oct18-96

ADAS Bulletin

Five new programs are ready. Two ADAS series 1 data entry and verification programs are operational. These are ADAS105 and ADAS106 for entry of ionisation data and they follow the same design principles as our trial case ADAS101. Then there are three programs from series 2. These programs are different from the usual ADAS codes in that they are really designed for background processing. Thus they draw their data from data files rather than from user data entered in a *processing options* widget. ADAS204 prepares collisional-radiative data in the 'bundle-nS' model for advanced population and ionisation balance calculations. ADAS211 prepares radiative recombination data and adds it to specific ion files of type *adf04*. ADAS212 does the same for dielectronic recombination. Note that ADAS211 and ADAS212 are new codes to ADAS and were not present in IBM-ADAS at JET. These three codes do the background work necessary to enable the advanced population code ADAS208 to operate in its full glory.

1. ADAS105

This is a program for examination of electron impact ionisation 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 ADAS105 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 fifth button to activate ADAS105.
- 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 ADAS105 analysis is /..../uid/adas/arch105/

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



- 1.5. The **processing options window** has the appearance shown below
 - 1.5.1. The button *Browse Index* remains available at the top of the window to display the archive index list.
 - 1.5.2. As described in the ADAS User Manual, the examination of input ionisation cross-sections is based on the generation of an approximate form for the cross-section variation with energy with which the input is compared. The approximate form is built from 'shell groups' and 'resonance groups designed to represent direct ionisation and autoionisation respectively. Scaling factors can be varied to attempt to optimise the fit of the approximate form to the input data.
 - 1.5.3. At a), the primary data on the nuclear and ion charges are entered. Make an appropriate choice at *Use default scaling parameters* if you wish the scaling parameters to be frozen at your initial settings (YES) or allowed to vary (NO). Click on the appropriate diamond button to display the parameters of either the *Shell* groups or *Resonance* groups in the sub-window to the right at b).
 - 1.5.4. Up to two shell or resonance groups may be prepared. Make this choice at *No. of shell groups* at the top of the sub-window at b). Then click on the button for the *1*st or 2nd. *Group* to display its parameter settings below. Enter the group parameters in the editable table. The definitions of the various parameters are given in the ADAS User Manual. Remember to enter a *Default scaling parameter*. 1.0 is a good first choice. Click on *Edit Table* to bring up the ADAS Table Editor widget in the usual manner.
 - 1.5.5. User input energies, cross-sections and required output temperatures are entered at c) with the currently selected units shown below at d). Click the *Edit table* button to 'drop down' the ADAS Table Editor for data input.
 - 1.5.6. 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 output temperatures.
 - 1.5.7. 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.

- 1.5.8. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window. The 'Escape to Menu' icon is also available for a quick exit at the bottom left hand corner.
- 1.6. The **output options window** is shown below.
 - 1.6.1. There is only one system of comparative display for ADAS105 at the moment. Unlike ADAS101, a 'Burgess option' is not available.
 - 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 ionisation rate coefficient at the user's temperatures.
 - 1.6.3. At a) select *Graphical Output* and insert a *Graph Title*. The latter appears as the index entry if you save the results of your analysis to archive. A graphic scaling parameter should be entered. This allows some movement in the x-direction on the comparative display along the lines of the Burgess 'C parameter'. Zero is a good initial choice.

1.6.4. Make the required choices of graph scaling and axes choices at b) for the comparative graph and at c) for the ionisation rate coefficient graph. For default scaling the *Ratio Graph Scaling* and *Ionis. Coefft. Scaling* buttons should not be activated.

-	ADAS105 OUTPUT OPTIONS	
	Data file name : /home/summers/adas/arch105/carbon.dat Browse Index	
a) b)	Graphical Output Select Device Graph Title Figure 1 Graphic scaling paramete Post-script HP-PCL HP-GL Warding Ionis. Coefft. Graph Scaling X-min : X-max : Y-min : Y-max :	
	□ Enable Hard Copy □ Replace File name graph.ps □ Text Output □ Replace Default file name File name paper.txt	c
	Cancel Done	

- 1.6.5. After making your choices on hard copy and text output click *Done* to show the comparative graph.
- 1.6.6. The comparative graph is displayed in the Graph Editor window as shown below. The graph displays the ratio of input cross-section to approximate form as circles with a spline drawn through these tabular points. The points can be modified by using the buttons a) beneath the graph in association with the mouse.
- 1.6.7. 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.

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

a)

h)

c)

- 1.6.9. 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, if any points are modified, the program cycles back to the Output Options window for reanalysis.
- 1.6.10. Click Done to display the final graphical output. The window appearance is as shown below.
- 1.6.11. Both the comparative plot and the final plot of ionisation rate coefficients may be displayed at a). Click *Show Plot 1* for the comparative plot and *Show plot 2* for the ionisation coefficient plot.
- 1.6.12. To store the results in the archive file, click *Archive*. To make a hard copy of the graph, click *Print*.
- 1.6.13. Click *Done* to return to the Output Options window. The *Escape to Menu* icon is available. Click on it to quit the program and return to the ADAS series 1 menu.



2. ADAS106

This is a program for examination of electron impact ionisation rate coefficient data from external sources and its interpolation to different temperatures 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 ADAS106 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.

2.1. 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.

- 2.2. 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.
- 2.3. Initiate ADAS, move to the series 1 menu and click on the sixth button to activate ADAS106.
- 2.4. The **archive selection window** appears first. It is slightly different in operation than the usual file selection window.
 - 2.4.1. The recommended root path for user archiving for ADAS106 analysis is /..../uid/adas/arch106/

which may be edited in the usual manner.

2.4.2. 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.

- 2.4.3. 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.
- 2.4.4. 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.
- 2.4.5. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window



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

- 2.5.1. The button *Browse Index* remains available at the top of the window to display the archive index list.
- 2.5.2. As described in the ADAS User Manual, the examination of input ionisation rate coefficients is based on the generation of an approximate form for the rate ceofficient variation with temperature with which the input is compared. The approximate form is built from 'shell groups' and 'resonance groups designed to represent direct ionisation and autoionisation respectively. Scaling factors can be varied to attempt to optimise the fit of the approximate form to the input data.
- 2.5.3. At a), the primary data on the nuclear and ion charges are entered. Make an appropriate choice at *Use default scaling parameters* if you wish the scaling parameters to be frozen at your initial settings (YES) or allowed to vary (NO). Click on the appropriate diamond button to display the parameters of either the *Shell* groups or *Resonance* groups in the sub-window to the right at b).
- 2.5.4. Up to two shell or resonance groups may be prepared. Make this choice at *No. of shell groups* at the top of the sub-window at b). Then click on the

button for the *I*st or 2nd. *Group* to display its parameter settings below. Enter the group parameters in the editable table. The definitions of the various parameters are given in the ADAS User Manual. Remember to enter a *Default scaling parameter*. 1.0 is a good first choice. Click on *Edit Table* to bring up the ADAS Table Editor widget in the usual manner.

- 2.5.5. User input temperatures, rate coefficients and required output temperatures are entered at c) with the currently selected units shown below at d). Click the *Edit table* button to 'drop down' the ADAS Table Editor for data input.
- 2.5.6. If an archive data set is opened, temperature, rate coefficients and output temperature values are filled from this. Otherwise the fields are empty. Pressing the *Default Temperature values* button inserts a default set of output temperatures.
- 2.5.7. 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.



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

The *Escape to Menu* icon is also available for a quick exit at the bottom left hand corner.

- 2.6. The **output options window** is shown below.
 - 2.6.1. There is only one system of comparative display for ADAS106 at the moment.
 - 2.6.2. Two graphs are presented. The first is a scaled comparative graph for assessing the rate coefficient data and making adjustments if appropriate. The second graph displays the final ionisation rate coefficient at the user's temperatures.
 - 2.6.3. At a) select *Graphical Output* and insert a *Graph Title*. The latter appears as the index entry if you save the results of your analysis to archive. A graphic scaling parameter should be entered. This allows some movement in the x-direction on the comparative display along the lines of the Burgess 'C parameter'. Zero is a good initial choice.
 - 2.6.4. Make the required choices of graph scaling and axes choices at b) for the comparative graph and at c) for the ionisation rate coefficient graph.

	ADAS106 OUTPUT OPTIONS	
	Data file name : /home/summers/adas/arch106/carbon.dat	
	Browse Index	
	□ Graphical Output Select Device Post-script	
a)	Graph Title Figure 1 Graphic scaling parameter 0.00	
b)	Ratio Graph Scaling Ionis. Coefft. Graph Scaling X-min : X-max : Y-min : Y-max : Y-min : Y-max :	
	☐ Enable Hard Copy ☐ Replace File name graph.ps	c)
	Text Output Replace Default file name File name paper.txt	
	Image: Cancel Done	

- 2.6.5. After making your choices on hard copy and text output click *Done* to show the comparative graph.
- 2.6.6. The comparative graph is displayed in the Graph Editor window as shown below. The graph displays the ratio of input rate coefficient to approximate form as circles with a spline drawn through these tabular points. The points can be modified by using the buttons a) beneath the graph in association with the mouse.
- 2.6.7. 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 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 a second time to terminate insertion operations.



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

c)

- 2.6.9. 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, if any points are modified, the program cycles back to the Output Options window for reanalysis.
- 2.6.10. Click Done to display the final graphical output. The window appearance is as shown below.

- 2.6.11. Both the comparative plot and the final plot of ionisation rate coefficients may be displayed at a). Click *Show Plot 1* for the comparative plot and *Show plot 2* for the ionisation coefficient plot.
- 2.6.12. To store the results in the archive file, click *Archive*. To make a hard copy of the graph, click *Print*.



3. **ADAS204**

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. There is no processing options window for ADAS204.
- 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.
 - 3.4.1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
 - 3.4.2. Graphical display is activated by the *Graphical Output* button a). 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 b) to allow

explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable. Plot A axes limits refer to the 'stick diagram and Plot B axes limits to the Doppler broadened profile.

- 3.4.3. Hard copy is activated by the *Enable Hard Copy* button c). The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a 'pop-up' window issues a warning.
- 3.4.4. A choice of output graph plotting devices is given in the Device list window d). Clicking on the required device selects it. It appears in the selection window above the Device list window.
- 3.4.5. 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.

Į	ADAS204 OUTPUT OPTIONS
	Data File Name : /disk2/adas/adas/adf08/radrec/blike/blike_c1ls.dat
	Browse comments
	Title for Run demonstration
a)	 ✓ Specific Ion Output □ Replace Default file name File Name /home/summers/adas/pass/data04.pass
up	Resolved Recombination Output Replace Default file name File Name /home/summers/adas/pass/data04.pass
	b) Text output File Name paper.txt
	Cancel Run Now Run in Batch
L	d)

4. **ADAS211**

The program calculates state-selective radiative recombination coefficients to LS-coupled terms in a one-electron Slater type model potential adjusted to observed energies. A template file must be supplied which lists the energy levels and their energies and supplies the electron temperatures at which the coefficients are to be calculated. The template files are built from the energy level lists at the head of adf04 files. The code provides two outputs. The first is a set of 'R-lines' with the radiative recombination coefficients which can be manually edited onto the end of the reference adf04 file. Secondly, it writes a file of ADAS data format adf08 with the tabulated results, suitable for archiving. adf08 files, without the computed results, that is just including the requested temperature lines are in fact the form of the input template files. Thus ADAS211 takes an incomplete adf08 file without the coefficients and returns the complete file.

4.1. 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 ADAS211 from the program selection menus in the usual manner.

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



- 4.2.1. *adf08* in template form is the appropriate format for use by the program ADAS211. Your template data should be held in such a file, in the same directory structure as central ADAS, but with your identifier replacing the first *adas*. You should finally, if the code operates correctly replace you *adf08* template file with the *adf08* type output file.
- 4.2.2. 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 isoelectronic sequence of the recombining ion. It is useful to use a naming convention for the final part of the file name which includes the ion and 'LS' (eg. blike/blike_c1ls.dat) to indicate that the data is for terms.
- 4.2.3. 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*.
- 4.2.4. Once a data file is selected, the set of buttons at the bottom of the main window become active.
- 4.2.5. 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.
- 4.2.6. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window
- 4.3. There is no processing options window for ADAS211.
- 4.4. The **output options window** is shown below. There is no graphical output possibility but in addition to the usual text file, two output data files may be produced.
 - 4.4.1. The data output file called the *Specific Ion Output* is activated by the button at a). The default file name is *data04.pass* and it is sent to your pass directory. It is prepared preformatted according to 'R-lines' for *adf04* files and can be patched directly into the *adf04* file, which was used as reference for the template input *adf08* file, at the foot of the transition list before the terminator. See central ADAS for examples.
 - 4.4.2. The second output file at b), called the *Resolved Recombination Output* is sent by default as *data08.pass* to your pass directory. Assuming the code has worked correctly, it is a direct replacement for the template *adf08* file. It simply includes all the state selective recombination coefficient results requested below the temperature lines in the template.

- 4.4.3. 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:
- 4.4.4. By pressing *Run Now* at d), 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. This is shown below. Once this has been done the calculations cannot be halted, but an execution time of less than 30 seconds can usually be expected.

	ADAS211 OUTPUT OPTIONS
	Data File Name : /disk2/adas/adas/adf08/radrec/blike/blike_c1ls.dat
	Browse comments
	Title for Run demonstration
	 □ Specific Ion Output □ Replace □ Default file name File Name /home/summers/adas/pass/data04.pass
a) /	Resolved Recombination Output Replace Default file name
	File Name /home/summers/adas/pass/data04.pass
	b)
	□ Text output □ Replace Default file name
	File Name paper.txt
	Cancel Run Now Run in Batch
	d)

By pressing Run in Batch the actual calculations required to produce the 4.4.5. 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 ADAS211 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.



5. ADAS212

The program adds state selective dielectronic recombination coefficient data to specific ion files of type adf04. To achieve this it, it opens the primary data archives for dielectronic recombination coefficient data of type adf09 and accesses the part of the data concerned with LS coupled low levels. 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 and the particular sub-library of relevance here is $a09_a04$. The result of the operation of the code is a fully specified adf04 file ready for immediate inclusion in your personal database.

- 5.1. 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. Initiate ADAS212 from the program selection menus in the usual manner.
- 5.2. The **file selection window** appears first. Its operation is as described in the bulletin *jan18-95*.

5.3.

- 5.3.1. An *adf18/a09_a04* format cross-referencing file is the appropriate input file for use by the program ADAS212. 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*.
- 5.3.2. 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 isoelectronic sequence of the recombined ion with a prefix which identifies the primary author of the actual dielectronic 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. nrb93#c/nrb93#c_c0ls.dat) to indicate that the data is for terms.
- 5.3.3. 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*.
- 5.3.4. Once a data file is selected, the set of buttons at the bottom of the main window become active.
- 5.3.5. 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.
- 5.3.6. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window



5.4. There is no processing options window for ADAS212.

5.5.

- 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
 - 5.5.1. The data output file is of specific ion file form, that is *adf04* and is sent to your pass directory as *adas213.pass*. It comprises the *adf04* file for which the cross-referencing was prepared but includes dielectronic data. It is the normal practice to use ADAS211 to put radiative recombination data in the specific ion file and then use ADAS212 to add the dielectronic data. The button at b) allows the choice of whether the dielectronic data should be added on to the radiative recombination 'R-lines' or replace them.
 - 5.5.2. By pressing *Run Now*, 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.

	ADAS212 OUTPUT OPTIONS	
	X-ref. File Name : /disk2/adas/adas/adf18/a09_a04/nrb93#c/nrb93#c_c0ls.da Browse comments	it
a)//	Add new recombination data to existing 'R' li YES in the specific ion file ?	
	Text output Replace Default file name File Name paper.txt	b)
	Cancel Run Now c)	

5.5.3. Since the code operates rapidly, we have removed the background execution operation available in the sister program ADAS211.

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