

## ADAS704: Postprocessor - Autostructure > adf18 file

This is a new code which provides one of the last links in the chain of processing required in the 'GCR Project' for the generation of complete collisional-radiative data for light elements (see also ADAS807 and 'GCR Project bulletin no. 2'). The code constitutes a third post-processing option on the Auger rate coefficient data output from ADAS701 (Autostructure). It creates a part of the cross-referencing file of type `../adas/adas/adf18/a09_p204/` which links dielectronic data into the bundle-nS population code ADAS204. The part in question is some supplementary data which allows for Auger breakup going from n-shells built on one parent metastable to a different metastable but not via a common spin system. Such Auger processes must occur via LS-coupling breakdown and, although small for light element ions, are sufficient to drop the high level populations markedly. To obtain these supplementary rates it is necessary to go back to basic ADAS701 calculations in intermediate coupling. ADAS704 then processes the intermediate coupling calculation data to give the required supplement.

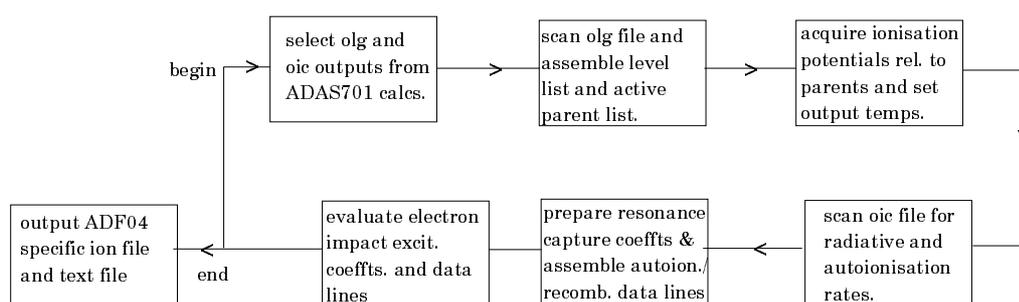
### Background theory:

To be added

### Program steps:

These are summarised in the schematic below.

Figure 8.4

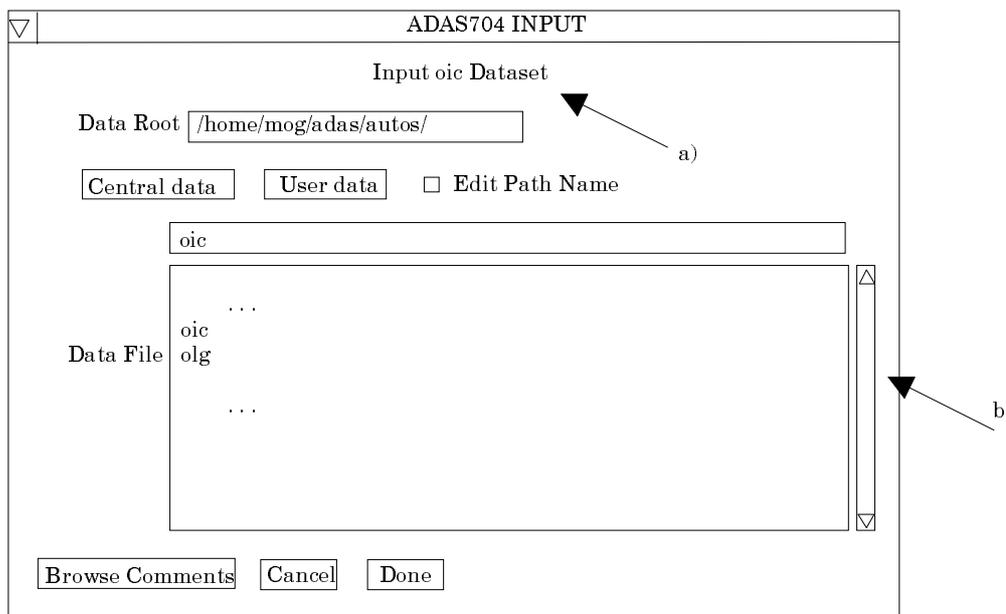


### Interactive parameter comments:

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 ADAS704 from the program selection menus in the usual manner.

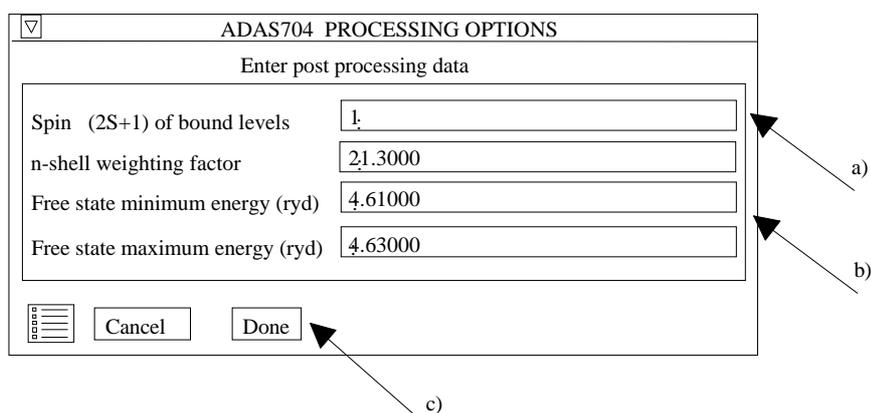
The **file selection window** has the appearance shown below

1. The input file is the intermediate coupling 'oic' file from the ADAS701 (Autostructure) run. Note that by convention a user should assign a separate '/autos/' sub-directory for such datasets from ADAS701 in his/her master '/adas/' directory rather than the usual '/pass' sub-directory. Note that the 'oic' file should be obtained for a set of n-shells in one-pass selected to match to representative levels and span n-shells up to some last n-shell from which extrapolation can safely be performed.
2. Buttons and controls follow the usual pattern



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

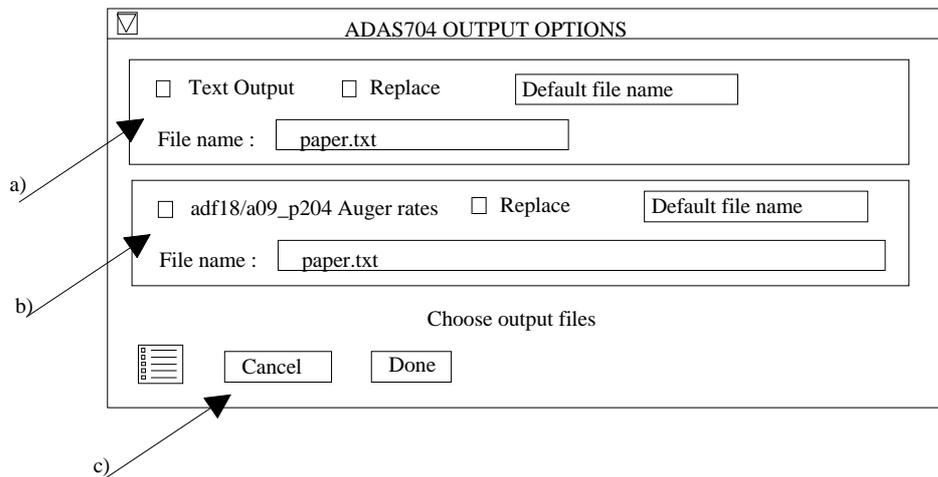
3. There are only limited options on the processing screen. At a), the *Spin* of the recombined system targetted is specified. That is spin system of the initial metastable + nI-electron system.
4. The *n-shell weighting factor* is a little complicated. It is defined as  $2 * (\text{indistinguishable composite metastable parent weight}) * (\text{spin system weight fraction of total possible spin weight for the composite parent}) / (\text{proportion of required metastable parent in the indistinguishable parent composite})$ . For example  $(2s^2 2p^3) n^{-1}$  for the  $^2D$  parent n-shell weighting factor = 12.8 arising from: composite parent weight = 16 ( $^2D$  and  $^2P$  are indistinguishable both contributing to the  $n^{-1}$  system); spin weight fraction = 0.25 (from  $1/[1+3]$  since singlet and triplet spin systems can result from these parents); proportion = 0.625 (since  $^2D$  is  $10/[10+6]$  of the indistinguishable composite parents). Further examples are given in the archived adf18 files.



5. At b), the 'Free state maximum and minimum energies' span the range of resonances (n-shells built on metastables) and must be used to isolate the band of free-electron energies which pick up the correct final metastable.

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

6. There is no graphical display.
7. The output file sought at b) is the supplementation data. Note that the rest (first part) of the /adf18/a09\_p204 cross-reference file is straightforward and existing samples can be modified quickly for other cases.



### Illustration:

The output *adf04* file from post-processing AUTOSTRUCTURE intermediate files for  $\text{Ar}^{+15}$  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 8-04a

Supplementary LS-breakdown autoionisation data between parent spin pairs					
(pmni, isysi ; pmnf)			ncut1	A Auger	slope
-----			-----	-----	-----
X	X	X	3	8.155E+10	
			4	8.891E+10	
			5	5.613E+10	
	.	.			
			28	1.071E+07	
			29	9.155e+06	
			30	7.884e+06	-5.00
4	8.891E+10				
4	8.891E+10				
4	8.891E+10				
4	8.891E+10				
-----					
C					
C					
C	Spin breakdown Auger rates calculated from AUTOSTRUCTURE				
C	using : XXXX				
C					
C	Code : ADAS704				
C	Producer: Martin O'Mullane				
C	Date: 21/09/00				
C					
C					
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### Notes: