oct18-97 **ADAS Bulletin**

In this release there are two new codes, ADAS410 developed by Martin O'Mullane and ADAS412 developed by Ricky Martin. ADAS410 is the missing interrogation code on our (now very extensive) state resolved dielectronic recombination data. These are of data class adf09 and Martin has also been preparing a lot of new data of this type. ADAS412 fills a gap in the computational chain involving G(Te) functions. The code performs the ionisation balance and population balance calculations and creates tables of G(Te) functions formatted according to the *adf20* specification. Thus you can now calculate your own G(Te) functions rather than being dependent on Alessandro and Peter McWhirter's production of them using the older off-line code. A substantial amount of new data has been added to the database. Also there have been the usual series of adjustments, dimension extensions and error corrections on existing codes.

1. **ADAS211 & ADAS212** Array dimensions and output formats on these codes have been altered to allow up to fourteen temperatures. Thus they are now consistent with the maximum number of temperatures allowed in the associated *adf04* datasets to which they add recombination rows.

2. **ADAS501 & ADAS503** We have allowed the numbers of temperature and density values to increase in a number of recently created *adf13* and *adf15* datasets beyond the old limits of 24. The code dimensions have been altered to accomodate this change.

3. **ADAS410** The code allows interrogation of state selective dielectronic recombination data of ADAS data format *adf09*. The ADAS data base now contains very large collections of such data spanning all the ions of elements up to neon. *adf09* includes state selective dielectronic data to resolved lower lying LS-coupled terms, dielectronic data to representative n-shells separated according to parents and spin systems and averaged Auger data. All of these data can be extracted and displayed by the new code.

   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 subdirectories of type *adf09*. 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.

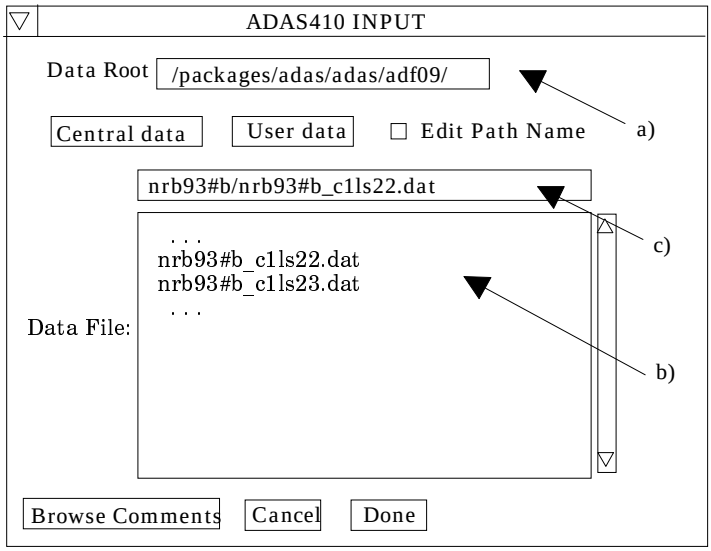
      3.1.2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

      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 datafiles are presented for selection. Datafiles all have the termination *.dat*. Note the notation used for dielectronic data file names, that is, *<ion>ls<nn'>* with *<ion>* the recombining ion, *<nn'>* denoting the parent n-shell transition class n-n'. *ls* indicates that the dielectronic data is at LS-resolution.

      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 datafile.



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 dataset being interrogated is also shown at a). The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.

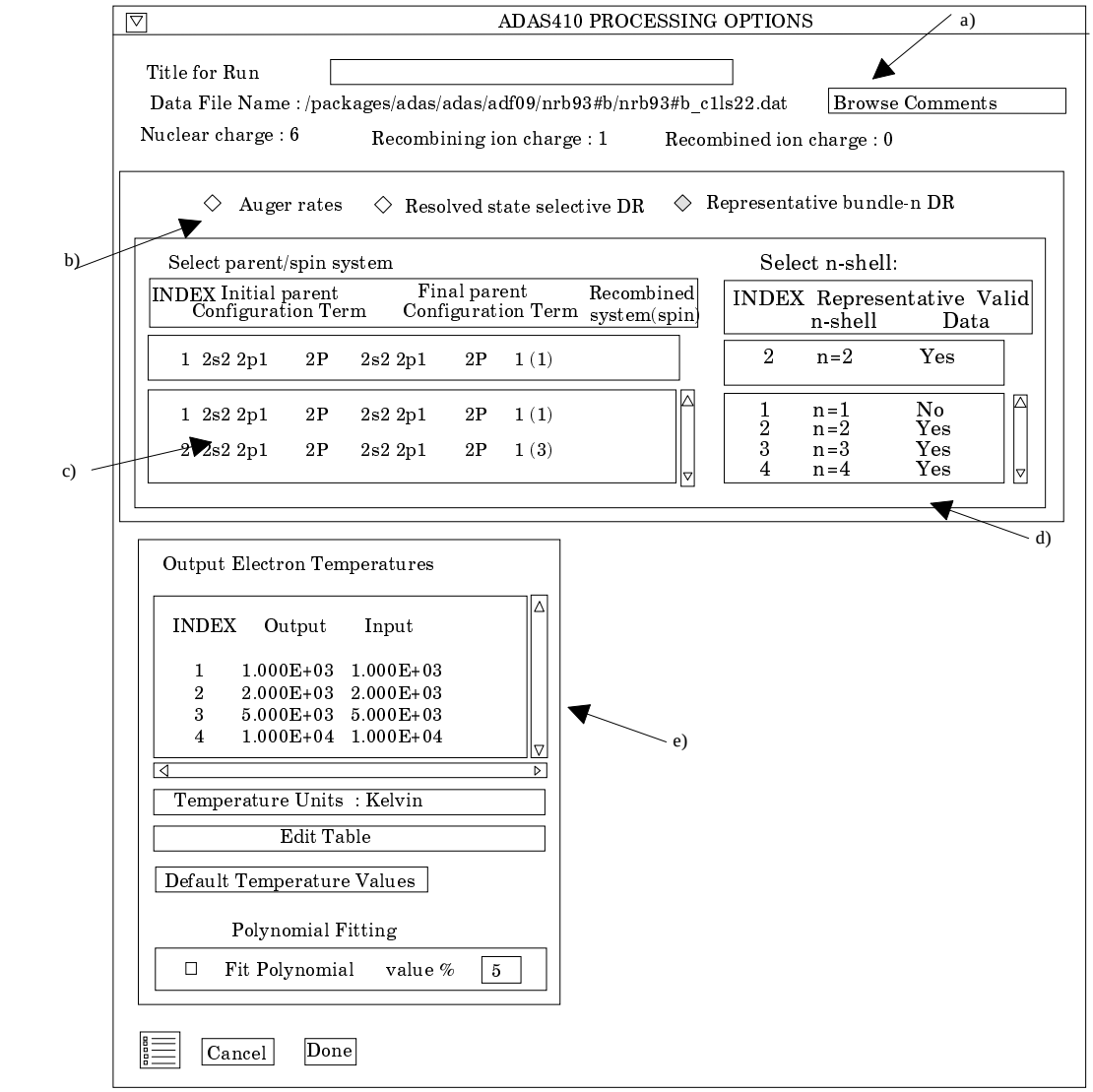
3.2.2. At b) the choice of the type of data to be extracted from the *adf09* file is selected by clicking the appropriate button. The sub-window below the buttons alters according to the choice made. The sub-window for *Representative bundle-n DR* is shown at c) and d). The schematics at f) and h) show the sub-windows for *Resolved state selective DR* and *Auger rates* respectively.

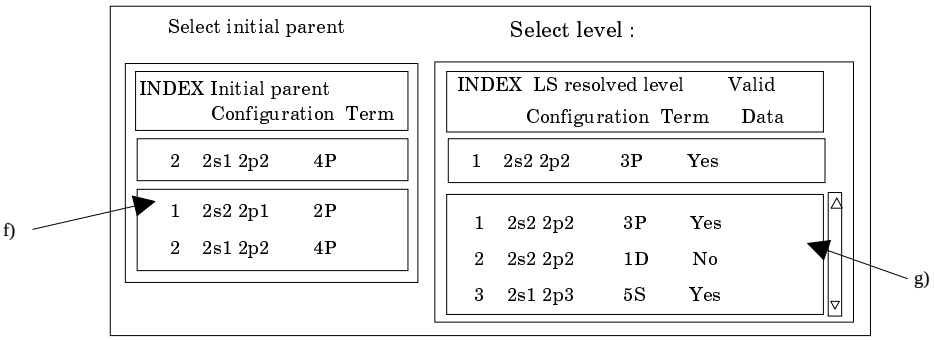
3.2.3. In the case of *Representative bundle-n DR*, select the initial parent and final parent/spin system combination first at c). Note that the dielectronic data is designed for the metastable resolved situation and so the choice of initial recombining (parent) metastable and then the recombined spin system and the parent it is built on matters. The adjacent window shows the n-shells for which data are available. These are representative n-shells up to around 1000. Data is not stored in the *adf09* file for every n-shell but only for a representative set. Codes which user the *adf09* datasets interpolate for non-representative n-shells. The selection table at d) indicates which n-shells have non-zero DR values.

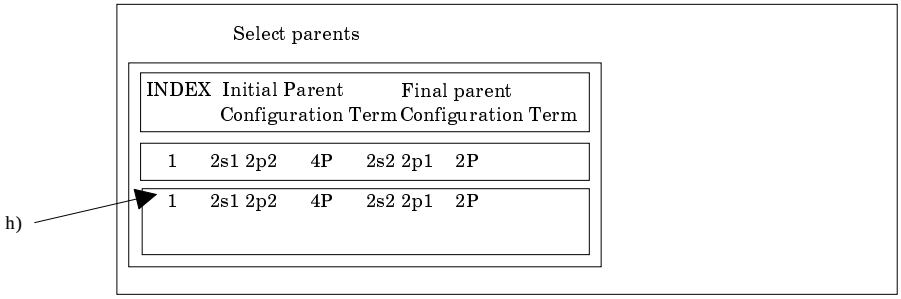
3.2.4. In the case of *Resolved state selective DR*, as illustrated at f), the situation is similar. However only the initial parent is identified, since the final recombined low levels may not have a clearly distinquished parent. The initial parent is selected at f). Then the final term of the recombined ion is selected at g). The *adf09* datasets contain fully LS resolved data for n-shells up to about 7.

3.2.5. at e), the electron temperatures at which you wish the dielectronic recombination data is chosen. Table editor is available to enter this data and default temperatures (equal to those in the *adf09* file) may be chosen by button click as usual.

3.2.6. The option of fitting a polynomial to the extracted data is offered just below the temperature selection widget.


ADAS410 PROCESSING OPTIONS
a)
Title for Run
Data File Name : /packages/adas/adas/adf09/nrb93#b/nrb93#b_c1ls22.dat
Browse Comments
Nuclear charge : 6
Recombining ion charge : 1
Recombined ion charge : 0
Auger rates
Resolved state selective DR
Representative bundle-n DR
b)
Select parent/spin system
INDEX Initial parent Configuration Term
Final parent Configuration Term
Recombined system(spin)
1 2s2 2p1 2P 2s2 2p1 2P 1 (1)
1 2s2 2p1 2P 2s2 2p1 2P 1 (1)
2 2s2 2p1 2P 2s2 2p1 2P 1 (3)
c)
Select n-shell:
INDEX Representative n-shell
Valid Data
2 n=2 Yes
1 n=1 No
2 n=2 Yes
3 n=3 Yes
4 n=4 Yes
d)
Output Electron Temperatures
INDEX Output Input
1 1.000E+03 1.000E+03
2 2.000E+03 2.000E+03
3 5.000E+03 5.000E+03
4 1.000E+04 1.000E+04
e)
Temperature Units : Kelvin
Edit Table
Default Temperature Values
Polynomial Fitting
Fit Polynomial
value %
5
Cancel
Done


Select initial parent
Select level :
INDEX Initial parent Configuration Term
2 2s1 2p2 4P
1 2s2 2p1 2P
2 2s1 2p2 4P
f)
INDEX LS resolved level Configuration Term
Valid Data
1 2s2 2p2 3P Yes
1 2s2 2p2 3P Yes
2 2s2 2p2 1D No
3 2s1 2p3 5S Yes
g)


Select parents
INDEX Initial Parent Configuration Term
Final parent Configuration Term
1 2s1 2p2 4P 2s2 2p1 2P
1 2s1 2p2 4P 2s2 2p1 2P
h)

3.2.7. The Auger data is stored for representative n-shells for recombined ion parent state and final ionised ion state pairs. The data is extracted for the complete set of representative n-shells so the choice at h) is only of the initial ionising ion parent core and final ionised parent. The choices are presented at h) for selection by clicking in the usual manner.

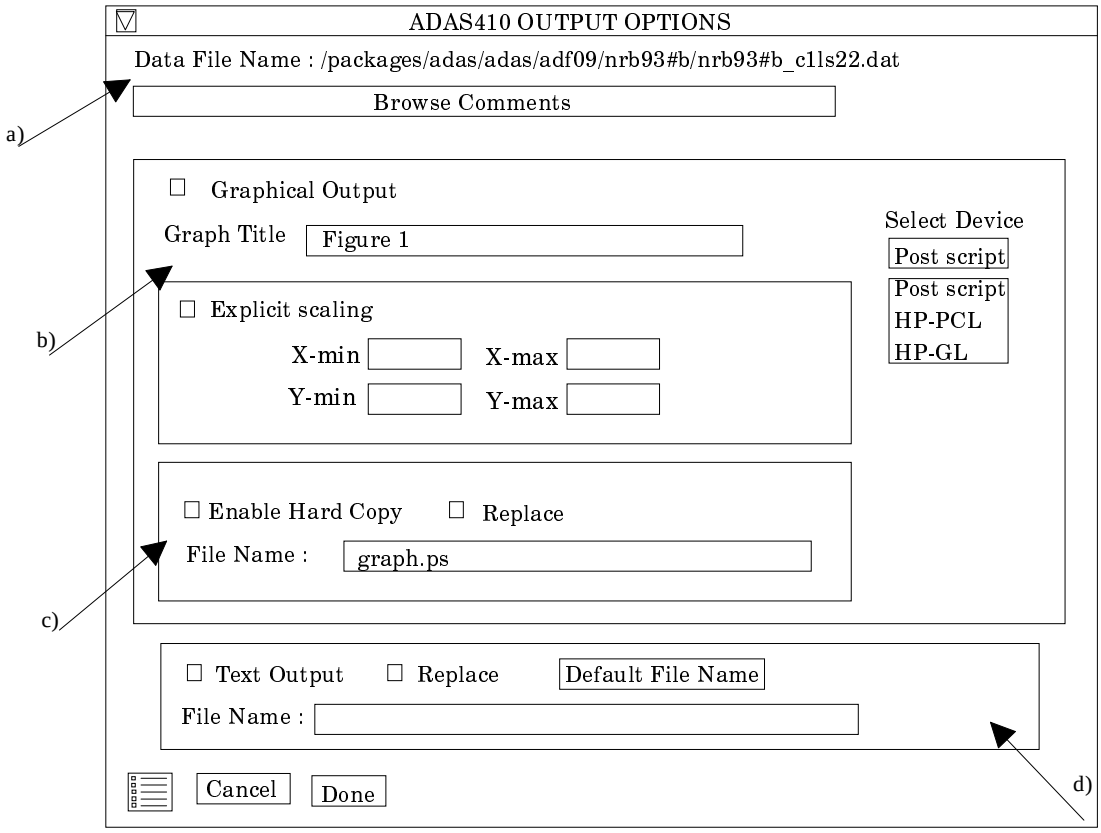
3.2.8. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

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.

3.3.2. Graphical display is activated by the *Graphical Output* button at b). This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.

3.3.3. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button at b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.



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

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

3.3.6. At d) output of the tabular record of the interrogation may be enabled. This is usually called *paper.txt* and it is created in the directory from which ADAS was launched.

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

3.3.8. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

4. **ADAS412** This new code allows the full calculation of solar astrophysical G(Te) functions. It does this by carrying out an excited population calculation from an *adf04* dataset in the manner of ADAS205, generating an ionisation balance from *adf11* datasets and finally assembling the G(Te) function. The code is the interactive implementation of the program used to create the main *adf20* datasets. The new code can create output data sets fully formatted to the *adf20* specification. Probable special uses of the code will be to check the sensitivity of G(Te) functions to small alterations in underlying collisional rates from *adf04* datasets or to focus on a restricted number of G(Te) functions. Thus we have allowed restriction of the number of G(Te) functions created by wavelength interval or by initial and final level. The theory of the G(Te) functions is given in the 'cds_manual' (*/.../adas/docs/cds-manual/...*).

4.1. The **file selection window** has the appearance shown below. It is composed of two sub-windows. The upper sub-window is a conventional file selection window used to select the specific ion file for the excited population part of the calculation, while the lower one allows an ionisation balance to be selected.

4.1.1. Data root a) shows the full pathway to the appropriate data subdirectories of type *adf04*. 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.

4.1.2. The Data root can be edited directly. Click the *Edit Path Name* button at b) first to permit editing.

4.1.3. Available sub-directories are shown in the large file display window c). Scroll bars appear if the number of entries exceed the file display window size.

4.1.4. Click on a name to select it. The selected name appears in the smaller selection window 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.

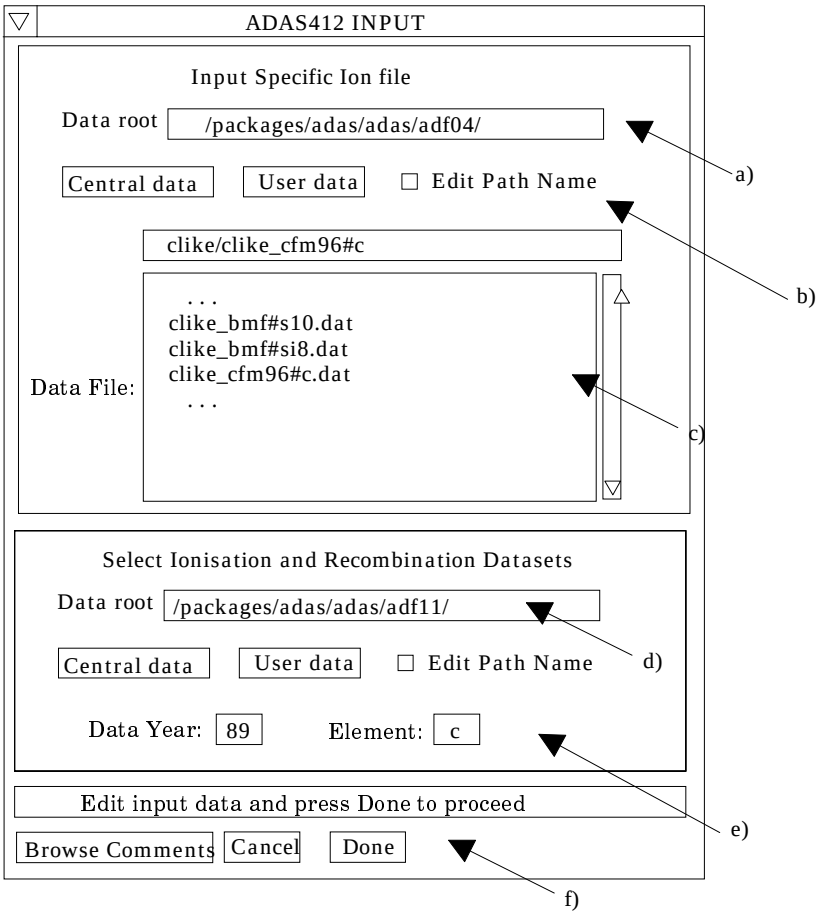
4.1.5. The ionisation balance is selected at d) and e). The appropriate data class is *adf11*.

4.1.6. Data root at d) shows the full pathway to the appropriate data subdirectories of type *adf11*. 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.

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

4.1.8. The particular ionisation and recombination data is selected by *Data Year* and then by *Element* at e). Enter the two digit year number. Note that the G(Te) code uses ionisation and recombination data unresolved by metastable. Thus it looks for sub-directories *acd<year>* and *scd<year>*, not acd<year>*r* and *scd<year>r*. Most of such data are in years '74', '85' and '89'.

4.1.9. Enter the element symbol at *Element*. The code will check that the same element is being used for the ionisation balance as for the excited population calculation.



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

4.1.11. Clicking on the *Browse Comments* button displays any information stored in the *adf04* file.

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

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

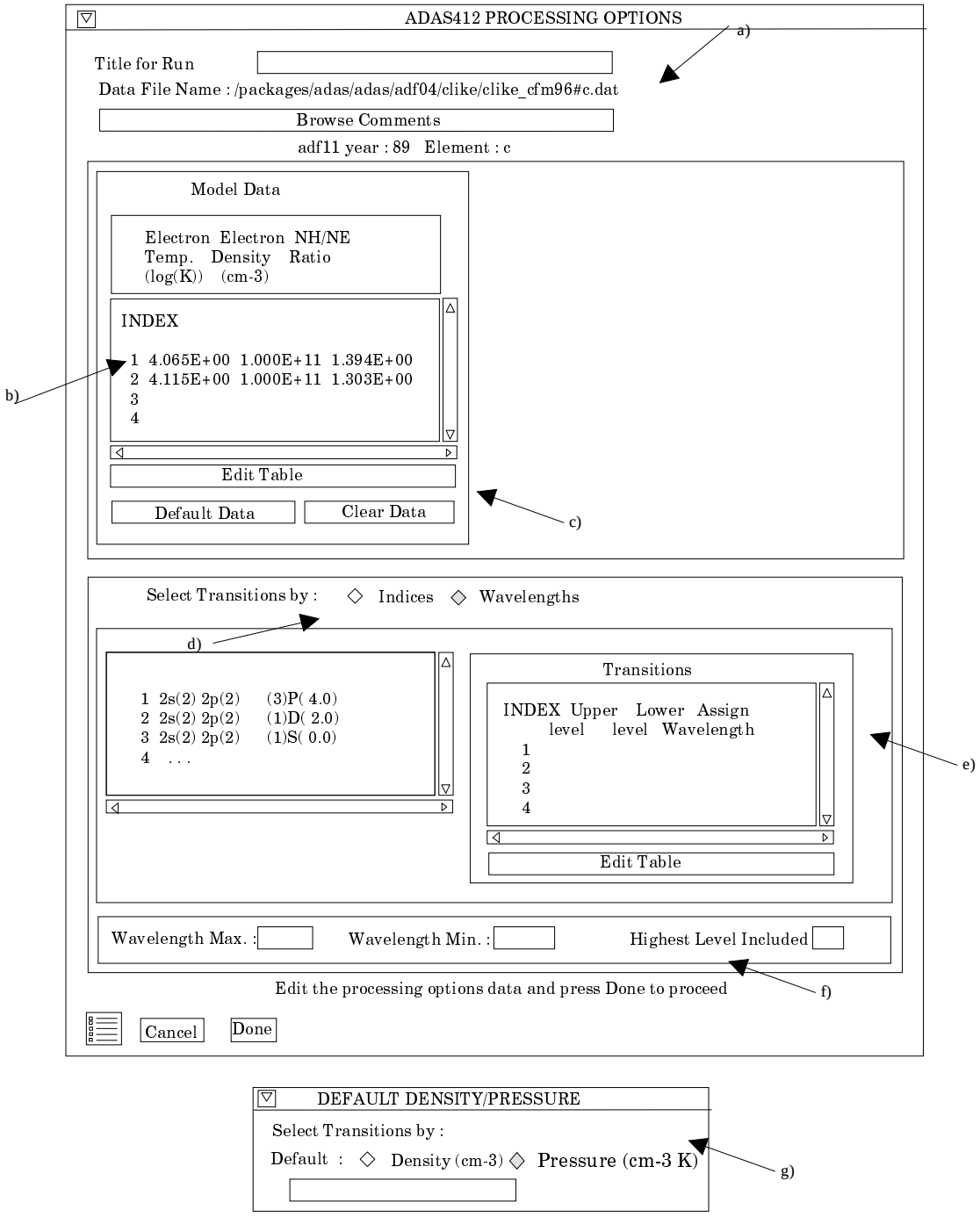
4.2.1. An arbitrary title may be given for the case being processed. For information the full pathway to the *adf04* dataset being used is also shown at a). The button *Browse comments* again allows display of the information field section at the foot of the selected *adf04* dataset, if it exists. Information on the ionisation and recombination data in use is given below.

4.2.2. At b) and c) the model data for the calculation are entered. The code will allow calculation of the G(Te) functions at either a fixed electron pressure or a fixed electron density.

4.2.3. Click the *Default Data* button to begin. A pop-up widget appears as shown at g). Select either *Density* or *Pressure*, enter a value in the editable box and press Return. Default model values of the selected type appear at b). The default temperature values come from the selected ionisation and recombination data sets. Note that the ratio of hydrogen to electron number densities is also inserted. This is required from the definition of the astrophysical type of G(Te) function. Standard solar atmosphere model data is used.

4.2.4. The model data is editable. Click on the *Edit Table* button to activate Table Editor. Note that the whole table becomes editable. It is the user's responsibility to modify the last column of N_H/N_e values according to changes in temperature. It is not recomputed from the standard built in atmosphere model.

4.2.5. The production of G(Te) functions is controlled and restricted by the selections at d). Activate the appropriate button at d) to enable selection by *Indices* or *Wavelengths*. The relevant part of the widget becomes activated.



4.2.6. Selecting by *Indices* is as shown at e). The complete indexed level list from the *adf04* file is shown on the left. In the editable table on the right, enter the upper and lower level indices of transitions you wish. Note that you must click the *Edit Table* button first to start Table Editor. The table allows you to enter the precise, spectroscopic accuracy wavelength of the line if you have it available. The output tables of the G(Te) function will provide the approximate theoretical wavelength from the *adf04* level energies. These are not of spectroscopic quality unless hand prepared. Browse the comments section of the adf04 file to see if this is so. The precise wavelength you

assign will appear in the output G(Te) tables along with the approximate theoretical one.

4.2.7. Selecting by Wavelengths activates the widgets at f). You can enter a *Minimum* and *Maximum* wavelength (in Angstroms) and further restrict by the *Highest level included*, that is the highest indexed level from the adf04 file which will be considered in setting up possible lines.

4.2.8. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

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

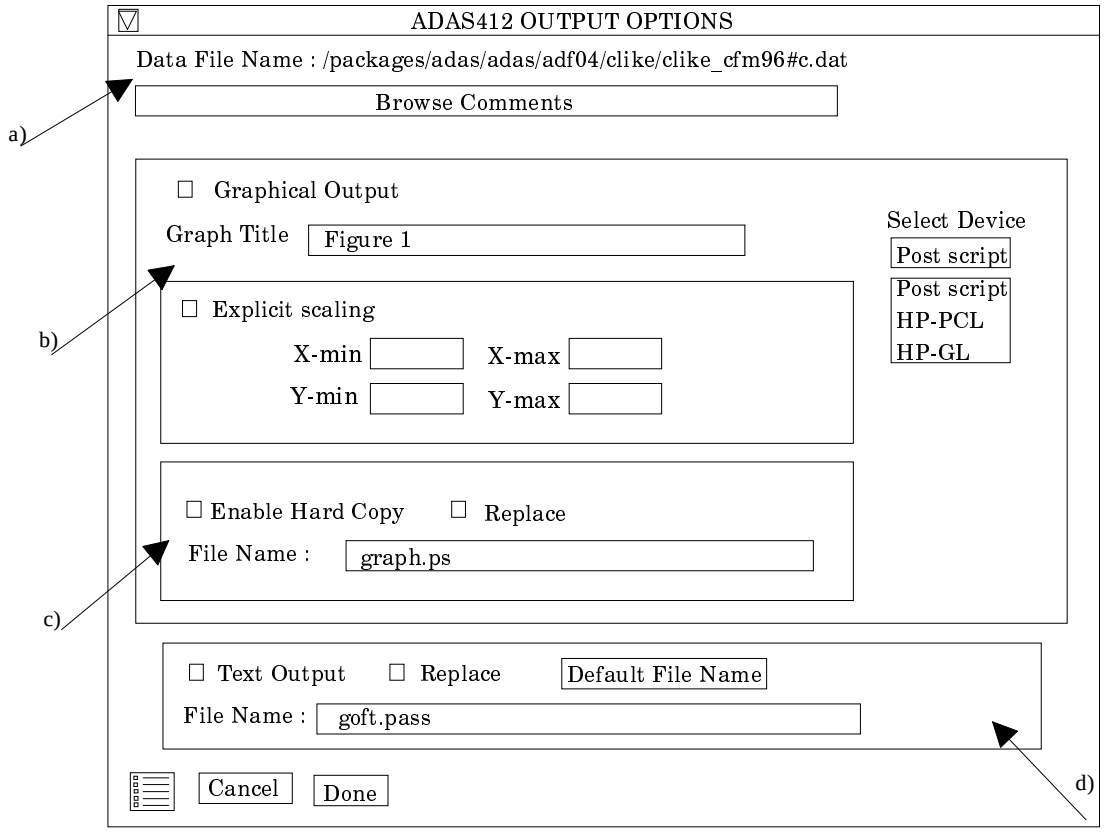
4.3.1. As in the previous window, the full pathway to the file being analysed is shown for information at a). Also the *Browse comments* button is available.

4.3.2. Graphical display of the G(Te) functions is activated by the *Graphical Output* button at b). This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.

4.3.3. 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.

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

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



4.3.6. The *Text Output* button at d) 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 is *goft.pass* and it is sent to your */../adas/pass* directory. Note that the

4.3.7. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

5. **ADF02** The data sets

/.../adas/adas/adf02/sia#h/sia#h_j97#h.dat
/.../adas/adas/adf02/sia#h/sia#h_tos#h.dat

have been updated by Harvey Anderson

6. **ADF04**

6.1. Errors were found in the energy levels of hydrogen-like datasets of the form

/.../adas/adas/adf04/copsm#h/...
and */.../adas/adas/adf04/copha#h/...*

These have been amended.

6.2. A fault in

/.../adas/adas/adf04/blike/blike_jl96#ne5.dat

detected by Ralph Dux has been corrected.

6.3. A substantial new body of data has been entered by Alessandro Lanzafame in various

/.../adas/adas/adf04/<ion>like/...

categories. They have the final part of their names as

/<ion>like_al97#<ion>.dat

6.4. A number of very old 'relic' faulty datasets have been removed from the *belike* directory.

7. **ADF09** Martin O'Mullane has amended and refreshed

/.../adas/adas/adf09/mom96#li

8. **ADF11** Data for krypton has been prepared by Martin O'Mullane and added as

/.../adas/adas/adf11/<code89>/<code89>_kr.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 ADAS411, ADAS213, ADAS205 and ADAS207.**

10.1. ADAS411 which interrogates the state selective radiative recombination data was not quite ready for the release. It will be issued at the next release.

10.2. Stuart Loch is preparing a utility, ADAS213, for modifying *adf04* files to include escape factors according to basic plane parallel and cylindrical plasma models. The code originator is Kurt Behringer. Stuart has converted it to FORTRAN and has nearly completed the IDL widgets for ADAS.

10.3. A development of ADAS205 and ADAS207 to include satellite lines is under test and will be included in the next release. It will come with a substantial body of new *adf04* data for lithium-like ions which includes the doubly excited levels. A further development into a spectral fitting code (tentatively called ADAS603) has still some way to go and will not be ready until late spring 1998.

H. P. Summers
29 October 1997