Two new programs are ready. Also extensive additional data has been placed in the ADAS database. Two ADAS series 3 collisional radiative processing programs are operational. These allow preparation of charge exchange spectroscopy effective emission coefficients (*adf12*) in a beam/plasma interaction region from fundamental charge exchange cross-section data (*adf01*). The corresponding interrogation programs on *adf01* and *adf12* data were made available and described in the *may18-95* bulletin. The first program in series 1 is now available. It is much more sophisticated than the old JET equivalent and sets the pattern for all the series 1 codes. I hope its capabilities will prove useful and appealing. It is David Brooks' masterpiece. A new utility in series 2 is also released which assists in 'level bundling' for series 2 excited population programs. There will be a corresponding 'level unbundling' program which we hope to have ready for the next issue. Finally the G(Te) interrogation and stacking program from series 5 is released. This is courtesy of Alessandro Lanzafame. It is of special relevance to astrophysical differential emission measure analysis. These are additional contributions to the sterling efforts of Tim Hammond with the main JET conversion.

1.   **ADAS101**

      This is a program for examination of electron collision cross-section data from external sources and its preparation as rate coefficients for permanent storage in the ADAS database. There is no central ADAS data class associated with input to this program, since new data is entered by hand in the program. However a mechanism is provided for storage and retrieval of the output from the ADAS101 analysis. The output from a case may be stored in an archive file. Such files are present only on the user's own space. Storage is sequential with an index.

    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 ADAS created output text file (*paper.txt* is the default) and graphic files (e.g. *graph.ps* if a postscript file) to be placed.

    1.3.   Initiate ADAS, move to the series 1 menu and click on the first button to activate ADAS101.

    1.4.   The **archive selection window** appears first. It is slightly different in operation than the usual file selection window.

        1.4.1.   The recommended root path for user archiving for ADAS101 analysis is

                    /..../uid/adas/arch101/

             which may be edited in the usual manner.

        1.4.2.   Click the appropriate button at a) for opening an old archive file, starting a new archive file or ignoring archiving. In the first case, the usual file display window shows existing archive files from which selection may be made. The selected file is displayed in the selection window. In the second case, the file display window is the same, but the selection window is editable for entry of a new archive file name. **Remember to press the *return* key on the keyboard to record an entered value**.

        1.4.3.   The capability is given for reworking or re-displaying the results of an earlier analysis stored in an archive file. At b) click on the *Refresh from archive* button. Then give the *Archive index number*. The selected data will be used as the default data in the subsequent processing and output windows. Archiving is strictly sequential. A new analysis is simply appended at the end of the archive file and the index updated. These is no data replacement or substitution.

        1.4.4.   Clicking on the *Browse Index* button displays the index list for the selected archive file. The possibility of browsing the index appears in the subsequent main window also.

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

```
┌─────────────────────────────────────────────────────────┐
│ ▽          ADAS101  INPUT                                 │
│  ┌──────────────────────────────────────────────────┐   │
│  │ Data root    /home/brooks/adas/arch101/           │   │
│  │              ☐ Edit Path Name                     │   │
│  └──────────────────────────────────────────────────┘   │
│                                                           │
│              ◇ Old Archive  ◇ New Archive  ◇ No Archive   │
│                                                           │
│  ┌──────────────────────────────────────────────────┐   │
│  │       ◇     Refresh from Archive                  │   │
│  │                                                    │   │
│  │    Archive Index Number         [        ]         │   │
│  └──────────────────────────────────────────────────┘   │
│                                                           │
│           ┌──────────────────────────────────────┐       │
│           │ db95fe19_001.dat                     │       │
│           └──────────────────────────────────────┘       │
│           ┌──────────────────────────────────────┐       │
│           │ . .                                  │       │
│           │ db95fe19_001.dat                     │       │
│           │   .                                  │       │
│  Archive File                                    │       │
│           │                                      │       │
│           │                                      │       │
│           │                                      │       │
│           │                                      │       │
│           └──────────────────────────────────────┘       │
│  [ Browse Index      ]   [Cancel]  [Done]                 │
└─────────────────────────────────────────────────────────┘
```
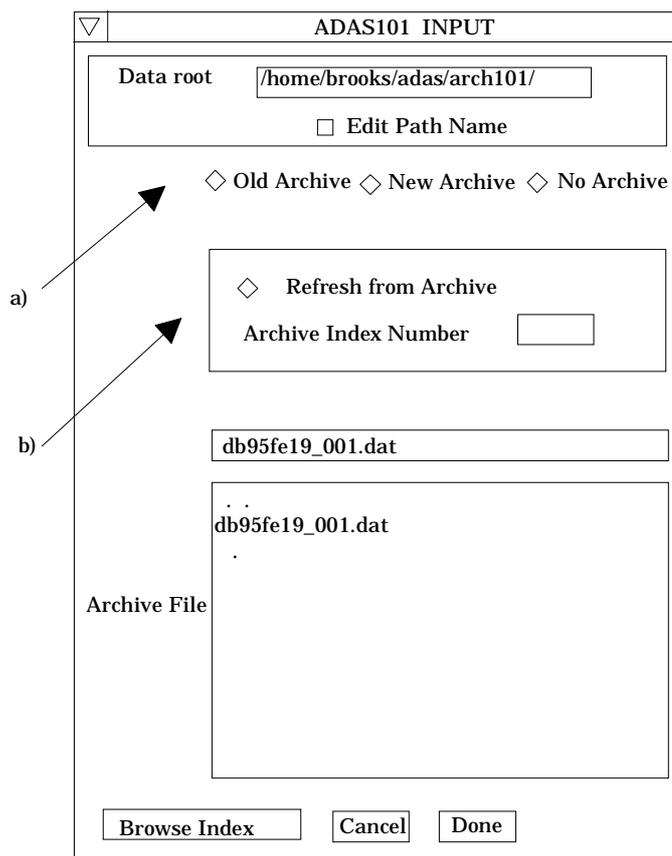
1.5.   The **processing options window** has the appearance shown below

1.5.1.   The button *Browse Index* at a) again allows display of the archive index list.

1.5.2.   As described in the ADAS Manual, four types of collision cross-section are allowed, namely 1-dipole, 2-non-dipole, 3-spin change and 4-other. Enter the *transition type* number at b). For dipole transitions the transition probability is required. Either the line strength (*S*), absorption oscillator strength (*f*) or Einstein A-value (*A*) forms are accepted. Click the appropriate button and enter the value.

1.5.3.   At c) details of the upper and lower levels of the transition are entered. The energies of levels are measured upwards from the lowest level of the ion. Click on the *Select energy form* button to indicate which units are being used for these energies. Note that full statistical weights (including spin parts in the case of terms) are required.

1.5.4.   User input cross-sections, energies and required output temperatures are displayed at d) with the currently selected units shown below. Click the *Edit table* button to 'drop down' the ADAS Table Editor for data input.

1.5.5.   If an archive data set is opened, energy, cross-section and temperature values are filled from this. Otherwise the fields are empty. Pressing the *Default Temperature values* button inserts a default set of temperatures.

1.5.6.   The ADAS Table Editor window follows the same pattern of operation as described previously. Note however the fairly wide selection of units in which data can be entered. This is to ease the problem of unit conversion for data from the general literature. Click on the buttons for the units with which you wish to work. The program internally converts to the threshold energy parameter *X* and the collision strength *Omega*. If data is returned from archive it will be in these forms. Click the *Done* button if editing is completed satisfactorily.

```
┌─────────────────────────────────────────────────────────────────────────┐
│ ▽                        ADAS101 PROCESSING OPTIONS                        │
│   Data file name :  /home/brooks/adas/ach101/db95fe19_001.dat             │
│   ┌─────────────────────────────────────────────────────────────────┐    │
│   │                          Browse Index                            │    │
│   └─────────────────────────────────────────────────────────────────┘    │
│        Nuclear Charge:     ┌──────────┐      Ion Charge:    ┌──────────┐   │
│                            └──────────┘                     └──────────┘   │
│   ┌─────────────────────────────────────────────────────────────────┐    │
│   │   Transition Type:    ┌────────┐   ┌──────────────────────────┐  │    │
│   │                       └────────┘   │ Transition Probability: ┌──┐│  │    │
│   │                                    │                         └──┘│  │    │
│   │                                    │  Form:   ◇ S   ◇ f   ◇ A  │  │    │
│   │                                    └──────────────────────────┘  │    │
│   └─────────────────────────────────────────────────────────────────┘    │
│   ┌─────────────────────────────────────────────────────────────────┐    │
│   │          Lower Level                        Upper Level          │    │
│   │       Index : ┌──────────┐              Index : ┌──────────┐     │    │
│   │       Stat. Wt. : ┌──────────┐          Stat. Wt. : ┌──────────┐ │    │
│   │   ┌───────────────────────────────────────────────────────────┐ │    │
│   │   │  Level Energy : ┌──────────┐      Level Energy : ┌────────┐│ │    │
│   │   └───────────────────────────────────────────────────────────┘ │    │
│   └─────────────────────────────────────────────────────────────────┘    │
│   ┌─────────────────────────────────────────────────────────────────┐    │
│   │   Select Energy Form :          ◇   cm-1        ◇   Rydbergs     │    │
│   └─────────────────────────────────────────────────────────────────┘    │
│   ┌─────────────────────────────────────────────────────────────────┐    │
│   │  ┌───────────────────────────────────────────────────────────┐△ │    │
│   │  │  INDEX   Input Energy   Input X-sect   Output Temp.        │  │    │
│   │  │    1     1.000E+00      1.000E+00      1.000E+05           │  │    │
│   │  │    2     2.000E+00      2.000E+00      2.000E+05           │  │    │
│   │  │    3     5.000E+00      5.000E+00      3.000E+05           │  │    │
│   │  │    4     1.000E+01      1.000E+01      4.000E+05           │  │    │
│   │  │    5     2.000E+01      2.000E+01      7.000E+05           │  │    │
│   │  │    6     5.000E+01      5.000E+01      8.000E+05           │  │    │
│   │  │    7     1.000E+02      1.000E+02      1.000E+06           │  │    │
│   │  │    8     2.000E+02      2.000E+02      2.000E+06           │▽ │    │
│   │  │◁                                                          ▷│  │    │
│   │  └───────────────────────────────────────────────────────────┘  │    │
│   │  Energy units : X .   X-section units : Omega .  Temperature units : Kelvin . │
│   │  ┌───────────────────────────────────────────────────────────┐  │    │
│   │  │                       Edit Table                           │  │    │
│   │  └───────────────────────────────────────────────────────────┘  │    │
│   │  ┌───────────────────────────────────────────────────────────┐  │    │
│   │  │               Default Temperature values                   │  │    │
│   │  └───────────────────────────────────────────────────────────┘  │    │
│   └─────────────────────────────────────────────────────────────────┘    │
│      Edit the processing options data and press Done to proceed           │
│   ┌────────────┐   ┌────────────┐                                         │
│   │   Cancel   │   │   Done     │                                         │
│   └────────────┘   └────────────┘                                         │
└─────────────────────────────────────────────────────────────────────────┘
```

a)

b)

c)

d)
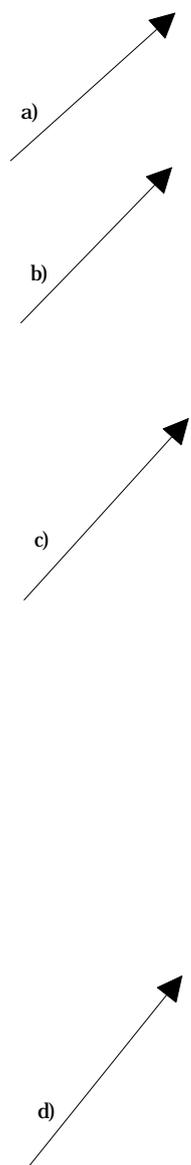
1.5.7. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

1.6. The **output options window** is more complex than in previous programs. It is shown below

1.6.1. There is a choice of method for examination and display of the input data. At a), click either the *ADAS analysis option* which corresponds to the JET analysis or the *Burgess analysis option*. The latter is an implementation of the technique developed by Alan Burgess which is popular in astrophysics. The sub-window at b) varies depending on this choice. Make the appropriate choices at b), c), d) and e) in the ADAS case or at b'), c') and d') in the Burgess case. The manual gives more details of how these options operate.

ADAS101 OUTPUT OPTIONS

Data file name : /export/home/adas/adas/adf13/sxb93#b3/sxb93#be_pju_be0.dat

Browse Index

◇ ADAS Analysis Option

◇ Burgess Analysis Option

a)

Optimisation Level : ◇ 1 ◇ 2   Optimisation Option : ◇ On ◇ Off

b)

Bad Point Option : ◇ On ◇ Off   Dipole X-sect. Fitting : ◇ Ratio ◇ Difference   d)

c)   e)

□ Graphical Output   Default Device

Graph Title   Figure 1   Post-script

□ 1st. Default Graph Scaling   □ 2nd. Default Graph Scaling   Post-script
X-min : [   ] X-max : [   ]   X-min : [   ] X-max : [   ]   HP-PCL
Y-min : [   ] Y-max : [   ]   Y-min : [   ] Y-max : [   ]   HP-GL

f)

□ Enable Hard Copy   □ Replace

File name : graph.ps

g)

□ Text Output   □ Replace   Default file name

File name : graph.ps

[Cancel]   [Done]

C-value [   ]

b')

Insert non-dipole point at infinity : ◇   Y-value : [   ]

c')

d')

1.6.2.   Two graphs are presented. The first is a scaled comparative graph for assessing the cross-section data and making adjustments if appropriate. The second graph displays the final *Upsilons* at the user's temperatures. Make the required choices of graph scaling and axes choices at f) for the comparative graph and at g) for the *Upsilon* graph.

1.6.3.   The comparative graph is displayed in the Graph Editor window as shown below. This introduces a new concept in ADAS, namely, the editable graph. The graph displays the scaled input values as circles with a spline drawn through these tabular points in the ADAS analysis option case. In the Burgess analysis option case, the spline is drawn through the special five knot points which are distinquished. The points can be modified by using the buttons a) beneath the graph in association with the mouse. In the Burgess

analysis option case, the knot points may only be moved vertically and a special button is present for this case.

```
┌──────────────────────────────────────────────────────────────────┐
│ ▽              ADAS101 : DIAGNOSTIC GRAPH EDITOR                    │
├──────────────────────────────────────────────────────────────────┤
│                                                                    │
│                                                                    │
│                                                                    │
│                                                                    │
│                                                                    │
│                                                                    │
│                                                                    │
│                                                                    │
│                                                                    │
│                                                                    │
│                                                                    │
│                                                                    │
│                                                                    │
├──────────────────────────────────────────────────────────────────┤
│  △  Move a Point      △  Delete a Point    △  Add X-point   △  Add Anywhere │
├──────────────────────────────────────────────────────────────────┤
│                                                                    │
│    Insert Point by Value :     X-val : [          ]                │
│                                                       △  Click to Insert │
│                                Y-val : [          ]                │
│                                                                    │
├──────────────────────────────────────────────────────────────────┤
│  [ Cancel ]     [ Print ]     [ Refresh ]    [ Help ]   [ Done ]   │
└──────────────────────────────────────────────────────────────────┘
```

a)
b)
c)
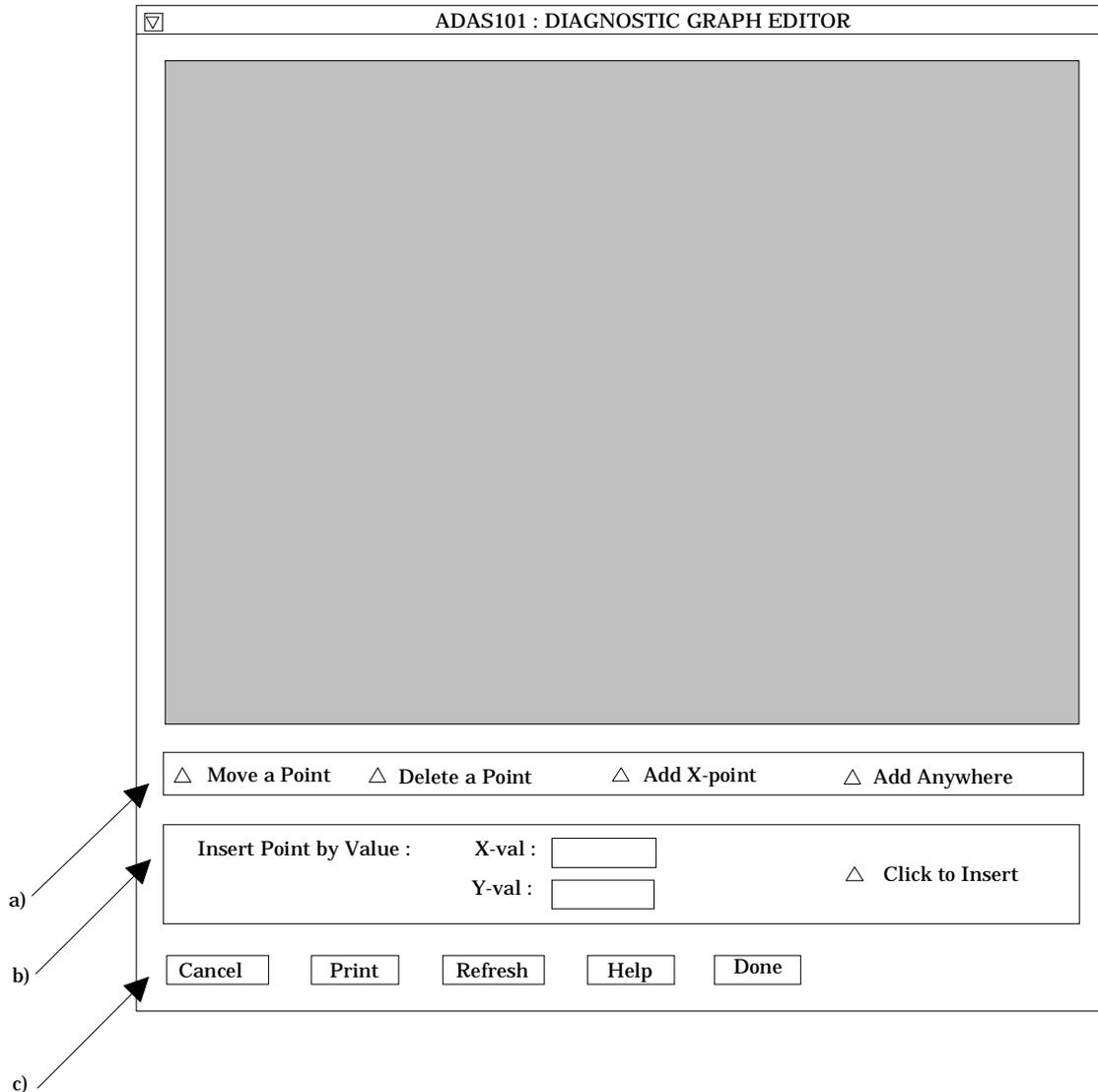
1.6.4.   To move a point, click the *move a point* button. Then use the *left* mouse button to pick and drag a point to a new position. Note that the x-ordering of points should be maintained although not forced by the editor. Each point has a small active zone around it for picking by the mouse. Terminate point moving operations by pressing the *right* mouse button. To delete a point, click the *delete a point* button. Then click the *left* mouse button with the pointer over the point to be deleted. Terminate point deletion operations by pressing the *right* mouse button. To add a new point in the x-ordered position between two existing points, click the *add X-point* button. Then click the *left* mouse button with the pointer at the position where the new point is to be inserted. Terminate point insertion operations by pressing the *right* mouse button. For completeness, the capability for adding a point anywhere is given although physically unreasonable. The operation is slightly different. Click the *add anywhere* button. With the *left* mouse button pick a point after which you wish the new point added. Press the *leftt* mouse button with the pointer at the insertion point. Multiple insertions may be made by continuing to click the *left* mouse button. Click the *right* mouse

button to terminate this particular insertion. Press the *right* mouse button a second time to terminate insertion operations.

    1.6.5.   To insert a point by value use sub-window b).

    1.6.6.   The buttons at c) provide the usual *cancel*, *print* and *done* options. In addition the *help* button displays some information on using the graph editing facilities. The original data and graph can be restored by clicking the *refresh* button. Note that after leaving the graph editor window with the *done* button, the modified and or additional points replace the original user input data. Note that with the ADAS analysis option, if any points are modified, the program cycles back to the Output Options window for reanalysis. With the Burgess analysis option, movement only of the spline knots does not force reanalysis.

    1.6.7.   The Upsilon graph is displayed after graph editing. There is no option to modify this output graph. The graph may be printed, using the *print* button. If the results of the analysis are acceptable and to be archived, click the *archive* button.

2.   **ADAS209**

This is a new code which is not part of JET-ADAS. It is designed to satisfy the need to work at different resolution levels in excited population structure. Specifically, in astrophysical work, LSJ resolution is usual, even for light species, whereas in fusion, LS resolution is usual. To avoid duplication of effort, the new code allows bundling of levels. It operates on specific ion files of type *adf04* and generates a new file of the same type but with levels grouped as specified by the user. Such an algorithm is also of value with very many level systems where there is a need to focus on the most important levels, for example metastables, and treat other levels more grossly.

ADAS209 PROCESSING OPTIONS

Data File Name : /disk2/lanzafam/adas/adf04/nlike_dhb94#o.dat

Browse Comments

Ion : O+1   Nuclear Charge : 8

Index	Configuration	Designation	Energy (cm-1)
1	2s2(1s0)	(1)0(0.0)	0.0
2	2s2p(3p0)	(3)1(0.0)	81942.5
3	2s2p(3p1)	(3)1(1.0)	87078.0
4	2s2p(3p2)	(3)1(2.0)	87542.0
6			
7			
8			
9			

a)

◇ Level Bundling   ◇ Parent Bundling

Cancel   Done

b)

2.1. The standard **file selection window** appears first. Its operation is as described in the bulletin *jan18-95*. The file selection window and relevant data format (*adf04*) is the same as for ADAS201.

2.2. The **processing options window** has the appearance shown above
　　2.2.1. A level list is displayed in the window at a). This is a simple transcription of the list from the head of the source *adf04* file.
　　2.2.2. At b), two buttons are present to allow bundling of the levels of the selected ion and then bundling of the parents of these levels. This latter option is non-trivial only when the advanced *adf04* specification is being used. More details are given in the ADAS Manual. Click the appropriate button to drop down the Bundling window. These are shown below.

ADAS209 : LEVEL BUNDLING

```
1   2s2(1s0)    (1)0( 0.0)       0.0
2   2s2p(3P0)   (3)1( 0.0)    81942.5
3   2s2p(3P1)   (3)1( 1.0)    87078.0
4   2s2p(3P2)   (3)1( 2.0)    87345.0
```

< Press return after each entry >
Finished allocation

ADAS209 : PARENT BUNDLING

```
1   (1S)        1.0         918657.0
```

< Press return after each entry >
Finished allocation

　　2.2.3. In the Level Bundling window, the index number, configuration specification, (2S+1)L(J) quantum numbers and the level energy (cm-1) are given for each level in a separate display window a) with an editable box to its right b). The editable box is for entering a bundle index number. That is levels which are to be grouped are given the same bundle index number. If no index number is given for a level, then the code treats the level as a distinct bundle. The code reindexes bundles as necessary for consistency. **Remember to press Return after entering each bundle index**.
　　2.2.4. Click the *Finished allocation* button when you are satisfied with you assignments.
　　2.2.5. The Parent bundling window has the same organisation and operation as the Level bundling window. It generally has less than five entries and if the advanced *adf04* format is not in use then only one. The information format is a little different from that of the levels. The first value is the index number, followed by the parent term character string (in brackets) as given

on the top line of the *adf04* file. The numerical value of the parent statistical weight follows with finally the parent energy (cm-1) relative to the lowest level of the ion. In the single parent case therefore this is just the ionisation potential.

2.2.6. Note that the organisation of all *adf04* datasets at present is such that although energy levels may be at the J-resolved intermediate coupling resolution, the parents are at term resolution. Thus there is usually no need to bundle parents unless there is a wish to focus for example on just the ground parent (lowest ionisation continuum). The latter may be the case if one wishes to bypass the complexities of metastables.

2.3. The **output options window** is of restricted form. It only offers the option of an output text file. This part is of the same layout as codes previously described.

2.3.1. The output is the bundled *adf04* file and is of the correct format for re-entry in the *adf04* database. The comments section at the end of the output *adf04* file details the unbundled source *adf04* file and the bundling imposed.

2.3.2. There is no graphical output option.

3. **ADAS308**

The program analyses line of sight spectral emissivities of charge exchange spectroscopy lines from hydrogic impurites occuring through neutral beam / plasma interaction, in terms of emission measure. In addition it predicts effective emission coefficients of charge exchange lines.

3.1. 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).

3.2. The **file selection window** appears first. Its operation is as described in the bulletin *jan18-95*.

3.2.1. *adf01* is the appropriate format for use by the program ADAS308. 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*.

3.2.2. 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.

3.2.3. 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*.

3.2.4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.

3.2.5. Once a data file is selected, the set of buttons at the bottom of the main window become active.

3.2.6. 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.

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

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

3.3.1. Information is given on the fully ionised impurity receiver and the neutral beam donor at a). The atomic mass of the receiver should also be entered at b).

3.3.2. The specification of beam parameters, details of observed line of sight spectral emissivities to be analysed and emissivities to be predicted are entered at c). Input data of each of these three types may be addressed in turn by activation of the relevant button. The window at d) then presents the appropriate table. The table may be edited by clicking on the *Edit Table* button. The *Observed spectrum lines* table is shown. In principle, a number of observed intensities are introduced here. It is possible to enter values which do not allow a consistent solution. The code advises of this but it is the responsibility of the user to check that the data is unblended etc. It is also a usual practice to enter just one line, possibly with a fictitious emissivity merely to obtain effective emission coefficients and line component details. The *Beam parameter information* button causes display of the window at d'). The table becomes editable in the usual way by clicking the *Edit Table* button. Note that no check is made that the various beam energy fractions sum to unity. This is the responsibility of the user. *The Required emissivity predictions* button causes the window at d'') to be displayed. This activates the predictive part of the code which becomes possible once the observed lines have been analysed in terms of emission measure. Then any set of lines within the N-shell limits may be predicted. The standard output includes the mean wavelength and effective emisison coefficient, but for up to five lines an extended tabulation of line component emissivities may be produced. Graphs may be produced for two selected line. Indicate these selections in the *Key* column.

3.3.3. At e) plasma parameters are entered. For ADAS308, *B Magn*. has no effect, but a value shuld be entered as a place holder.

3.3.4.   The final window at f) allows model and theory choices. Details are given in the ADAS Manual. For each type, clicking on the selection window drops down a short menu of choices. Click on the appropriate choice. The ADAS data base source numerical data of type adf01 is the most usual, that is the *Use input data set* choice button. Note that the *Select emission measure* model choice includes *Electron impact excitation* as well *as Charge exchange*.

3.4.   The **Output options window** follows the usual pattern. Note that two plots are produced if required. The *Plot A* is the stick diagram of component line-of-sight emissivities. The *Plot B* is of the Doppler broadened profile of the line at the plasma ion temperature. Separate explicit scaling is possible for the two plots.

```
            Beam parameter information
    INDEX      Fraction     Energy (eV/amu)
      1         0.100         4.00e+04
      2         0.100         3.00e+04
      3           . .            . .
      4
      5

.d')

                    Edit Table

        Note : It is left to the user to ensure the sum
                of the fractions is correct.
```

```
          Required emissivity predictions
    INDEX      Upper      Lower      Key
              level N    level N'

      1         6          4          1
      2         5          4
      3         4          3          1
      4
      5

.d")

                    Edit Table

Note :maximum allowed N quantum no. : 20
        minimum allowed N quantum no.  : 1

Key:  1 = graphical and tabular output (max. 2)
       2 = tabular output only (max. 5 non-blank entries)

Blank  = summary only.
```

4.   **ADAS309**
The program computes sets of effective emission coefficients for transitions in hydrogenic impurities following charge exchange from neutral beam donors. They are prepared over one-dimensional scans of plasma parameters around a reference set and assembled directly for inclusion in the ADAS database as data type *adf12*.

4.1.   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 effective emission coefficient file formatted to adf12 specification. There is no graphic output from this program.

4.2.   The **file selection window** appears first. Its operation is as described in the bulletin *jan18-95*.

4.2.1.   *adf01* is the appropriate format for use by the program ADAS309. 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*.

4.2.2.   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.

4.2.3.   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*.

4.2.4.   Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.

4.2.5.   Once a data file is selected, the set of buttons at the bottom of the main window become active.

4.2.6.   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.

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

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

4.3.1.   The user input follows broadly that required for ADAS308. The reference plasma parameters are specified at a) with the beam reference energy entered just below. Note that a reference value is usually taken centralised in the one dimensional scan for that parameter. In such one dimensional scans, the other parameters are kept at their reference values. The actual scans are entered by clicking on the appropriate button at b). The selected scan table is displayed at e) and may be edited in the usual manner

4.3.2.   At c), the particular transition for which the tabulation is to be prepared is entered. This is analagous to ADAS308 but only one transition is treated at a time. At d), the usual model options are available..

4.4.   The **output options window** is shown below. There is no graphical output possibility but in addition to the usual text file, the data output file may be produced a). It is prepared preformatted according to *adf12* for direct addition to the ADAS database. Since it may be desired to patch the data in to existing *adf12* data sets, the transition count is left blank. More details are given in the ADAS Manual. As the calculations may take some time, the option is given of executing in the background. There are therefore two ways in which output can be generated:

4.4.1.   By pressing *Run Now* b), you can wait for the output to be generated before continuing. When this option is taken a small information box opens showing the progress the program has made. Once this has been done the calculations cannot be halted, but an execution time of less than 30 seconds can usually be expected.

ADAS309 : PROCESSING OPTIONS

Title for Run

Data File Name :   /disk2/hammond/adas/adf01/qcx#h0/qcx#h0_old#b5.dat

Browse Comments

		-----------Receiver-----------		------Neutral donor------		
Symbol	Nuclear charge	Initial ion charge	Final ion charge	Symbol	Nuclear charge	
B	5	5	4	H	1	

Please input the following receiver information

Atomic mass number of receiver

Input reference plasma parameter information :-

Ion temp. (eV)   :   Elec. temp. (eV) :

Ion dens. (cm-3) :   Elec. dens. (cm-3) :

Z effective   :   B Magn. (T)   :

a)

Input reference beam parameter information :-

Beam energy (eV/amu) :

Input selected transition :-

Upper N level :   Lower N level :

Note : maximum allowed N quantum no. :   20
          minimum allowed N quantum no. :   1

c)

Select charge exchange theory   :

Select donor states   :

Select emission measure model   :

d)

Input scan information :-

◇   Beam energy scan

◇   Ion density scan

◇   Ion temperature scan

◇   Plasma effective Z scan

◇   Magnetic induction scan

b)

Beam energy scan

INDEX	Energy (eV/amu)
1	4.000E+04
2	
3	
4	
5	

Edit Table

e)

Cancel   Done

4.4.2. By pressing *Run in Batch* the actual calculations required to produce the output are run at a later time, but it is necessary for a batch file containing all relevant data to be created or updated. Again a small information box opens showing the progress made in doing this. The process will normally be considerably quicker than when pressing *Run Now*. A larger batch job can be built up by returning to the Processing Options Window and making new selections before returning to the Output Options Window and again clicking on *Run in Batch*. When you exit the Processing Options Window of ADAS309 by clicking on *Cancel* to return to the Input Options Window, the program takes this as a signal that the batch job is completed and submits it for execution. A small information box opens giving the name of the job and information on when execution will begin. Calculations run in this way will normally run more quickly than those run using the *Run Now* button. When the batch job is complete, the output files are generated and a mail message sent from the operating system to say that it is finished. This will normally contain a simple message which says 'Your batch job has completed successfully'. It is possible to build a queue of batch jobs by submitting one as described above, constructing another and submitting that in the same way, but due to the relatively short time taken by the calculations it is not anticipated that this will happen very often.

4.4.3. Note that care must be taken with filenames when using ADAS309. Whenever the *Replace* option is selected and output then produced, the program automatically deselects the *Replace* option again to prevent the output being accidentally overwritten. When running batch jobs, the program goes one step further . After *Run in Batch* has been selected the first time, the *Append* option is always automatically selected for subsequent output. It is possible to override this and even to send output to different files from the same batch job. However, if the *Replace* button is selected

once the contruction of a batch file has begun then any earlier output stored in the batch file will be deleted when the job executes.

```
┌─────────────────────────────────────────────────────────────────────┐
│ ▽                    ADAS309  OUTPUT OPTIONS                          │
│                                                                       │
│   Data file name  :  /disk2/adas/adas/adf01/qcx#h0/qcx#h0_gyt#h1..dat │
│   ┌─────────────────────────────────────────────────────────────┐    │
│   │                     Browse comments                          │    │
│   └─────────────────────────────────────────────────────────────┘    │
│   ┌─────────────────────────────────────────────────────────────┐    │
│   │  ☐  Data Output     ☐  Append     ☐  Replace   ┌────────────┐│    │
│   │                                                │Default File │││    │
│   │                                                │   Name     ││    │
│   │  File name  :  ┌──────────────────────────────────────┐     ││    │
│   │                │ /disk2/hammond/adas/adas/pass/data.pass│    ││    │
│   │                └──────────────────────────────────────┘     ││    │
│   └─────────────────────────────────────────────────────────────┘    │
│   ┌─────────────────────────────────────────────────────────────┐    │
│   │  ☐  Text Output     ☐  Append     ☐  Replace   ┌────────────┐│    │
│   │                                                │Default File ││    │
│   │                                                │   Name     ││    │
│   │  File name  :  ┌──────────────────────────────┐             ││    │
│   │                │ paper.txt                     │             ││    │
│   │                └──────────────────────────────┘             ││    │
│   └─────────────────────────────────────────────────────────────┘    │
│   ┌─────────┐    ┌─────────┐     ┌──────────────┐                     │
│   │ Cancel  │    │ Run Now │     │ Run in Batch │                     │
│   └─────────┘    └─────────┘     └──────────────┘                     │
└─────────────────────────────────────────────────────────────────────┘
```

a)

b)

5.   **ADAS506**
        The program interrogates G(Te) functions from the ADAS database. It has the secondary purpose of allowing the user to collect a set of G(Te) functions into a compact simplified data set for use directly into differential emission measure analysis.

5.1.   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), the graphic file if saved (e.g. *graph.ps* if a postscript file) and the collection file.

5.2.   The **file selection window** appears first. Its operation is as described in the bulletin *jan18-95*.

5.2.1. *adf20* is the appropriate format for use by the program ADAS506. 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.*

5.2.2.
        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. They are named by iso-electronic sequence (eg. *gft95#li*). specific file names include a source indfetifier (eg. *al*) the specific ion symbol (eg. *c3*) and the pressure (eg. *p3e14*).

5.2.3. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then the individual datafiles are presented for selection. Datafiles all have the termination *.dat* (eg. *gft95#li_al#c3_p3e14.dat*).

5.2.4. Once a data file is selected, the set of buttons at the bottom of the main window become active.

5.2.5. 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.

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

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

5.3.1. Transitions for which G(Te) 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 a) just above the line list display window.

5.3.2. Your settings of electron temperatures (output) are shown in the temperature display window d). The temperature values at which the G(Te) coefficients are stored in the datafile (input) are also shown for information.

5.3.3. 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

5.3.4. 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.

5.3.5. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

▽ ADAS506 PROCESSING OPTIONS

Title for run   Test title for ADAS506

Data File Name : /home/lanafam/adas/adf20/gft95#li/gft95#li_al_c3_p3e14.dat

Browse comments

Number of Electron Impact Transitions : 29
Number of Index Energy Levels : 15

Polynomial fitting

◇   Fit Polynomial   value % :   5

Select Transition

TRANSITION INDEX	--------UPPER LEVEL--------		--------LOWER LEVEL--------		APPROXIMATE WAVELENGTH	SPECTROSCOPIC WAVELENGTH
	INDEX	DESIGNATION	INDEX	DESIGNATION		
1	1	2s1 (2)S(0.5)	1	2p1 (2)P(0.5)	1550.800	0.000
1	1	2s1 (2)S(0.5)	1	2p1 (2)P(0.5)	1550.800	0.000

. . .

a)

Select Temperature for Output File   ◇

Output Electron Temperatures

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

◁   ▷

Temperature units : eV

Edit Table

Default Temperature values

Edit the processing options data and press Done to proceed

Cancel   Done

5.4. The **output options window** appearance is shown below:

    5.4.1. The graph is displayed in a following **graphical output** window. This is similar to that for ADAS201.

    5.4.2. Writing to the collection file is activated by clicking the *Collection File* button at a). The operation is slightly different from the usual text output. The collection file is composed of blocks of data for each spectrum line. Each block includes a header line which enables the code to construct an indexed list of lines present in the collection file. A line which is already present in the collection. Thus the G(Te) collection file is dissimilar to the archive files described for ADAS101 above where appending only can be done.

```
┌─────────────────────────────────────────────────────────────────────────┐
│ ▽                      ADAS506  OUTPUT OPTIONS                             │
│                                                                           │
│   Data file name : /home/lanzafam/adas/adf20/gft95#li/gft95#li_al#c3_p3e14.dat │
│                                                                           │
│   ┌───────────────────────────────────────────────────────────────────┐ │
│   │                       Browse Comments                             │ │
│   └───────────────────────────────────────────────────────────────────┘ │
│                                                                           │
│   ┌───────────────────────────────────────────────────────────────────┐ │
│   │  ☐   Graphical Output                         Default Device       │ │
│   │  Graph Title    ┌──────────────────────┐     ┌──────────────┐      │ │
│   │                 │   Figure 1           │     │ Post-script  │      │ │
│   │                 └──────────────────────┘     └──────────────┘      │ │
│   │   ┌──────────────────────────────────────┐   ┌──────────────┐      │ │
│   │   │ ☐  Explicit Scaling                  │   │ Post-script  │      │ │
│   │   │          X-min:[    ]  X-max:[    ]  │   │ HP-PCL       │      │ │
│   │   │          Y-min:[    ]  Y-max:[    ]  │   │ HP-GL        │      │ │
│   │   └──────────────────────────────────────┘   └──────────────┘      │ │
│   │   ┌──────────────────────────────────────┐                         │ │
│   │   │ ☐  Enable Hard Copy  ☐  Replace      │                         │ │
│   │   │  File name :  graph.ps               │                         │ │
│   │   └──────────────────────────────────────┘                         │ │
│   └───────────────────────────────────────────────────────────────────┘ │
│                                                                           │
│   ┌───────────────────────────────────────────────────────────────────┐ │
│   │ ☐  Text Output   ☐  Replace   [Default file name]                 │ │
│   │  File name :  paper.txt                                           │ │
│   └───────────────────────────────────────────────────────────────────┘ │
│   ┌───────────────────────────────────────────────────────────────────┐ │
│   │ ☐  Collection File  ☐  Replace                                    │ │
│   │  File name :  [                          ]                        │ │
│   └───────────────────────────────────────────────────────────────────┘ │
│                                                                           │
│   [ Cancel ]   [ Done ]                                                   │
└─────────────────────────────────────────────────────────────────────────┘
```

a)

6. New data have been entered into the central database as follows:

    6.1. *adf01*. The charge exchange data for neutral helium ground state beam donors to impurities have been replaced. These data are based on conversion from the corresponding neutral deuterium donor. Some additional specific calculations (W. Fritsch and R. Olson) have enabled the conversion algorithm to be corrected and substantially improved. R. Hoekstra & F. Bliek (KVI, Groningen) have collaborated with me at JET on this upgrade.

    6.2. *adf04*. A very substantial collection of files for specific elements, under the sub-directory structure */adf04/copmm#<el>/...* where *<el>* is the element nuclear charge number, has been placed. These are LS-coupled data sets of moderate accuracy (based on Cowan's structure code with level rebundling to terms and Born collision rates). They do not include true exchange spin changing collision cross-sections although they have such entries through LS-coupling breakdown. Such data sets we

find very useful as templates to which improved data can be added. Also they give a first cut at new systems. They are designed for automatic processing with mnemonic fields for the energy level configurations (Eissner notation) and will be used by some later ADAS codes (ADF407, ADF408). Martin O'Mullane, JET Joint Undertaking prepared these data. Incidentally, the intermediate coupling versions also exist, but are very large. Martin can produce such data for arbitrary complex systems quite quickly and semi-automatically.

6.3. *adf05*. A new general Z data file for the beryllium-like ions, neon to iron, n=2-2, 2-3 and 3-3 has been prepared called */adf05/belike/belike_jl1995.dat*. It is for levels in intermediate coupling. *adf04* files have been produced from it using ADAS203 (not yet available) and have been gathered in a dedicated subdirectory with data set names such as */adf04/copjl#be/copjl#be_jj#c2.dat*. The *jj* is used here to denote j-resolved data. It is fully up-to-date using the latest published cross-section data. It is the product of a major effort by Jim Lang, Rutherford-Appleton Laboratory. It is being used to prepare G(Te) functions - see below.

6.4. *adf20*. Large collections of G(Te) functions are being put in position. This is an on-going task. These are suited for differential emission measure analysis and can be interrogated by ADAS506. They are prepared by iso-electronic sequence and for a number of electron pressures. A typical data set name is */adf20/gft95#b/gf95t#b_al#c1_p1e10.dat*. The *al* denotes Alessandro Lanzafame who has done all the work of preparing these files, the *p1e10* denotes a pressure of 1.0×10^{10} (K cm-3), the *c1* denotes the boron like ion C^{+1}.

6.5. *adf23*. For the first time we are starting to bring together proper initial and final state resolved (LS term) ionisation rate coefficient data allowing a consistent view of metastables. This is a large task led by Don Griffin and Mitch Pindzola with Nigel Badnell and Tom Gorczyca. Light elements, which do not have significant excitation-autoionisation contributions are being calculated first. The new data are in data files such as */adf23/griffin/belike/belike_th_b1ls.dat* where *th* denotes normalisation to theoretical total cross-section and *b1ls* denotes ionisation from LS coupled terms of the beryllium-like ion B^{+1}.

For the next release, we shall turn to ADAS series 4 programs. They are concerned with ionisation and recombination. We shall begin as usual with the interrogative programs on the database and then move on to the proccessing programs.

H. P. Summers
7 July 1995