

ADAS703: Postprocessor - Autostructure > adf04 file

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 redistributive collision data, in a simple impact parameter approximation are also produced and added to the *adf04* file.

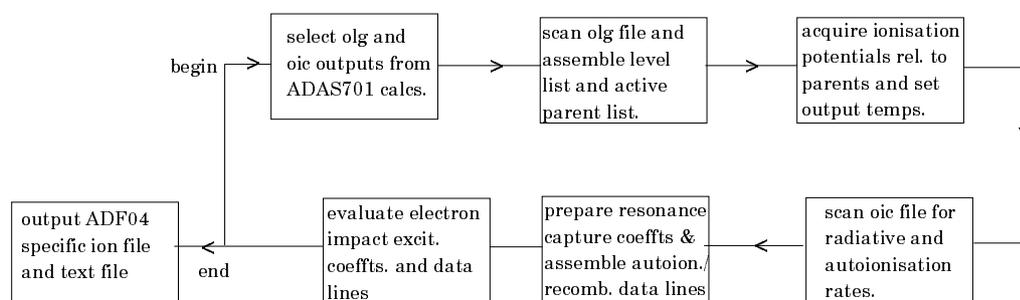
Background theory:

Within ADAS, calculation of the population structure of excited states of an ion in a plasma has previously been restricted to bound states or to states which are uncoupled to continua in which they are embedded. This has prevented explicit calculation of the populations of doubly excited states which participate in dielectronic recombination or excitation/auto-ionisation. The ADAS population code ADAS705 releases this constraint by allowing inclusion of resonance capture coefficients, Auger break-up rates and inner-shell excitation rate coefficients in its rate equations. In practice, such data must be provided in the input specific ion file of data format *adf04* upon which ADAS705 works. The doubly excited states of interest may be divided into (i) the individually resolved group and (ii) the bundled group following the pattern and usual analysis methods for satellite line spectra. Thus group (i) contains the upper doubly excited levels for which the stabilising radiative transition gives a satellite line which is spectrally resolved from the parent resonance line. (ii) contains doubly excited levels involving higher shell spectators whose stabilising spectral emissions are not resolvable one from another and/or from the parent resonance line. ADAS has a specified approach to 'level bundling' (cf. ADAS209 and ADAS210) and in this context group (i) levels should be handled individually and group (ii) levels should be bundled. From the point-of view of precision of spectral analysis, data for group (i) should be provided at the best available accuracy whereas group (ii) can use less precise data. The present code is designed to prepare a specific ion file of type *adf04* for group (i) levels incorporating the best available resonance capture, radiative and autoionisation rates from ADAS701 (AUTOSTRUCTURE). The code ADAS704 adds bundled shell contributions to the *adf04* file, while the code ADAS213 adds electron impact inner shell excitation data.

Program steps:

These are summarised in the schematic below.

Figure 8.3

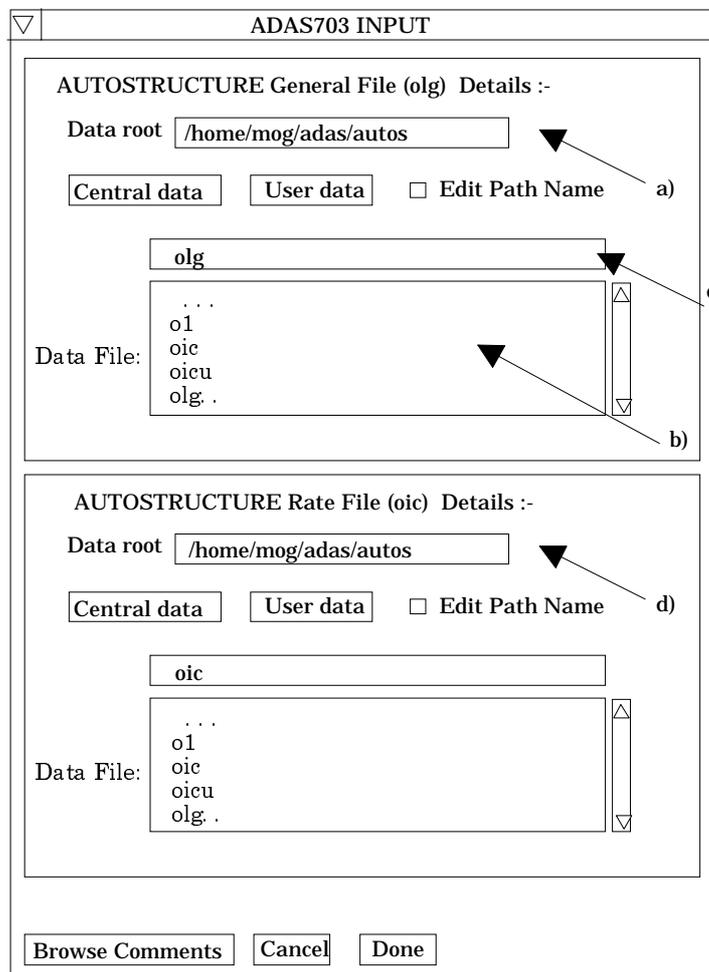


Interactive parameter comments:

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.

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

1. Two data files must be selected in indential manner at a) and d).
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 performs 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.
3. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
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.
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.



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

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

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

9. 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 coeff. calculation to establish approximate target sizes for strong coupling corrections.
10. 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).

ADAS703 PROCESSING OPTIONS

Title for Run

Input Ionisation Potentials for Parent :-

1s 2s

1s 2p

1s 1s

Eissner style energy levels : Yes No

Temperature Values

INDEX	Output	Input
1	3.200E+05	3.200E+04
2	6.400E+05	6.400E+04
3	1.280E+06	1.280E+05
3	3.200E+06	3.200E+05

Temperature Units : Kelvin

Edit Table

Default Temperature Values

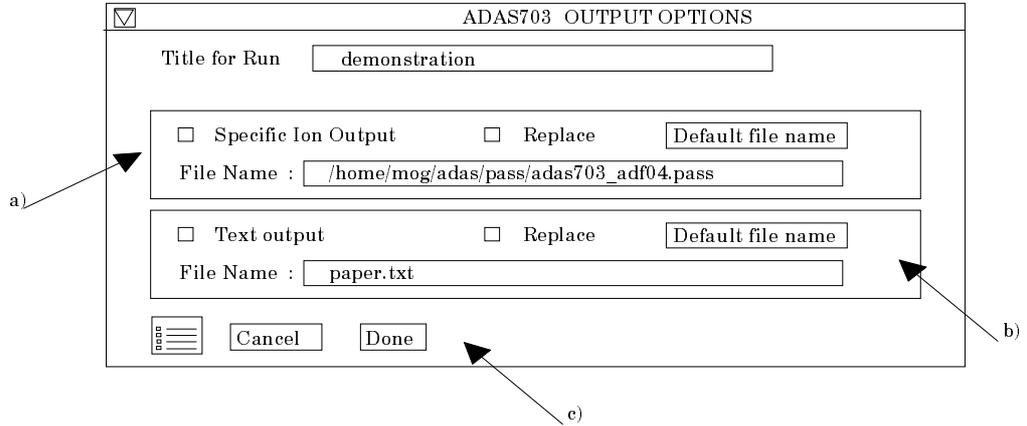
Edit the processing options data and press Done to continue

11. 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.
12. 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.
13. 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.

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

14. 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*.

15. 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.**



16. 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.

Illustration:

The output *adf04* file from post-processing AUTOSTRUCTURE intermediate files for Ar^{+15} is shown in table 2-03a. Levels 4 and above are autoionising. R-lines are generated for resonance capture into these double excited states as a function of electron temperature with the autoionising rate entered into the column immediately following the transition indices. There is only a single parent state ($1S$) in this case.

Table 2-03a

AR+15	18	16	7404400.0																			
1	21512		(2)0(0.5)																		0.0	
2	21513		(2)1(0.5)																		257884.9	
3	21513		(2)1(1.5)																		289300.4	
4	11522		(2)0(0.5)																		24860800.0	
17	11523		(2)1(0.5)																		25374048.0	
18	11523		(2)1(1.5)																		25399152.0	
19	11523		(2)0(0.5)																		25531792.0	
-1	301.92	68.10	66.40	173.21	173.21	173.21	173.21	173.21	173.21	173.21	173.21	173.21	173.21	173.21	173.21	173.21	173.21	173.21	173.21	173.21	173.21	173.21
16.00	3	1.28+05	2.56+05	5.12+05	1.28+06	2.56+06	5.12+06	1.28+07	2.56+07	5.12+07	1.28+08	2.56+08	5.12+08	1.28+09	2.56+09	5.12+09	1.28+10	2.56+10	5.12+10	1.28+11	2.56+11	5.12+11
2	1	1.13+09	2.56-01	2.61-01	2.90-01	3.24-01	3.52-01	3.99-01	4.81-01	5.54-01	6.28-01	7.21-01	7.88-01	8.81-01	9.91-01	1.07+00	1.22+00	1.40+00	1.54+00	1.72+00	1.91+00	2.12+00
3	1	1.59+09	5.09-01	5.19-01	5.66-01	6.34-01	6.88-01	7.75-01	9.31-01	1.07+00	1.22+00	1.40+00	1.54+00	1.72+00	1.91+00	2.12+00	2.33+00	2.56+00	2.81+00	3.08+00	3.37+00	3.68+00
19	13	2.49+09	3.64-01	3.72-01	4.03-01	4.51-01	4.89-01	5.50-01	6.61-01	7.62-01	8.66-01	9.98-01	1.09+00	1.22+00	1.40+00	1.54+00	1.72+00	1.91+00	2.12+00	2.33+00	2.56+00	2.81+00
19	14	4.65+09	7.06-01	7.21-01	7.83-01	8.77-01	9.51-01	1.07+00	1.29+00	1.48+00	1.68+00	1.94+00	2.12+00	2.33+00	2.56+00	2.81+00	3.08+00	3.37+00	3.68+00	4.00+00	4.34+00	4.70+00
R 15	+1	1.49+14	1.00-78	2.28-53	6.38-32	2.22-19	1.88-15	1.03-13	5.37-13	5.20-13	3.05-13	1.04-13	4.08-14	1.22-14	4.77-14	1.22-15	4.77-15	1.22-16	4.77-16	1.22-17	4.77-17	1.22-18
R 12	+1	1.74+12	1.00-78	5.42-55	1.06-33	2.99-21	2.36-17	1.25-15	6.36-15	6.12-15	3.57-15	1.22-15	4.77-16	1.22-17	4.77-17	1.22-18	4.77-18	1.22-19	4.77-19	1.22-20	4.77-20	1.22-21
R 5	+1	1.57+10	1.00-78	8.80-57	7.43-36	1.26-23	8.42-20	4.09-18	1.98-17	1.88-17	1.09-17	3.69-18	1.44-18	4.28-18	1.67-18	5.12-18	1.83-19	2.16-19	2.56-19	2.99-19	3.52-19	4.00-19
R 8	+1	1.83+13	1.00-78	3.26-54	4.88-33	1.17-20	8.73-17	4.49-15	2.25-14	2.16-14	1.26-14	4.28-15	1.67-15	5.12-15	1.83-16	2.16-16	2.56-16	2.99-16	3.52-16	4.00-16	4.77-16	5.54-16
R 13	+1	8.42+13	1.00-78	8.38-54	1.68-32	4.79-20	3.80-16	2.01-14	1.03-13	9.89-14	5.77-14	1.97-14	7.71-15	1.22-15	4.77-16	1.22-17	4.77-17	1.22-18	4.77-18	1.22-19	4.77-19	1.22-20
-1																						
-1	-1																					

C Specific ion file generated from AUTOSTRUCTURE list file																						
C																						
C Program: JETSHP.STRIP.FORT(GCPSAJ91)																						
C Producer: JETABU																						
C Date: 29/08/96																						

Notes: