

may18-95

ADAS Bulletin

Two ADAS series 3 programs are now ready. Together they allow interrogation of fundamental charge transfer collision cross-section data in the database from neutral donors to full ionised ions and then of the effective emission coefficients of charge exchange spectroscopy derived from them. In this bulletin, I wish to give an overview of the user interface to these programs.

Firstly, some advice - when we put up a new release which includes amendments to existing programs, your defaults data sets may become inappropriate. This usually manifests itself by an ADAS program which you have initiated simply stopping and sending you back to the main selection menu. In these circumstances, delete the existing defaults data set for that program in your `./../adas/defaults/` directory. ADAS will create a new one for you.

1. ADAS301

This is a conventional interactive interrogation program. Its broad operation is as for ADAS201 (cf. bulletin *mar18-95*).

- 1.1. 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.

- 1.2. 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)
- 1.3. Initiate ADAS, move to the series 3 menu and click on the first button to activate ADAS301.
- 1.4. The **file selection window** appears first. Its appearance is as described in the bulletin *jan18-95*.
 - 1.4.1. Note that each type of data is stored according to its ADAS data format (*adf* number). *adf01* is the appropriate format for use by the program ADAS301. 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*.
 - 1.4.2. Available sub-directories are shown in the large file display window. Scroll bars appear if the number of entries exceed the file display window size. There are a large number of these. They are stored in sub-directories by donor which is usually neutral but not necessarily so (eg. *qcx#h0*). The individual members are identified by the subdirectory name, a code and then fully ionised receiver (eg. *qcx#h0_old#c6.dat*). The data sets generally contain *nl*-resolved cross-section data but *n*-resolved and *nlm*-resolved are handled. Resolution levels must not be mixed in datasets.
 - 1.4.3. The codes distinguish different sources. The first letter *o* or the code *old* has been used to indicate that the data has been produced from JET compilations which originally had parametrised *l*-distribution of cross-sections. The *nl*-resolved data with such code has been reconstituted from them. Data of code *old* is the preferred JET data. Other sources codes include *ory* (old Ryufuku), *ool* (old Olson), *ofr* (old Fritsch) and *omo* (old molecular orbital). There are new data such as *kvi*.
 - 1.4.4. Click on a file name in the file display window to select it. The selected name appears in the smaller selection window above the file display window. Then the individual datafiles are presented for selection. Datafiles, as distinct from directories, all have the termination *.dat*.
 - 1.4.5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
 - 1.4.6. 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 has gone into the dataset and the attribution of the dataset. The possibility of browsing the comments appears in the subsequent main window also.

1.4.7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

1.5. The **processing options window** has the appearance shown below

▼
ADAS301 PROCESSING OPTIONS

Title for Run

Data File Name : /export/home/adas/adas/adf01/qcx#h0/qcx#h0_c6.dat

Polynomial fitting

Fit Polynomial value % :

Select velocities/energies for Output File

Output Collision velocities/energies

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

Select quantum numbers for processing

	Range	Total
Principal quantum no. N (1-12)	<input type="checkbox"/>	[0]
Orbital quantum no. L (0-N-1)	<input type="checkbox"/>	[-1]
Azimuthal quantum no. M (0-L)	<input type="checkbox"/>	[-1]

Data is N and L resolved

Edit the processing options data and press Done to continue

1.5.1. 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.

1.5.2. The output data extracted from the datafile, a 'charge exchange cross-section', may be fitted with a polynomial. This is as a function of relative collision energy per atomic mass unit (eV/amu). Clicking the *Fit Polynomial* button 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.**

1.5.3. You may operate in velocity units or energy units as you find convenient. Your settings of collision velocity/energy (output) are shown in the display window. The velocity/energy values at which the charge exchange coefficients are stored in the datafile (input) are also shown for information.

1.5.4. The program recovers the output velocities/energies you used when last executing the program. Pressing the *Default Velocity/Energy values* button inserts a default set of velocities/energies equal to the input velocities/energies

1.5.5. The Velocity/Energy 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 the *18nov-94* bulletin.

- 1.5.6. The specific cross-section data to be extracted is specified by the window to the right at a). The level or resolution of the data source is shown at c). Activate the *Select quantum numbers for processing* button to allow new settings of these quantum numbers. The values in the three smaller windows b) become editable depending also on the resolution of the dataset. Note that the *Range* of the data in the dataset is displayed. There are special codes to be used to obtain summed cross-sections over sub-quantum numbers. These are indicated in brackets under the *Total* column and should be entered into the editable window if required.
- 1.5.6. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.
- 1.6. The **output options window** appearance is of the standard form described in bulletin *jan18-95*.
 - 1.6.1. The graph is displayed in a following **Graphical Output** window.

2. **ADAS303**

This is conventional interactive interrogation program. Its broad operation is as for ADAS301 above. It interrogates effective emission coefficients for charge exchange spectrum lines. These depend on plasma conditions which are specified in the interrogation.

- 2.1. The **file selection window** appears first and follows the standard pattern..
 - 2.1.1. *adf12* is the appropriate format for use by the program ADAS301. Details of the organisation of such data is given in the ADAS Manual.
 - 2.1.2. Available sub-directories are shown in the large file display window. Scroll bars appear if the number of entries exceed the file display window size. There are a large number of these. They are stored in sub-directories by donor which is usually neutral but not necessarily so (eg. *qef93#h*). The individual members are identified by the subdirectory name, a code and then fully ionised receiver (eg. *qef93#h_be4.dat*). The data sets generally contain many individual spectrum lines.
 - 2.1.3. Such data is generally stored by year number (eg. *93*) with the most recent data to be preferred.
- 2.2. The **processing options window** has the appearance shown below:
 - 2.2.1. The usual title entry and polynomial fitting facilities are present.
 - 2.2.2. A transition display window with selected transition window above is present at a). This follows the same pattern as ADAS201 but with different information fields. Click as usual on the transition to be selected.
 - 2.2.3. Output energies for the neutral donor are displayed at b). This follows the pattern of ADAS301 above. Click the *Edit Table* button to activate the ADAS Table Editor. Note that final graphed results are of effective emission coefficient versus beam energy (eV/amu).
 - 2.2.4. Effective emission coefficients for the *adf12* database are calculated at one dimensional scans in various plasma parameters relative to a reference set of plasma conditions. Details are given in the manual. The required values of the plasma parameters for output are specified in the window to the right at c).
 - 2.2.5. To alter the settings, activate the *Select supplementary plasma parameters* button at c). The sub-windows below at d) become active with the data entry box in each editable. For information, the reference value of each plasma parameter is given together with the range of the parameter in its one-dimensional scan. Values outside the range should not be entered.
 - 2.2.6. For data prepared using processing code ADAS309, the B magnetic field parameter has no effect, but is simply used for place holding. The scan in *B Magnetic* is of zero length.

ADAS303 PROCESSING OPTIONS

Title for Run

Data File Name : /export/home/adas/adas/adf13/qef93#h/qef93#h_be4.dat

Polynomial Fitting

Fit polynomial Value % :

Selection data Block

INDEX	Transition N - N'	Donor	Receiver	QCX File Source	Processing Code	Emission Type
1	3 - 2	H(1s)	BE+4	OLD#BE4	ADAS309	CX
1	3 - 2	H(1s)	BE+4	OLD#BE4	ADAS309	CX
2	4 - 3	H(1s)	BE+4	OLD#BE4	ADAS309	CX
3	5 - 4	H(1s)	BE+4	OLD#BE4	ADAS309	CX
4	6 - 5	H(1s)	BE+4	OLD#BE4	ADAS309	CX
5	7 - 6	H(1s)	BE+4	OLD#BE4	ADAS309	CX

Neutral Beam Donor Energy Values

INDEX	Output	Input
1	5.000E+03	5.000E+03
2	7.000E+03	7.000E+03
3	1.000E+04	1.000E+03
4	1.500E+04	1.500E+04
5	2.000E+04	2.000E+04

Energy/Velocity Units : eV/amu

Select supplementary plasma parameters

	Output Value:	Reference Value:	----- Minimum	----- Maximum
Ion Density (cm-3)	<input type="text" value="2.500E+13"/>	2.500E+11	1.000E+11	1.000E+14
Ion Temperature (eV)	<input type="text" value="5.000E+03"/>	5.000E+03	1.000E+03	3.000E+04
Z Effective	<input type="text" value="2.000E+00"/>	2.000E+00	1.000E+00	6.000E+00
B Magnetic (T)	<input type="text" value="3.000E+00"/>	3.000E+00	3.000E+00	3.000E+00

Edit the processing options data and press Done to proceed

2.3. The **output options window** appearance is of the standard form described in bulletin *jan18-95*.

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

At the next release, due at the beginning of July, the collisional radiative codes ADAS308 and ADAS309 which prepare data of type *adf12* from charge exchange cross-section data of type *adf01* will be made available. Together with the codes described here, a basic capability for charge exchange spectroscopy atomic modelling will then be in place.

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