Graphical output' checkbox, a 'Graph Title' field (set to 'Figure 1'), and three radio buttons for plot types: 'Scaled transition wave number vs. ion charge', 'Scaled A-value vs. ion charge', and 'Scaled rate parameter vs. z-scaled electron temperature'. A 'Scaled A-value plot' section contains an 'Explicit scaling' checkbox and four input fields for X-min, X-max, Y-min, and Y-max. Below this is a 'Label Lines with indices on rate parameter plot' section with 'No' and 'Yes' radio buttons. The bottom section of the dialog has 'Enable Hard Copy' and 'Replace' checkboxes, a 'File Name' field (set to 'Graph.ps'), and a 'Select Device' dropdown menu with options 'Post script', 'HP-PCL', and 'HP-GL'. At the very bottom are buttons for 'Back to Processing', 'View Graph', 'Output and Exit', and 'Output and Return Here'. Annotations a-e point to various parts of the interface: 'a)' points to the 'Graphical output' checkbox, 'b)' to the plot type radio buttons, 'c)' to the 'Label Lines...' radio buttons, 'd)' to the 'Output and Return Here' button, and 'e)' to the 'Text Output' section below the main dialog.

a)  Graphical output  
Graph Title

b)  Scaled transition wave number vs. ion charge  
 Scaled A-value vs. ion charge  
 Scaled rate parameter vs. z-scaled electron temperature

Scaled A-value plot :-  
 Explicit scaling  
X-min :  X-max :   
Y-min :  Y-max :

c) Label Lines with indices on rate parameter plot :  No  Yes

Enable Hard Copy  Replace  
File Name :

Select Device

d)  COPASE Passing File  Replace   
File Name :

e)  Text Output  Replace   
File Name :

### Illustration:

The illustration is from a lithium-like general-z file spanning from carbon to iron. The z-interpolation shown here is to nitrogen. Figure 3.3a shows the scaled Upsilon plot Vs scaled electron temperature. The interpolated ADF04 file for lithium-like nitrogen created by the code is shown in table 3.3a. The summary information is given in the standard text output file shown in table 3.3b.

Figure 3.3a.

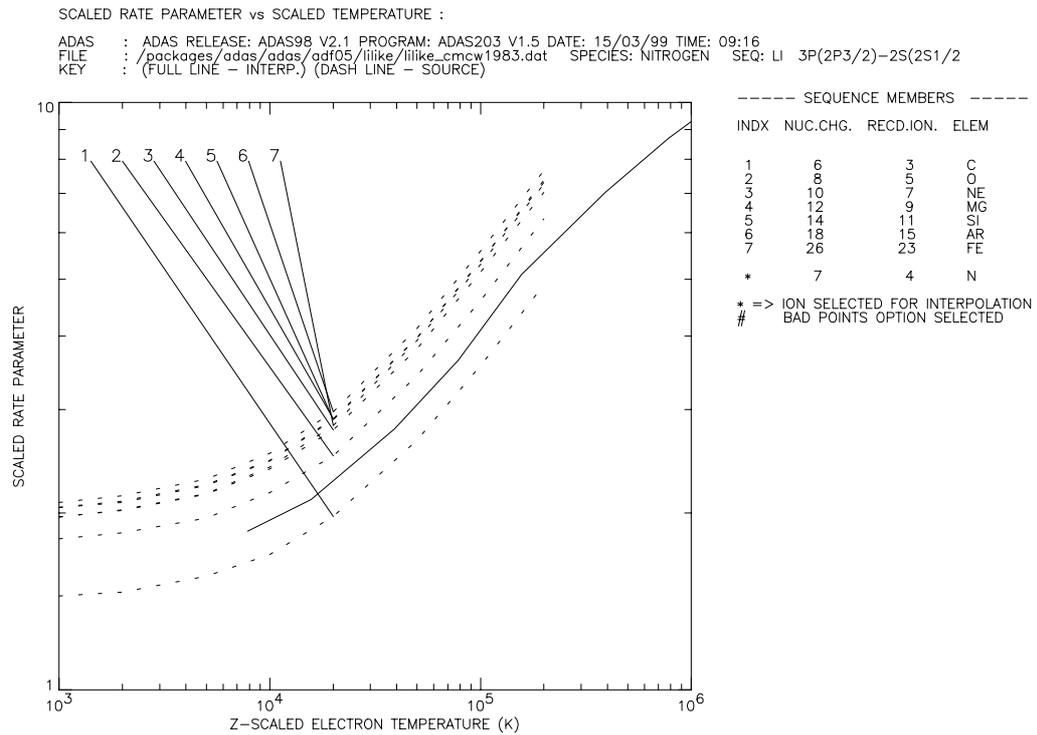


Table 3.3a.

n + 4	7	5	789029.							
1	1S2 2S(1/2)	(2)0( 0.5)						0.0		
2	1S2 2P(1/2)	(2)1( 0.5)						80476.7		
3	1S2 2P(3/2)	(2)1( 1.5)						80667.3		
4	1S2 3S(1/2)	(2)0( 0.5)						455806.5		
5	1S2 3P(1/2)	(2)1( 0.5)						477486.2		
6	1S2 3P(3/2)	(2)1( 1.5)						477556.1		
7	1S2 3D(3/2)	(2)2( 1.5)						483915.3		
8	1S2 3D(5/2)	(2)2( 2.5)						483946.6		
-1										
5.00	3	1.96+05	3.92+05	9.80+05	1.96+06	3.92+06	9.80+06	1.96+07	3.92+07	
2	1	3.34+08	2.43+00	2.61+00	2.99+00	3.40+00	3.86+00	4.64+00	5.31+00	6.03+00
3	1	3.50+08	4.82+00	5.19+00	5.93+00	6.75+00	7.67+00	9.23+00	1.06+01	1.20+01
4	1	0.00+00	2.67-01	2.74-01	2.85-01	2.93-01	3.02-01	3.02-01	3.02-01	3.02-01
5	1	1.14+10	5.85-02	6.62-02	8.71-02	1.14-01	1.59-01	2.20-01	2.71-01	3.27-01
6	1	1.14+10	1.21-01	1.37-01	1.80-01	2.36-01	3.30-01	4.56-01	5.64-01	6.80-01
7	1	0.00+00	1.48-01	1.56-01	1.79-01	1.98-01	2.31-01	2.35-01	2.35-01	2.35-01
8	1	0.00+00	2.95-01	3.13-01	3.57-01	3.96-01	4.62-01	4.69-01	4.69-01	4.69-01
5	2	0.00+00	3.87-01	3.87-01	3.87-01	3.87-01	3.87-01	3.87-01	3.87-01	3.87-01
6	3	0.00+00	7.77-01	7.77-01	7.77-01	7.77-01	7.77-01	7.77-01	7.77-01	7.77-01
4	2	3.19+09	5.75-02	6.06-02	6.92-02	8.09-02	1.02-01	1.31-01	1.57-01	1.85-01
4	3	6.40+09	1.15-01	1.21-01	1.39-01	1.62-01	2.04-01	2.62-01	3.14-01	3.70-01
7	2	3.59+10	1.31+00	1.42+00	1.72+00	2.10+00	2.64+00	3.47+00	4.20+00	4.99+00
7	3	7.18+09	2.61-01	2.85-01	3.45-01	4.19-01	5.27-01	6.92-01	8.38-01	9.97-01
8	3	4.30+10	2.35+00	2.56+00	3.11+00	3.77+00	4.74+00	6.23+00	7.54+00	8.97+00
-1										
-1	-1									
C	-----									
C	Specific ion file created from general Z excit. file									
C	Processing code: ADAS203									
C	General Z excit. source file: /packages/adas/adas/adf05/lilike/lilike_cmcw1983.dat									
C	Scaling parameter adjustments from source file defaults:									
C	Indx	IEC1	IAC1	IAC2	FAC2	IGC1	FGC2	LBPTS		
C	5	1	1	1	4.00	1	-1.70	T		
C	Prepared by: •jl barwani - /home/									
C	Date : 15/03/99									
C	-----									

Table 3.3b

```

ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS203 V1.5 DATE: 15/03/99 TIME: 09:16
**** TABULAR OUTPUT FROM GENERAL Z EXCIT. FILE PROGRAM: ADAS203 - DATE: 15/03/99 ****

INPUT GENERAL Z EXCIT. FILE NAME: /packages/adas/adas/adf05/lilike/lilike_cmcw1983.dat

SELECTED      NUCLEAR      RECOMBINING      ----- IONIZATION POTENTIAL -----
ION           CHARGE (Z0)      ION CHARGE (Z1)  (wave number <cm-1>) (rydbergs)
-----
n + 4         7                5                789029.          7.1901797

----- ENERGY LEVELS -----
INDEX  CONFIGURATION  (2S+1)L(J)  ----- ENERGY RELATIVE TO LEVEL 1 ----- ENERGY RELATIVE TO IONISATION
POTENTIAL                                     (wave number <cm-1>) (rydbergs) (wave number <cm-1>) (rydbergs)
-----
1  1S2 2S(1/2)    (2)0( 0.5)      0.          0.0000000      789029.        7.1901797
2  1S2 2P(1/2)    (2)1( 0.5)      80477.        0.7333596      708553.        6.4568201
3  1S2 2P(3/2)    (2)1( 1.5)      80667.        0.7350961      708362.        6.4550836
4  1S2 3S(1/2)    (2)0( 0.5)      455807.       4.1536237      333223.        3.0365560
5  1S2 3P(1/2)    (2)1( 0.5)      477486.       4.3511840      311543.        2.8389957
6  1S2 3P(3/2)    (2)1( 1.5)      477556.       4.3518211      311473.        2.8383586
7  1S2 3D(3/2)    (2)2( 1.5)      483915.       4.4097700      305114.        2.7804097
8  1S2 3D(5/2)    (2)2( 2.5)      483947.       4.4100553      305083.        2.7801244

INPUT GENERAL Z FILE INFORMATION:
-----
ISOELECTRONIC SEQUENCE NEUTRAL MEMBER = LI
NUMBER OF ELECTRON IMPACT TRANSITIONS = 14
NUMBER OF IONS IN GENERAL Z FILE      = 7

----- INPUT MEMBERS -----
INDEX  NUCLEAR  RECOMBINED  ELEMENT
      CHARGE  ION CHARGE  SYMBOL
-----
1      6        3          c
2      8        5          o
3     10        7          ne
4     12        9          mg
5     14       11          si
6     18       15          ar
7     26       23          fe

-- INPUT GENERAL Z TEMPERATURES AT SELECTED ION --
INDEX  (Kelvin)  (eV)  (Reduced)
-----
1      2.500D+04  3.100D+00  1.000D+03
2      5.000D+04  6.199D+00  2.000D+03
3     1.250D+05  1.550D+01  5.000D+03
4      2.500D+05  3.100D+01  1.000D+04
5      5.000D+05  6.199D+01  2.000D+04
6     1.250D+06  1.550D+02  5.000D+04
7     2.500D+06  3.100D+02  1.000D+05
8     5.000D+06  6.199D+02  2.000D+05

OUTPUT SPECIFIC ION FILE INFORMATION:
-----
---- OUTPUT TEMPERATURES FOR SPECIFIC ION FILE ---
INDEX  (Kelvin)  (eV)  (Reduced)
-----
1      1.960D+05  2.430D+01  7.840D+03
2      3.920D+05  4.860D+01  1.568D+04
3      9.800D+05  1.215D+02  3.920D+04
4     1.960D+06  2.430D+02  7.840D+04
5     3.920D+06  4.860D+02  1.568D+05
6     9.800D+06  1.215D+03  3.920D+05
7     1.960D+07  2.430D+03  7.840D+05
8     3.920D+07  4.860D+03  1.568D+06

-- SCALING PARAMETER ADJUSTMENTS FROM SOURCE FILE DEFAULTS --
INDEX  IEC1  IAC1  IAC2  FAC2  IGC1  FGC2  LBPTS
-----
5      1    1    1    4.00  1    -1.70  T

```

Notes: