

ADAS413: Collisional ionisation – graph and fit data

The code allows interrogation of state selective collisional ionisation rate coefficient data of ADAS data format *adf23* which distinguish initial state of the ionising ion and final state of the ionised ion. These data can be extracted and displayed by the new code.

Background theory:

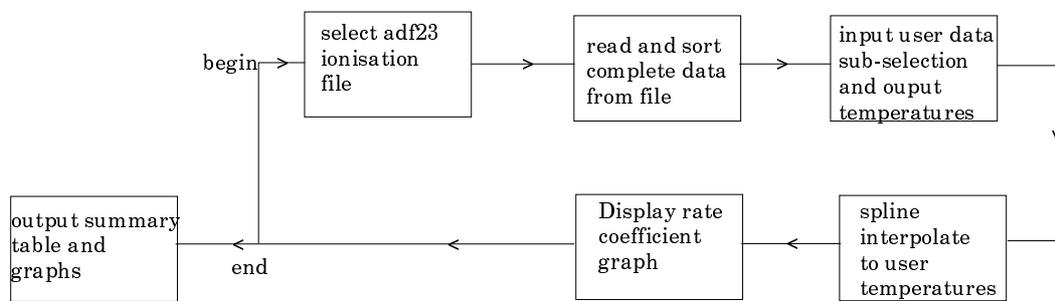
The code and background theory is being extended to include the planned new intermediate coupling ionisation data. The following notes are incomplete.

The detailed ionisation models and data for access by the code are described in ADAS213. Spline interpolation as a function of temperature is used to provide the interrogation results here.

Program steps:

These are summarised in figure 5.13.

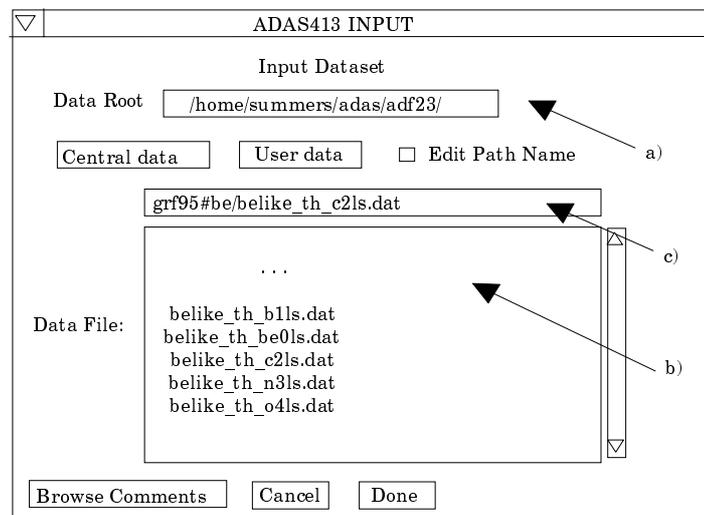
Figure 5.13



Interactive parameter comments:

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

1. Data root a) shows the full pathway to the appropriate data subdirectories of type *adf23*. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. 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*. Note the notation used for radiative recombination data file names, that is, $\langle ion \rangle ls$ with $\langle ion \rangle$ the recombining ion. *ls* indicates that the radiative recombination data is at LS-resolution.
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.
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.

▼
ADAS413 PROCESSING OPTIONS
a)

Title for Run

Data File Name : /home/summers/adas/adf23/grf95#be/belike_th_c2ls.dat

Nuclear charge : 6 Ionised ion charge : 3 Ionising ion charge : 2

◇ Direct Ionis.
◇ Excit. to Autoion. Levels
◇ Excit. to Autoion. n-shells

Select Ionising Level

INDEX	Ionising Level	Term	Configuration
2	*2s1 2p1	1P	
1	*2s2 2p0	1S	
2	*2s1 2p1	3P	

Select Ionised Parent

INDEX	Ionised Parent	Term	Valid Data
1	2s1 2p0	2S	T
1	*2s1 2p0	2S	T
2	*2s0 2p1	2P	T

Output Electron Temperatures

INDEX	Output	Input
1		
2		
3		
4		

Temperature Units : Kelvin

Edit Table

Default Temperatures

Polynomial Fitting

Fit Polynomial Value % :

Edit the processing options data and press Done to proceed

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b)

d)

f)

g)

a)

c)

e)

8. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being interrogated is also shown at b). The button *Browse comments* at a) again allows display of the information field section at the foot of the selected dataset, if it exists.
9. At c), there are three types of data for selection, *Direct Ionis.*, *Excit. To Autoion. Levels* and *Excit. to Autoion. N-shells*. In the case of *Direct Ionis.*, as illustrated at d), the initial ionising state is selected at d) by clicking on an entry in the selection window. Then the final parent, that is the final ionised ion state is selected at e).
10. At this time there is no sample data of the other two types in the adf23 files.
11. At f), the electron temperatures at which you wish the collisional ionisation data is chosen. Table editor is available to enter this data and default temperatures (equal to those in the *adf23* file) may be chosen by button click as usual.
12. The option of fitting a polynomial to the extracted data is offered just below the temperature selection widget.
13. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

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

14. As in the previous window, the full pathway to the file being analysed is shown for information at a). Also the *Browse comments* button is available.
15. Graphical display is activated by the *Graphical Output* button at b). 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.
16. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button at b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.

The screenshot shows the 'ADAS413 OUTPUT OPTIONS' window. At the top, there is a checked box and the title 'ADAS413 OUTPUT OPTIONS'. Below the title, the 'Data File Name' is displayed as '/home/summers/adas/adf23/grf95#be/belike_th_c2ls.dat'. A 'Browse Comments' button is located below the file name. The main area contains several sections:

- A section with a checked box for 'Graphical Output'. It includes a 'Graph Title' field with the text 'Figure 1' and a 'Select Device' dropdown menu with options 'Post script', 'Post script HP-PCL', and 'HP-GL'.
- A section with a checked box for 'Explicit scaling'. It contains four input fields for 'X-min', 'X-max', 'Y-min', and 'Y-max'.
- A section with two unchecked checkboxes: 'Enable Hard Copy' and 'Replace'. Below them is a 'File Name' field containing 'graph.ps'.
- A section with two unchecked checkboxes: 'Text Output' and 'Replace'. It includes a 'Default File Name' button and an empty 'File Name' field.

 At the bottom of the window are three buttons: a menu icon, 'Cancel', and 'Done'. Annotations 'a)', 'b)', 'c)', and 'd)' point to the 'Browse Comments' button, the 'Graphical Output' section, the 'Explicit scaling' section, and the 'Text Output' section respectively.

17. Hard copy is activated by the *Enable Hard Copy* button at 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.
18. A choice of output graph plotting devices is given in the Device list window to the right. Clicking on the required device selects it. It appears in the selection window above the Device list window.
19. At d) output of the tabular record of the interrogation may be enabled. This is usually called *paper.txt* and it is created in the directory from which ADAS was launched.
20. The graph is displayed in a following Graphical Output window.
21. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

Illustration:

Figure 5.13a

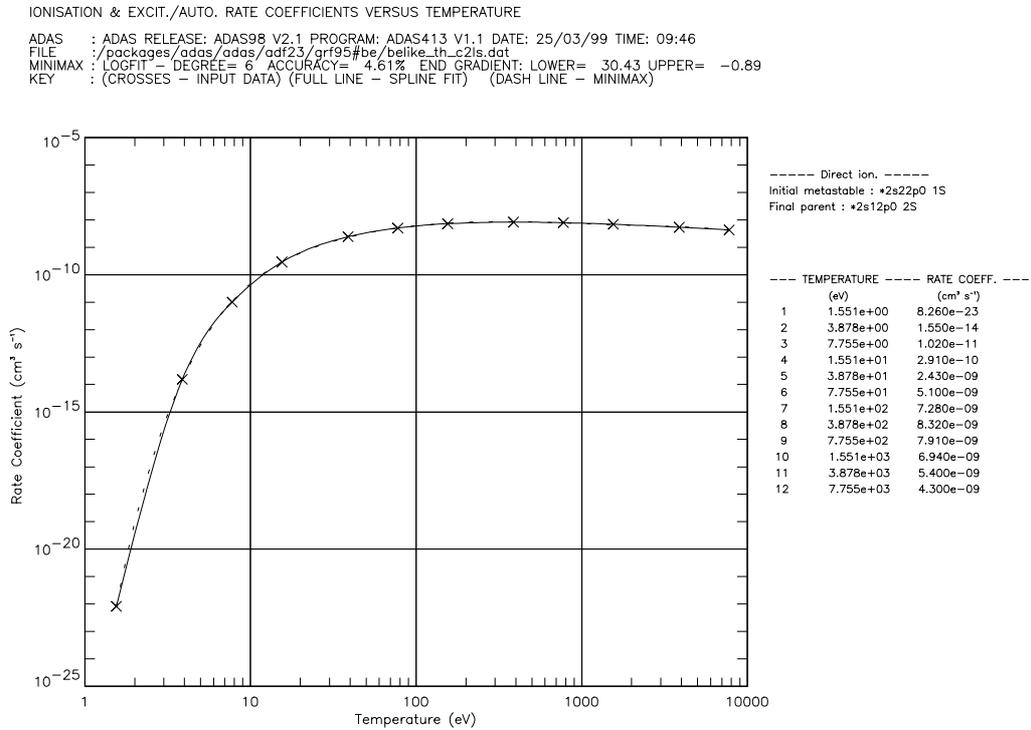


Table 5.13a

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ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS413 V1.1 DATE: 25/03/99 TIME: 09:46

**** TABULAR OUTPUT FROM IONISATION EXCIT/AUTOION. RATE-COEFFICIENTS IN PROGRAM: ADAS413 - DATE: 25/03/99
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IONISATION & EXCIT./AUTO. RATE-COEFFICIENTS AS A FUNCTION OF TEMPERATURE
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DATA GENERATED USING PROGRAM: ADAS413
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FILE : /packages/adas/adas/adf23/grf95#be/belike_th_c21s.dat

Element          : CARBON
Nuclear charge   (Z0) : 6
Ionised ion charge (Z1) : 3
Ionising ion charge (Z) : 2
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Initial metastable : *2s22p0 1S
Final parent       : *2s12p0 2S

----- TEMPERATURE ----- RATE COEFFICIENT

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Kelvin	eV	cm**3/sec
1.800D+04	1.551D+00	8.2600D-23
4.500D+04	3.878D+00	1.5500D-14
9.000D+04	7.755D+00	1.0200D-11
1.800D+05	1.551D+01	2.9100D-10
4.500D+05	3.878D+01	2.4300D-09
9.000D+05	7.755D+01	5.1000D-09
1.800D+06	1.551D+02	7.2800D-09
4.500D+06	3.878D+02	8.3200D-09
9.000D+06	7.755D+02	7.9100D-09
1.800D+07	1.551D+03	6.9400D-09
4.500D+07	3.878D+03	5.4000D-09
9.000D+07	7.755D+03	4.3000D-09

NOTE: * => RATE-COEFFICIENT EXTRAPOLATED FOR THIS TEMPERATURE VALUE

A(1) = -2.910672271D+01	A(2) = 4.419277516D+01
A(3) = -4.202710354D+01	A(4) = 2.242739120D+01
A(5) = -6.850384550D+00	A(6) = 1.110077863D+00
A(7) = -7.375975341D-02	

LOGFIT - DEGREE= 6 ACCURACY= 4.61% END GRADIENT: LOWER= 30.43 UPPER= -0.89

Notes: