jun18-98   **ADAS Bulletin**
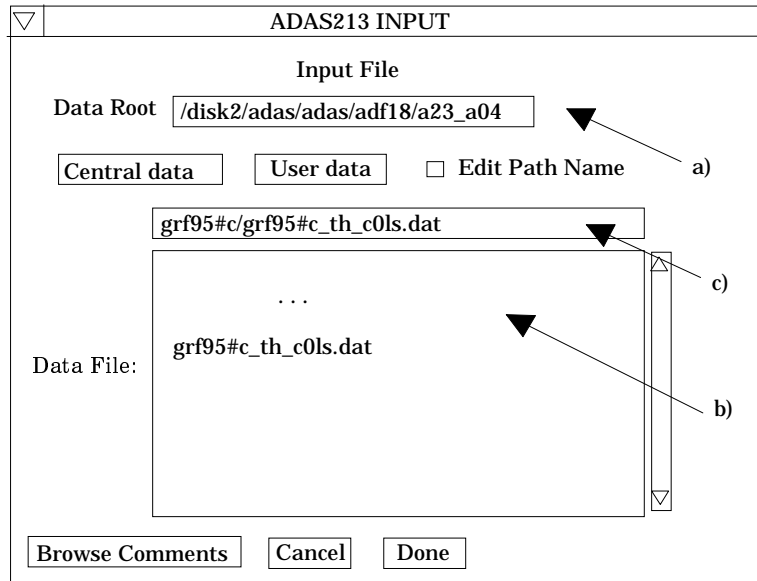

In this release there are seven new codes, ADAS213 ADAS214, ADAS215, ADAS413, ADAS701,ADAS702 and ADAS703.

1.   **ADAS213**   The program adds state selective electron impact ionisation data to specific ion files of type *adf04* and electron impact excitation data to levels of the *adf04* file which are auto-ionising . To achieve this it, it opens the primary data archives for Maxwell averaged ionisation/excitation-autoionisation coefficient data of type *adf23* The mapping of the data into the *adf04* files makes use of a cross-referencing file which must be set up prior to execution. Such cross-referencing files are archived in data format *adf18/a23_a04*. The result of the operation of the code is a fully specified *adf04* file ready for immediate inclusion in a personal database. The code includes an added capability for mapping LS-resolved ionisation data to J-resolved levels rather than terms. Also the code is internally set up for mapping from true J-resolved intermediate coupling *adf23* data archives to *adf04* files, when these become available.
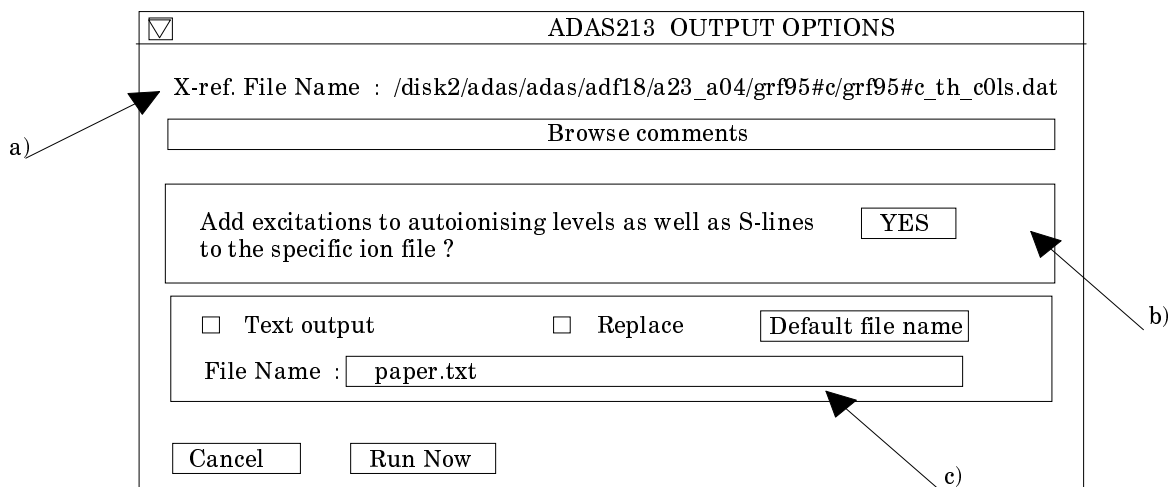
Move to the directory in which you wish the output text file produced after executing any ADAS program (*paper.txt* is the default) to appear. There is no graphical output from this code and text output is brief. Initiate ADAS213 from the program selection menus in the usual manner.

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

1.1.1.   An *adf18/a23_a04* format cross-referencing file is the appropriate input file for use by the program ADAS213. Your cross-referencing data should be held in such a file, in the same directory structure as central ADAS, but with your identifier replacing the first *adas.*

1.1.2.   Available sub-directories are shown in the large file display window at b). Scroll bars appear if the number of entries exceed the file display window size. There are a large number of these. They are usually stored in sub-directories by iso-electronic sequence of the recombined ion with a prefix which identifies the primary author of the actual ionisation data accessed. It is useful to use a naming convention for the final part of the file name which includes the ion and 'LS' (eg. grf95#c/grf95#c_th_c0ls.dat) to indicate that the data is for terms. Note the extra '*th*' in the file name which indicates that the state-selective data is in fact normalised to a total theoretical cross-section

1.1.3.   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.*

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

1.1.5.   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.

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

```
┌─────────────────────────────────────────────────────────────┐
│ ▽              ADAS213 INPUT                                   │
├───────────────────────────────────────────────────────────────┤
│                         Input File                            │
│  Data Root  ┌─────────────────────────────────┐               │
│             │ /disk2/adas/adas/adf18/a23_a04  │      ▼         │
│             └─────────────────────────────────┘                │
│  ┌──────────────┐   ┌───────────┐   ☐ Edit Path Name     a)   │
│  │ Central data │   │ User data │                              │
│  └──────────────┘   └───────────┘                              │
│             ┌─────────────────────────────────┐               │
│             │ grf95#c/grf95#c_th_c0ls.dat     │   ▼            │
│             └─────────────────────────────────┘         ▲  c)  │
│             ┌─────────────────────────────────┐    ┌┐          │
│             │           . . .                 │    └┘          │
│             │                            ▼                     │
│  Data File: │  grf95#c_th_c0ls.dat                             │
│             │                                          b)      │
│             │                                                  │
│             │                                          ▼       │
│             └─────────────────────────────────┘               │
│  ┌──────────────────┐  ┌────────┐  ┌──────┐                   │
│  │ Browse Comments  │  │ Cancel │  │ Done │                   │
│  └──────────────────┘  └────────┘  └──────┘                   │
└───────────────────────────────────────────────────────────────┘
```

There is no processing options window for ADAS213.

1.2. The **output options window** is shown below. There is no graphical output possibility but in addition to the usual text file, an output data file is always produced.

1.2.1. The data output file is of specific ion file form, that is *adf04*, It's name is specified in the cross-reference file and so is not sought in the output options window. It is usually sent to the pass directory as *adas213_adf04.pass* for checking and re-naming later. It comprises the complete *adf04* file for which the cross-referencing was prepared but includes electron impact ionisation data.

1.2.2. The button at b) allows the choice of whether electron impact excitation data should be added to the output *adf04* file. This is a special situation for *adf04* files which have been set up for the study of doubly excited states and satellite spectrum lines. It will only be fully implemented with the release of the second phase of ADAS series 7 codes. The present answer is 'NO'.

1.2.3. Text output is selected at c). *paper.txt* is the default text file name.

1.2.4. The code is quite quick in execution and so only the immediate foreground execution option is implemented. Press *Run Now* and wait for the output to be generated before continuing. A small information box opens showing the progress the program has made.

```
┌─────────────────────────────────────────────────────────────────────┐
│ ▽              ADAS213  OUTPUT OPTIONS                                 │
├───────────────────────────────────────────────────────────────────────┤
│ ▼                                                                     │
│     X-ref. File Name : /disk2/adas/adas/adf18/a23_a04/grf95#c/grf95#c_th_c0ls.dat │
│ a)  ┌───────────────────────────────────────────────────────────────┐ │
│     │                     Browse comments                           │ │
│     └───────────────────────────────────────────────────────────────┘ │
│     ┌───────────────────────────────────────────────────────────────┐ │
│     │ Add excitations to autoionising levels as well as S-lines  ┌─────┐│ │
│     │ to the specific ion file ?                                 │ YES ││▼│
│     │                                                            └─────┘│ b)│
│     └───────────────────────────────────────────────────────────────┘ │
│     ┌───────────────────────────────────────────────────────────────┐ │
│     │ ☐  Text output          ☐  Replace        ┌───────────────────┐│ │
│     │                                            │ Default file name ││ │
│     │ File Name : ┌────────────────────────────┐ └───────────────────┘│ │
│     │             │  paper.txt                 │                      │ │
│     │             └────────────────────────────┘                      │ │
│     └───────────────────────────────────────────────────────────────┘ │
│     ┌────────┐  ┌─────────┐                                           │
│     │ Cancel │  │ Run Now │                                      c)   │
│     └────────┘  └─────────┘                                           │
└───────────────────────────────────────────────────────────────────────┘
```

2. **ADAS214** ADAS214 calculates escape factors for spectral line emission along a given line-of-sight, Θ_L, and for collisional radiative population calculations of excited levels in

atoms and ions, Θ_p, on the basis of some simplifying approximations. A wide choice of spectral line profiles, spatial emission profiles and plasma geometry cases are available in the code. Doppler, Lorentz or Holtsmark profiles can be used, as well as convolutions and superpositions of different types and widths, in order to account for various line broadening mechanisms and particle groups with different temperatures. The spatial emission profiles of radiation are approximated by a polynomial fit and the code can be run for constant emission, a linear or a parabolic decrease from the plasma centre to the edge. The population escape factor can be calculated in the centre of a plasma sphere, in the mid-plane of a disk, or on the axis of a cylinder. The underlying definitions of the present escape factor analysis and the approximations in the solution of the equation of radiative transfer are explained in the background theory below. Normalised escape factors for Θ_L, and Θ_p for the described cases are shown and the consequences of the different models are discussed. An example of the use of the code is also given, with emphasis on the choice of input parameters. In the past, the described program had already been applied to many other studies of opacity including the calculation of ionisation, recombination and radiation coefficients on the basis of the ADAS atomic data base.

Move to the directory in which you wish the standard ADAS created files to appear. For ADAS214, these are the output text file (*paper.txt*), and adas214.pass, the modified *adf04* file. The graphical output from the code are as described previously. Initiate ADAS214 from the program selection menus in the usual manner.

2.1.   The **file selection window** appears first as illustrated below.

    2.1.1.   ADAS214 may access many data-sets during its operation. Buttons are present at a) to set the data root to that of the *Central data* or to your personal *User data* (provided it is in ADAS organisation). Alternatively, the data root may be edited explicitly
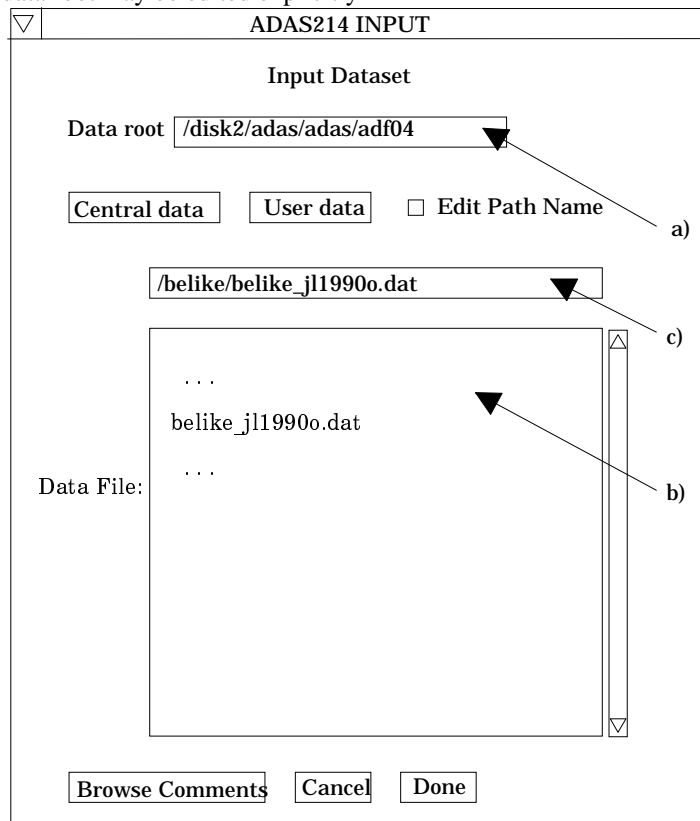
    2.1.2.   At b) identify and select the relevant *adf04* file for the ion in question.

    2.1.3.   c) displays the *adf04* file that has been selected from the relevant directory.

    2.1.4.   Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous Series 2 menu. Clicking

the browse button brings up any existing comments on the selected *adf04* file.

2.2.   The **processing options window** is shown below.

    2.2.1.   A summary of the *adf04* data file selected is given at a).

    2.2.2.   The selection of temperatures, densities and other plasma parameters are made at b). The following parameters need to be entered: atomic mass number, electron temperature (this is only used to calculate the Boltzmann density distribution), gas temperature, density, length of plasma (b in fig 5), aspect ratio (a/b in fig 5), line profile, density distribution across plasma and plasma geometry.

2.2.3.   The table to select the transitions to be observed for their variation in emergent flux ratios the may be edited by clicking on the *Edit Table* button. The ADAS Table Editor is then presented with the usual set of editing operations available. The normalised escape factor plot will show the predicted optical depths for the transitions chosen here. If scanning is enabled, then emergent flux line ratios can be plotted for each transition with respect to the first one selected in the table.

2.2.4.   In the metastable and Boltzmann deviation window, c), one can enter at d) a factor to alter the Boltzmann density of the respective levels. If no multiplier is entered, the level is assumed to be underpopulated to 1/10th of its Boltzmann value. This is only used to get an initial estimate of the populations, to be used to calculate the population escape factors.

2.2.5.   If scanning is not selected, the code is run for the values selected. If scanning is selected, then the code is run for a range of column densities, the range being given by the maximum and minimum factors entered below the scanning button for the number of steps chosen.

2.2.6.   Clicking the *Done* button causes the next output options window to be displayed. *Cancel* takes you back to the previous window and the *Escape to Menu* icon is also available for a quick exit at the bottom left hand corner.

2.2.7. The **output options window** is shown below.

2.2.8. 11. Information is again given of the input *adf04* file at a).

2.2.9. 12. The *graphical output* button at b) must be selected to enable the generation of graphs. The graph title is also entered at b).

2.2.10. 13. If the *explicit scaling* button is selected, the plotting range can be forced manually, the ranges being entered in the boxes provided. If scaling isn't selected, the program finds the most relevant range itself to plot the chosen graph.

2.2.11. 14. The output graph to be generated is selected in the box to the right of the explicit scaling box. Graph 1 is the Normalised escape factor vs. Optical depth curve. Graph two is of the line profile and graph 3 is the emergent flux intensity ratio as a function of column density for the selected transitions and is only available if the scanning option is selected.

2.2.12. 15. The *hard copy* button enables the generated graph to be sent to file for printing. The filename is entered in the box provided, and the printer device selected from the list. It is to be noted that the *print* button on the graph window will still have to be pressed for the graph to be sent to file.

▽ ADAS214 OUTPUT OPTIONS

Data File Name : /disk2/adas/adas/adf04/belike/jl1990c.dat

Browse Comments

a)

☐ Graphical Output

Graph Title [   ]

Select Graph

Graph1

☐ Explicit scaling

Graph1
Graph2
Graph3

b)

X-min [   ]   X-max [   ]

Y-min [   ]   Y-max [   ]

Select Device

Postscript

Post script
HP-PCL
HP-GL

☐ Enable Hard Copy   ☐ Replace

File Name [graph.ps   ]

c)

☐ Text Output   ☐ Replace   [Default File Name]

File Name [paper.txt   ]

d)

☐ ADF04 File   ☐ Replace   [Default File Name]

File Name [adas214_adf04.pass]

N.B. Only when you exit ADAS214 will ADF04 output be sent to this file

e)

[Cancel] [Done]

2.2.13. 16. The usual text output file summarising the processing may be produced. Make the required selections at d).

2.2.14. 17. The modified *adf04* file can be written to file by making the required selection at e)

2.2.15. 18. Clicking the *Done* button causes the calculation to commence. Clicking the *Cancel* button takes the user back to the previous window and clicking the *Escape to Menu* button returns to the ADAS menu screen

3. **ADAS215** This is a new code which is not part of JET-ADAS. It alters the electron collisional rate coefficient (Upsilon) data in a specific ion file of format *adf04* to a different set

of electron temperatures for which it creates a new specific ion file. Extrapolation may be attempted with the code and this is an indeterminate error amplifying process in general. The code seeks to minimise this by supporting interpolation and extrapolation using Burgess-Tully C-plot parameters, selective display of collision rate coefficients and adjustment of Burgess-Tully types and C parameters.

Move to the sub-directory in which you wish graphic or text output from this program to appear. Initiate ADAS215 from the program selection menus in the usual manner.

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

    3.1.1. Data root a) shows the full pathway to the appropriate data sub-directories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. The appropriate ADAS data format for input to this program is ADF04 ('specific ion files'). 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.

    3.1.2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
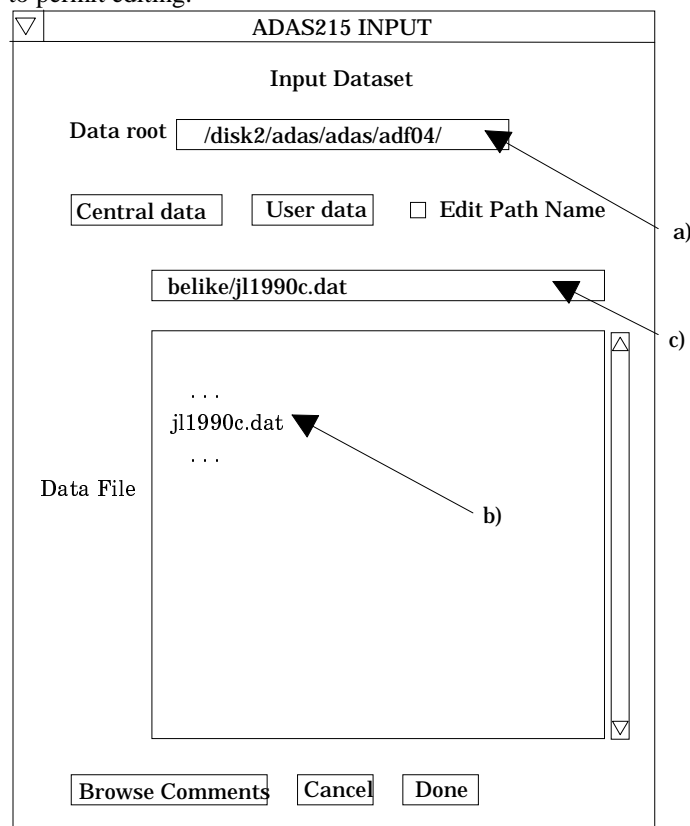
    3.1.3. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.

    3.1.4. 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 data files are presented for selection. Data files all have the termination *.dat*.

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

    3.1.6. Clicking on the *Browse Comments* button displays any information stored with the selected data file. It is important to use this facility to find out what is broadly available in the data set. The possibility of browsing the comments appears in the subsequent main window also.

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

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

    3.2.1.   An arbitrary title may be given for the case being processed. For information the full pathway to the *adf04* file selected for temperature re-gridding is also shown. The button *Browse comments* a) allows display of the information field section at the foot of the selected *adf04*, if it exists.
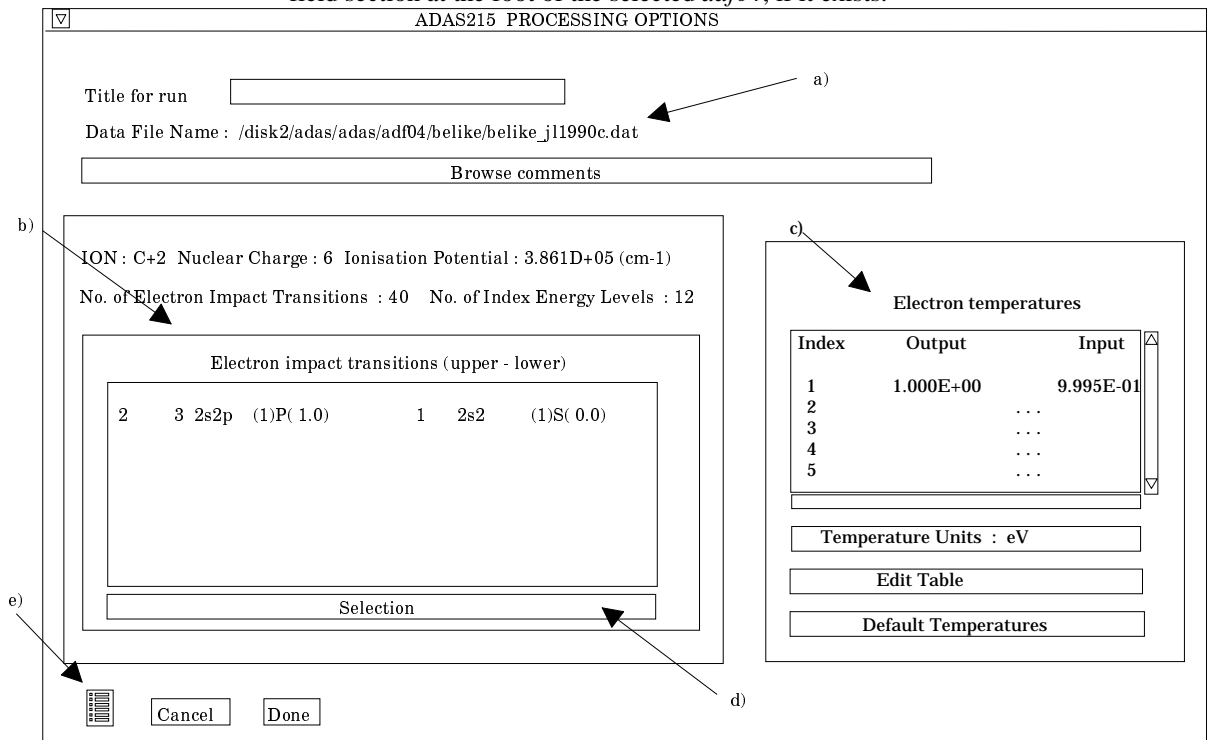
    3.2.2.   The sub-window at c) shows the *Input* temperatures from the *adf04* file and the *Output* temperatures at which the new *adf04* file is to be produced. Click on the *Edit Table* button to change the output values. Click on the *Default Temperatures* button to insert the default output temperature set. Note that the default set of temperatures is the standard 'z-scaled' set used for iso-electronic sequences preparation since 1997.

    3.2.3.   The number of electron impact excit./de-excit. rate coefficients isolated form the *adf04* file is shown at b) and those selected for graphing are shown in the display window just below.

    3.2.4.   Click on the Selection button to alter those selected for display and the change the initial Burgess & Tully types and C-values assigned automatically by the code.

    3.2.5.   A pop-up window appears as shown below. It displays the complete set of electron impact transitions showing the transition index number and the upper and lower level quantum numbers. Three small editable boxes are present at the beginning of each transition row. The first is for selecting graphical display of the scaled Upsilon for the transition. The choices are *blank* for do not display and '*P*' or '*p*' for display.

    3.2.6.   The adjacent two boxes allow the Burgess & Tully type (choices 1-4) and the C-value to be altered. It is expected that you will move forward to output graphical display and then return to this screen if necessary to adjust or experiment with these settings.

Electron impact transitions

```
1    2  2s2p    (3)P( 4.0)    1    2s2    (1)S( 0.0)
2    3  2s2p    (1)P( 1.0)    1    2s2    (1)S( 0.0)
3    4  2p2     (3)P( 4.0)    1    2s2    (1)S( 0.0)
4    5  2p2     (1)D ( 2.0)   1    2s2    (1)S( 0.0)
```

Col. 1 : insert 'p' to plot ; Col2 : Burgess and Tully class ; Col 3: C-value .   Make a Maximum of 20 selections

Cancel   Done

3.2.7.   Click *Done* at b) to return to the main *Processing Options* window

3.2.8.   Click *Done* in the *Processing Options* window to initiate the interpolation to the new temperatures and advance to the next screen in the usual manner.

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

3.3.1.   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. Graphical display is activated by the *Graphical Output* button 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. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.

3.3.2.   Hard copy is activated by the *Enable Hard Copy* button c). The File name box then becomes editable. If the output graphic file already exists and the *Replace* button has not been activated, a 'pop-up' window issues a warning.

3.3.3.   A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.

3.3.4.   At d) the *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.

3.3.5.   At e) output of the re-gridded *adf04* file may be enabled. The *Default file* is set up at the first pass through this window. Note that the actual output is deferred. This is to allow further adjustment of rate coefficient interpolations before the final complete *adf04* is written. The re-gridded *adf04* file is placed by default in your */pass* directory as *adas215_adf04.pass*.

3.3.6.   **N.B. In the re-gridded *adf04* file all transition lines other than electron impact transitions between bound states are deleted.** That is 'R-lines', 'S-lines', 'H-lines', 'P-lines' and 'I-lines'. Interpolation /extrapolation for these categories is much less secure than recreating the data. Temperature re-gridding should be done as the first step in the chain of processing.

```
┌─────────────────────────────────────────────────────────────────────────┐
│ ▽            ADAS215  OUTPUT OPTIONS                                       │
│   Data File Name :  /disk2/adas/adas/adf04/belike/jl1990c.dat             │
│   ┌─────────────────────────────────────────────────────┐                │
│   │              Browse Comments                          │                │
│   └─────────────────────────────────────────────────────┘                │
│                                                                           │
│   ┌───────────────────────────────────────────────────────────────────┐ │
│   │   ☐  Graphical Output                        Select Device         │ │
│   │                                              ┌──────────┐           │ │
│   │  Graph Title  ┌──────────────────────────┐  │ Postscript │          │ │
│   │               └──────────────────────────┘  └──────────┘           │ │
│   │   ┌─────────────────────────────────────┐   ┌──────────┐           │ │
│   │   │ ☐  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                  │                       │ │
│   └───────────────────────────────────────────────────────────────────┘ │
│   ┌───────────────────────────────────────────────────────────────────┐ │
│   │  ☐ ADF04 File       ☐ Replace   ┌────────────────┐                 │ │
│   │                                 │ Default File Name │               │ │
│   │    File Name ┌────────────────────────────┐                        │ │
│   │              │ adas215_adf04.pass         │                        │ │
│   │    N.B.  Only when you exit ADAS215 will ADF04 output be sent to this file │ │
│   └───────────────────────────────────────────────────────────────────┘ │
│   ┌──┐ ┌────────┐  ┌──────┐                                               │
│   │≡ │ │ Cancel │  │ Done │                                               │
│   └──┘ └────────┘  └──────┘                                               │
└─────────────────────────────────────────────────────────────────────────┘
```

a)
b)
c)
d)
e)

3.3.7.   The graph is displayed in a following Graphical Output window.

3.3.8.   At the base of the graph window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 2 menu. *Done* takes you back to the previous output options screen. The final output of the re-gridded *adf04* file and the *paper.txt* file is held over until adjustments are completed. To complete, click *Done* in the graph window to return to the output options window, then click the *Exit to Menu* button on that window.

4.   **ADAS413**

5.   **ADAS701**   The code is a full implementation of the program AUTOSTRUCTURE developed by N. R. Badnell. The entire capability of the original program for arbitrary structure, Auger rate and Radiative rate calculation has been retained. However input driver file selection, driver templates, output selection and output routing have been enabled within the ADAS framework to simplify the production of two types of data, namely dielectronic recombination rates and data for doubly excited state (satellite line) models. Move to the sub-directory in which you wish text output from this program to appear. Initiate ADAS701 from the program selection menus in the usual manner.

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

5.1.1.   Data root a) shows the full pathway to the appropriate data sub-directories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. The appropriate ADAS data format for input to this program is *adf27* ('AUTOSTRUCTURE drivers'). Click the *User Data* button to insert the pathway to your own data. *User Data* is the default. Central ADAS contains samples from which the user can build his/her own

driver. 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.

5.1.2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

5.1.3. 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. The practice in ADAS is to store drivers in sub-directories according to iso-electronic sequence of the recombining ion (eg. /*belike*).

```
 ▽           ADAS701 INPUT

    Data Root  /disk2/adas/adas/adf27/          ▼

     Central data     User data     □ Edit Path Name      a)

              helike/ne8ic_sat.dat              ▼
            ┌──────────────────────────────────┐ △
            │  . . .                            │        c)
            │  ne8ic_sat.dat                    │
            │  . . .                      ▼     │
            │                                   │        b)
  Data File:│                                   │
            │                                   │
            │                                   │
            │                                   │ ▽
            └──────────────────────────────────┘

   Browse Comments    Cancel     Done
```
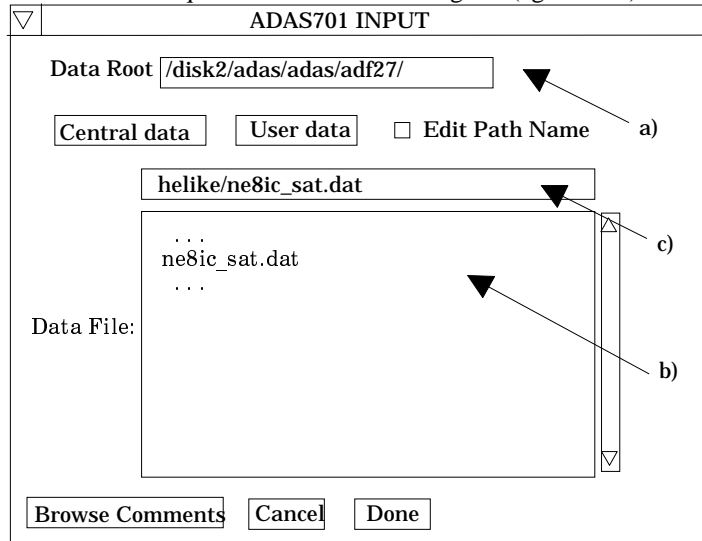
5.1.4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. The individual data files all have the termination *.dat*. The purpose of the driver data set is indicated by the pattern of the file name as

5.1.5. /*<ion><coupling>{<prt-trans>}{-<n-shell>}{_<task>}.dat*

5.1.6. where   *<ion>* denotes the recombining ion (eg. 'o4' for O^{+4})

   <coupling> denotes the coupling scheme ('*ls*' for LS-coupling, '*ic*' for intermediate coupling)

 <prt-trans> denotes the parent n-n' shell transition (eg. '*23*'). This name portion does not appear for task '*sat*' below

   <n-shell> denotes the outer n-shells treated, which may be a single shell (as eg. '3') or all n-shells (as eg. 'n') This name portion does not appear for tasks '*.str*' and '*.sat*' below.

   <task> denotes the objective ('*str*' for the baseline structure calculation, '*sat*' for satellite line preparation) If the field is blank then the main Auger and radiative rate calculations for dielectronic rates take place.

5.1.7. Thus '*o4ls23_str.dat*' is a driver for the n=2-3 parent transition related LS-coupled term structure calculation used to establish the resonance positions. '*o4ls23-3.dat*' and '*o4ls23-n.dat*' are for the dielectronic rate calculations with only the n=3 outer electron present and for all outer n-shells respectively. '*o4ls_sat.dat*' is for the preparation of Auger/radiative data for satellite line modelling.

5.1.8. Once a data file is selected, the set of buttons at the bottom of the main window become active.
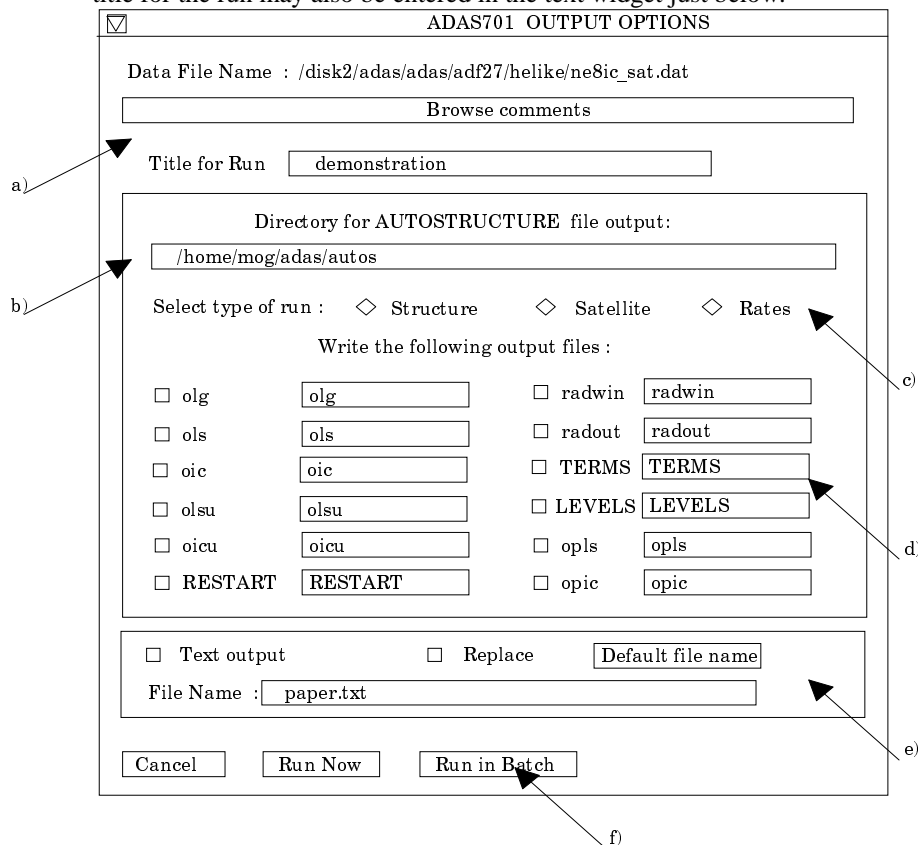
5.1.9. Clicking on the *Browse Comments* button displays any information stored with the selected data file. It is important to use this facility to find out what is broadly available in the data set. The possibility of browsing the comments appears in the subsequent main window also.

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

There is no **processing options window**

5.2.   The **output options window** appearance is shown below. Note that there is no graphical output in this case

5.2.1.   The full pathway to the driver data set to be used is shown for information at the top of the window and at a) the *Browse comments* button is available. A title for the run may also be entered in the text widget just below.

```
┌────────────────────────────────────────────────────────────────────┐
│ ▽                    ADAS701  OUTPUT OPTIONS                         │
│                                                                      │
│   Data File Name  :  /disk2/adas/adas/adf27/helike/ne8ic_sat.dat     │
│   ┌──────────────────────────────────────────────────────────────┐  │
│   │                    Browse comments                           │  │
│   └──────────────────────────────────────────────────────────────┘  │
│                                                                      │
│    Title for Run    ┌─────────────────────────────────┐             │
│                     │   demonstration                 │             │
│                     └─────────────────────────────────┘             │
│   ┌───────────────────────────────────────────────────────────────┐ │
│   │            Directory for AUTOSTRUCTURE  file output:           │ │
│   │   ┌───────────────────────────────────────────────────────┐   │ │
│   │   │  /home/mog/adas/autos                                 │   │ │
│   │   └───────────────────────────────────────────────────────┘   │ │
│   │                                                               │ │
│   │    Select type of run :   ◇  Structure    ◇  Satellite   ◇  Rates │
│   │                  Write the following output files :           │ │
│   │                                                               │ │
│   │    □ olg    ┌────────┐         □ radwin  ┌──────────┐         │ │
│   │            │  olg   │                   │  radwin  │         │ │
│   │            └────────┘                   └──────────┘         │ │
│   │    □ ols    ┌────────┐         □ radout  ┌──────────┐         │ │
│   │            │  ols   │                   │  radout  │         │ │
│   │            └────────┘                   └──────────┘         │ │
│   │    □ oic    ┌────────┐         □ TERMS   ┌──────────┐         │ │
│   │            │  oic   │                   │  TERMS   │         │ │
│   │            └────────┘                   └──────────┘         │ │
│   │    □ olsu   ┌────────┐         □ LEVELS  ┌──────────┐         │ │
│   │            │  olsu  │                   │  LEVELS  │         │ │
│   │            └────────┘                   └──────────┘         │ │
│   │    □ oicu   ┌────────┐         □ opls    ┌──────────┐         │ │
│   │            │  oicu  │                   │  opls    │         │ │
│   │            └────────┘                   └──────────┘         │ │
│   │    □ RESTART ┌────────┐        □ opic    ┌──────────┐         │ │
│   │            │ RESTART │                  │  opic    │         │ │
│   │            └────────┘                   └──────────┘         │ │
│   └───────────────────────────────────────────────────────────────┘ │
│   ┌───────────────────────────────────────────────────────────────┐ │
│   │   □  Text output        □  Replace      ┌──────────────────┐  │ │
│   │                                         │ Default file name │  │ │
│   │                                         └──────────────────┘  │ │
│   │   File Name  : ┌─────────────────────────────────────────┐    │ │
│   │               │  paper.txt                              │    │ │
│   │               └─────────────────────────────────────────┘    │ │
│   └───────────────────────────────────────────────────────────────┘ │
│   ┌─────────┐   ┌──────────┐   ┌──────────────┐                     │
│   │ Cancel  │   │ Run Now  │   │ Run in Batch │                     │
│   └─────────┘   └──────────┘   └──────────────┘                     │
└──────────────────────────────────────────────────────────────────────┘
```
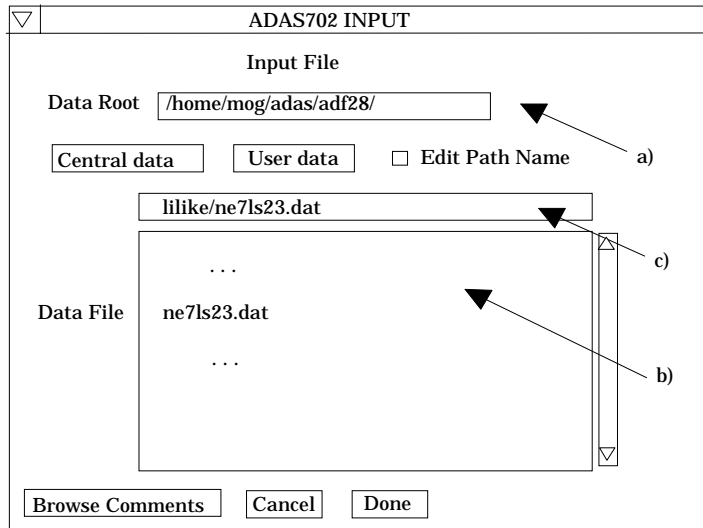
a)   b)   c)   d)   e)   f)

5.2.2.   The sub-window at b) allows selection of which output files from ADAS701 are to be kept and the names to be assigned to them. Up to twelve output files are available in principle. The default file names are shown and their contents are as follow:

5.2.3.   *olg*   detailed (diagnostic) output.

ols   energies & radiative and autoionisation rates between terms (formatted).

oic   energies & radiative and autoionisation rates between levels (formatted).

olsu   energies & radiative and autoionisation rates between terms (unformatted).

oicu   energies & radiative and autoionisation rates between levels (unformatted).

RESTART   restart file   .

radwin   input file of externally prepared radial orbitals.

radout   output file of internally calculated radial orbitals.

TERMS   term labelling.

LEVELS   level labelling.

opls   LS-coupling photo-ionisation cross-sections.

opic   intermediate coupling photo-ionisation cross-sections.
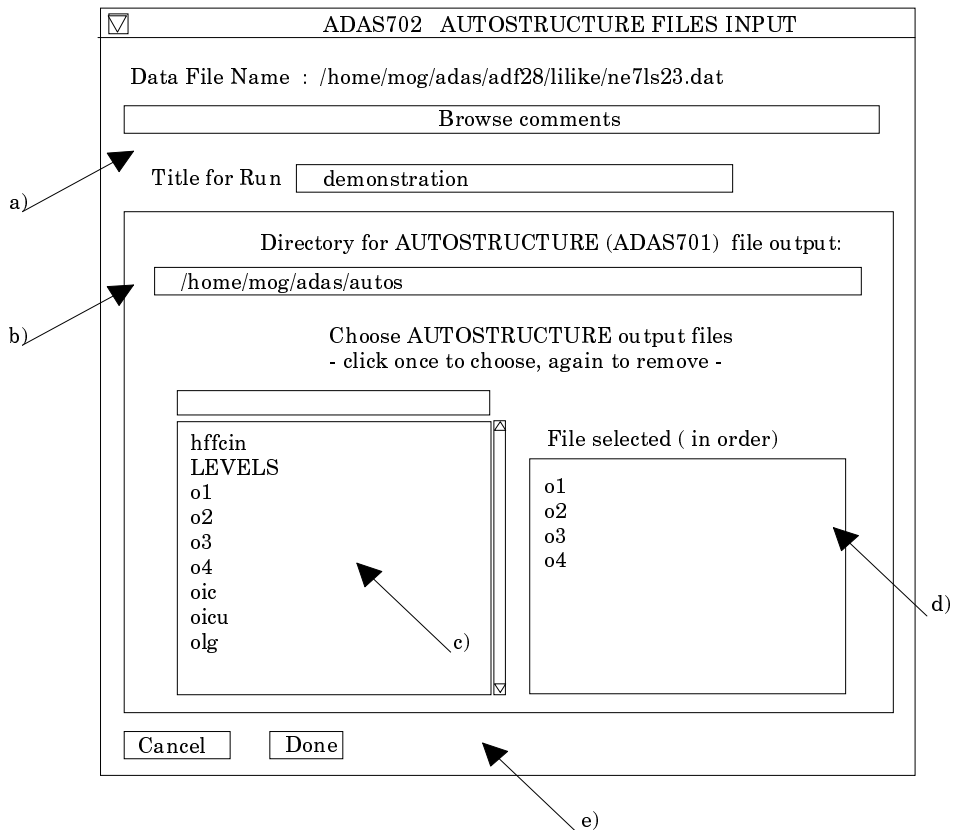
5.2.4.   The pathway to the directory where you wish to place the saved files in entered at b). The default is to the sub-directory *'/.../<user>/adas/autos'* . This is a sub-directory like the usual */pass* sub-directory but is dedicated to ADAS7 series.   The output may be quite substantial and exceed small

workstation capacities. The text widget is editable, so an alternative path may be substituted for the default.

5.2.5. At c) , the button for the type of run is clicked. This matches the driver data set names '*str*', '*sat*' and '' described above. According to your choice, various of the temporary output files are selected for saving. The text widgets are editable and you can replace default names by names of your choice. Warnings may be issued below the file names if a file already exists and will be over-written. This is simply a warning for the user to take action before proceeding if desired. There is no further protection. Note that the same standard names are always used by default and so the user must rename if he wishes to keep data. Deselected output files will be eliminated in a clean-up after the code has completed. For dielectronic rate production, it is usual to do the calculation in a number of stages (cf. the drivers *o4ls23-3.dat* and *o4ls23-n.dat*). The Auger & radiative rate coefficient files ,'*ols*' - for LS coupling or '*oic*' for intermediate coupling, should be renamed for each stage successively as '*o1*', '*o2*', etc. This is the responsibility of the user. Note that both formatted (eg. '*oic*') and unformatted (eg. '*oicu*') forms of the files can be produced. For large runs it is much more economical to use the unformatted forms and they are similarly renamed (eg. '*o1u*').

5.2.6. At d) the *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.

5.2.7. At the base of the graph window, buttons are available for selection of foreground execution (*Run Now*), or batch submission (*Run in Batch*). Click *Cancel* to return to the input driver selection window without execution.

6. The code accesses intermediate data sets of energy levels, autoionization rates and radiative rates created by ADAS701. It re-organises and collects these data to generate tables of state resolved and metastable resolved dielectronic recombination coefficients according to ADAS data format *adf09*. The code handles both (LS) coupling and intermediate coupling (IC) data. The original background version of the code was (and is) known as ADASDR.

There is no graphic output from this program. Initiate ADAS702 from the program selection menus in the usual manner.

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

6.1.1. Data root a) shows the full pathway to the appropriate data subdirectories. The appropriate ADAS data format for input to this program is *adf28*. 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. It is expected that the user would prepare his/her own driver *adf28* data. Central ADAS of this type contains templates which can form the basis for creating one's own drivers.

```
┌─────────────────────────────────────────────────────────┐
│ ▽           ADAS702 INPUT                                 │
│                   Input File                              │
│  Data Root  ┌──────────────────────────┐   ▼             │
│             │ /home/mog/adas/adf28/    │              a)  │
│                                                           │
│  ┌─────────────┐   ┌─────────────┐   □ Edit Path Name     │
│  │ Central data│   │ User data   │                        │
│             ┌──────────────────────────┐ ▼                │
│             │ lilike/ne7ls23.dat       │             c)   │
│             ┌──────────────────────────┐┌─┐              │
│             │        . . .             ││△│              │
│  Data File  │                          │└─┘              │
│             │  ne7ls23.dat      ▼      │                  │
│             │                          │            b)    │
│             │        . . .             │                  │
│             │                          │┌─┐              │
│             │                          ││▽│              │
│             └──────────────────────────┘└─┘              │
│  ┌──────────────────┐  ┌────────┐  ┌──────┐              │
│  │ Browse Comments  │  │ Cancel │  │ Done │              │
│  └──────────────────┘  └────────┘  └──────┘              │
└─────────────────────────────────────────────────────────┘
```

6.1.2.

6.1.3.   The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

6.1.4.   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.

6.1.5.   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*.

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

6.1.7.   Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.

6.1.8.   Clicking the *Done* button moves you forward to the next window, which comprises a second stage of data file selection. Clicking the *Cancel* button takes you back to the previous window.

6.1.9.   The second stage (AUTOSTRUCTURE output file selection) widget is shown below.

6.1.10.   The name of the driver data set selected in the previous step is displayed at a) and its comments lines can be browsed by clicking the *Browse Comments* button. Also a title may be entered for the run in the text widget directly below.

6.1.11.   Selection of the output files from the prior runs of ADAS701 (AUTOSTRUCTURE) which are required for post-processing are selected at b).

6.1.12.   The default directory pathway is */.../<userid>adas/autos/* consistent with the default operation of ADAS701. The directory pathway is editable.

6.1.13.   Available files for selection are shown in the scrollable selection window at c). Files generated by mutiple runs of ADAS701 would normally be renamed as '*o1*', '*o2*' etc. or their unformatted versions '*o1u*', '*o2u*' etc. Click on a file to select it and click on it again to de-select. Selected files appear in the adjacent *Files selected* window at d). If more than four files are selected, a warning is issued. At least one file must be selected before the code will proceed.

```
┌─────────────────────────────────────────────────────────────────────────┐
│ ▽                    ADAS702   AUTOSTRUCTURE FILES INPUT                   │
│                                                                           │
│     Data File Name  :  /home/mog/adas/adf28/lilike/ne7ls23.dat            │
│     ┌───────────────────────────────────────────────────────────────┐    │
│     │                     Browse comments                            │    │
│     └───────────────────────────────────────────────────────────────┘    │
│     Title for Run    ┌───────────────────────────────────────┐           │
│                      │   demonstration                       │           │
│                      └───────────────────────────────────────┘           │
│     ┌───────────────────────────────────────────────────────────────┐    │
│     │          Directory for AUTOSTRUCTURE (ADAS701)  file output:   │    │
│     │  ┌─────────────────────────────────────────────────────────┐  │    │
│     │  │ /home/mog/adas/autos                                    │  │    │
│     │  └─────────────────────────────────────────────────────────┘  │    │
│     │               Choose AUTOSTRUCTURE output files               │    │
│     │               - click once to choose, again to remove -       │    │
│     │  ┌──────────────────────────────┐                             │    │
│     │  └──────────────────────────────┘                             │    │
│     │  ┌───────────────────────────┐   File selected ( in order)    │    │
│     │  │ hffcin                    │  ┌──────────────────────────┐   │    │
│     │  │ LEVELS                    │  │ o1                       │   │    │
│     │  │ o1                        │  │ o2                       │   │    │
│     │  │ o2                        │  │ o3                       │   │    │
│     │  │ o3                        │  │ o4                       │   │    │
│     │  │ o4                        │  │                          │   │    │
│     │  │ oic                       │  │                          │   │    │
│     │  │ oicu                      │  │                          │   │    │
│     │  │ olg                       │  │                          │   │    │
│     │  └───────────────────────────┘  └──────────────────────────┘   │    │
│     └───────────────────────────────────────────────────────────────┘    │
│     ┌─────────┐   ┌───────┐                                               │
│     │ Cancel  │   │ Done  │                                               │
│     └─────────┘   └───────┘                                               │
└─────────────────────────────────────────────────────────────────────────┘
```
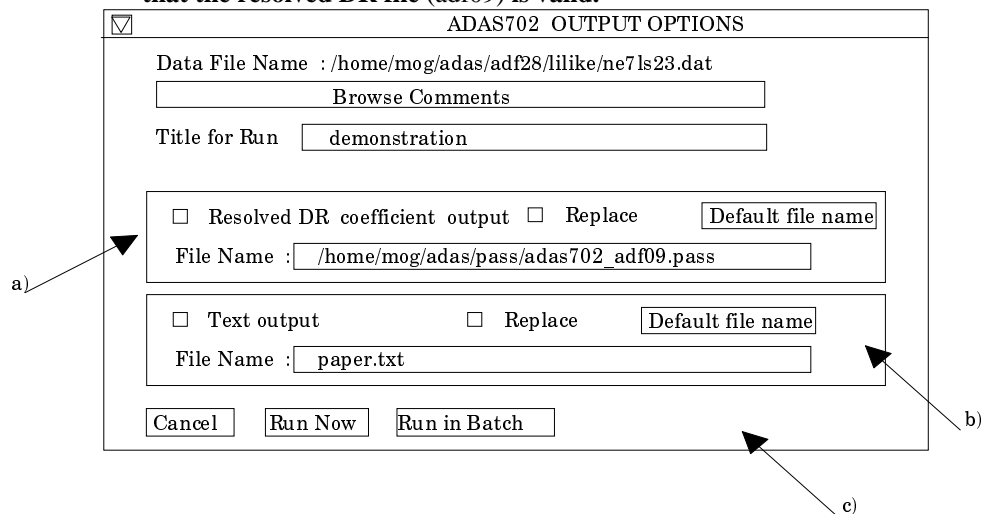
6.1.14. Click *Done* to advance to the *Output Options* screen in the usual manner.

6.1.15. There is no processing options window for ADAS702.

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

6.2.1.   At a) output of the *adf09* file may be enabled. The *Default file name* and *Replace* options are available. By default, the output file is sent to your */pass* directory as */.../adas/pass/adas702_adf09.pass*.

6.2.2.   At b) the *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated. **NB. It is essential to look at the** *paper.txt* **file to ensure that the code has operated as planned and hence that the resolved DR file** (adf09) **is valid.**


```
┌─────────────────────────────────────────────────────────────────────────┐
│ ▽                        ADAS702  OUTPUT OPTIONS                           │
│                                                                           │
│     Data File Name  : /home/mog/adas/adf28/lilike/ne7ls23.dat             │
│     ┌───────────────────────────────────────────────────────────┐        │
│     │                     Browse Comments                        │        │
│     └───────────────────────────────────────────────────────────┘        │
│     Title for Run    ┌───────────────────────────────────────┐           │
│                      │   demonstration                       │           │
│                      └───────────────────────────────────────┘           │
│     ┌───────────────────────────────────────────────────────────────┐    │
│     │  □  Resolved DR  coefficient  output  □   Replace  ┌──────────┐│    │
│     │                                                    │Default file name││
│     │  File Name :  ┌─────────────────────────────────────┐          │    │
│     │               │ /home/mog/adas/pass/adas702_adf09.pass│        │    │
│     │               └─────────────────────────────────────┘          │    │
│     └───────────────────────────────────────────────────────────────┘    │
│     ┌───────────────────────────────────────────────────────────────┐    │
│     │  □  Text output                  □   Replace   ┌──────────────┐│    │
│     │                                                │Default file name││
│     │  File Name :  ┌─────────────┐                                   │    │
│     │               │ paper.txt   │                                   │    │
│     │               └─────────────┘                                   │    │
│     └───────────────────────────────────────────────────────────────┘    │
│     ┌─────────┐  ┌──────────┐  ┌──────────────┐                           │
│     │ Cancel  │  │ Run Now  │  │ Run in Batch │                           │
│     └─────────┘  └──────────┘  └──────────────┘                           │
└─────────────────────────────────────────────────────────────────────────┘
```

6.2.3.   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 7 menu. Remember that

Done takes you forward to the next screen while *Cancel* takes you back to the previous screen.

7.   **ADAS703**   The program isolates energy level, Auger rate and radiative rate data from ADAS701 calculations. It assembles these into specific ion files of type *adf04* which include data lines for energy levels of doubly excited states and data lines for free-bound resonance capture and Auger break-up. These specific ion files are the precursors for doubly excited population calculation and dielectronic satellite line emissivity prediction. Only specific ion files in intermediate coupling (J-resolution) may be created. Supplementary electron impact re-distributive collision data, in a simple impact parameter approximation are also produced and added to the *adf04* file. Move to the directory in which you wish the output text file produced after executing any ADAS program (*paper.txt* is the default) to appear. There is no graphic output from this program. Initiate ADAS703 from the program selection menus in the usual manner.

   7.1.   The **file selection window** has the appearance shown below
      7.1.1.   Two data files must be selected in indentical manner at a) and d).

      7.1.2.   Data root a) shows the full pathway to the appropriate data subdirectory. Click the *Central Data* button to insert the default central ADAS pathway to the data   or click the *User Data* button to insert the pathway to your own data. It would be the normal practice to access your own data produced by running ADAS701 since central ADAS perfoms no archiving of the ADAS701 intermediate output files. It is recommended that you use a special passing file directory for ADAS series 7 called */.../<userid>/adas/autos/*. This is the default pathway for ADAS703.
      7.1.3.   The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

7.1.4. Available sub-directories and files are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.

7.1.5. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Datafiles produced directly by ADAS701 have no extension unlike the usual *.pass* for temporary files.

7.1.6. Select the *olg* AUTOSTRUCTURE general file at a) and the *oic* radiative and autoionisation rate file at d). Once the data files are selected, the set of buttons at the bottom of the main window become active.

7.1.7. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.

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

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

7.2.1. An arbitrary title may be given for the case being processed.

7.2.2. Parent configurations obtained from analysis of the input files are displayed at a). The approximate ionisation potentials, that is the energies (cm^{-1}) of these parents relative to the ground state of the recombined ion, are required. It is sufficient to use term averages as these data are only used in the impact parameter electron impact excitation rate coefft. calculation to establish approximate target sizes for strong coupling corrections.

7.2.3. Specific ion files of data format *adf04* contain a character field for the configuration associated with each energy level. In the output *adf04* file written by the code, the configuration may be written in standard form as $n_1l_1q_1$ $n_2l_2q_2$ ...... or in the compact notation of Eissner used in the SUPERSTRUCTURE/AUTOSTRUCTURE data entry. The choice is made with the buttons at b).

7.2.4. Electron temperatures for the output *adf04* file are specified at c). The *Input* values constitute the 1997 standard reduced ADAS temperature set which are hard-wired in the code. The *olg* and *oic* files passed from the AUTOSTRUCTURE run contain no electron temperature data. The program recovers the output temperatures you used when last executing the program. Pressing the *Default Temperatures Values* button copies the *Input* temperatures as the *Output* temperatures.

7.2.5. The Temperature Values are editable. Click on the *Edit Table* button if you wish to change the values. Note that you can work in a choice of temperature units.

7.2.6. 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 7 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

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

7.3.1. At a) output of the *adf04* file may be enabled. The *Default file name* and *Replace* options are available. By default, the output file is sent to your */pass* directory as */.../adas/pass/adas703_adf04.pass*.

7.3.2. At b) the *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated. **NB. in the current ADAS release no information is sent to the *paper.txt* file**.
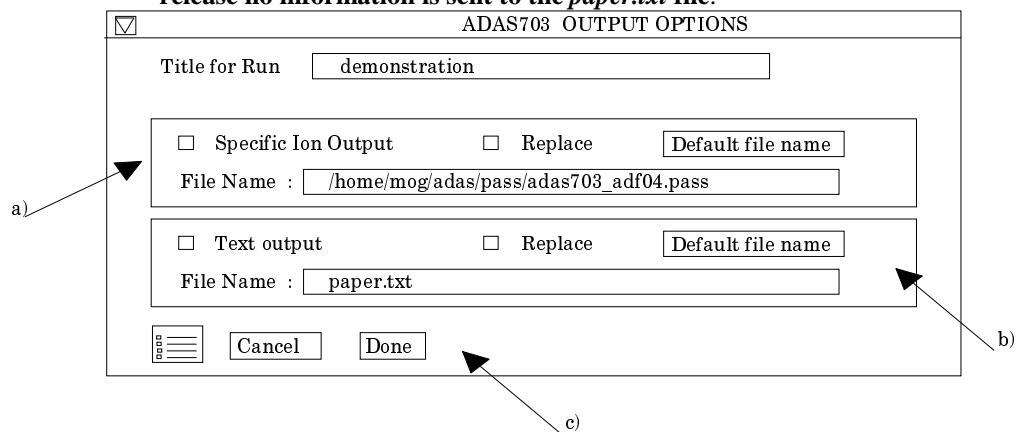
7.3.3. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 7 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

8. **ADF11** Data for xenon has been prepared by Martin O'Mullane and added as
   /.../adas/adas/adf11/<code89>/<code89>_xe.dat

9. Note that the state of the database in broad terms is described and updated in
   /.../adas/docs/datastatus/adf_stat

10. **Plans for ADAS705 and ADAS706.**

H. P. Summers
25 June 1998