
ADAS808: Create a composite set of adf34, adf40 and adf41 iso-nuclear driver files

The program uses the IDL graphical user interface to automate preparation of the driver datasets required for large-scale off-line production of *ADAS Baseline Atomic Data* for complex atoms. Drivers for many or all of the ionisation stages of a heavy element may be generated at the one time. The drivers produced are the input datasets for offline running (usually on massively-parallel computers) of the codes ADAS801, ADAS407 and ADAS810. Subsequent to ADAS808, the offline calculations may be executed automatically under the control of a master script with final delivery of complete data in the ADAS data format classes ADF04, ADF03, ADF11, ADF15 and ADF40. The code allows the user to assess and regulate the subsequent size of the offline calculations on the basis of experimental spectral regions of interest, available machine size and strategies in atomic structure modelling.

Background theory:

The fundamental part of the *ADAS Baseline Atomic Data* consists of ADF04 files for each ion of an element, archived in iso-nuclear collections. Each file comprises energy levels and A-values for an ion computed using Cowan Atomic Structure Code and electron impact Maxwell averaged collision strengths in the Born approximations. Implementation within ADAS is via the code ADAS801. This code has the Cowan Atomic Structure Code at its core but includes an IDL front end to acquire the input data (the ADF34 driver), and subroutines to organize output in ADAS standard forms (ADF04 files) and nomenclatures. For medium/ heavy element ions, with many electrons, the ADAS801 calculations must be performed in intermediate coupling and include many configurations. For such systems the preparation of configuration lists for the ADF34 drivers is prohibitively tedious and the calculations are massive. Automated handling followed by offline execution on massively parallel machines is essential. In ADAS, the automated, high throughput is achieved by firstly sophisticated interactive set-up of the ADF34 drivers. ADAS808 fulfills this latter purpose.

The complete *ADAS Baseline Atomic Data* includes also various derived data classes. In simple systems, these other data are generated by interactive execution of the codes ADAS407, ADAS408 and ADAS208. For medium/heavy element systems, it is convenient to use ADAS808 to set up additional drivers so that these codes also may be executed automatically offline. Finally, the complexity of heavy element emission, means in practice that spectral analysis must often be carried out on unresolved or only partially resolved transition array features rather than on individual spectrum lines. In ADAS, a new derived quantity, called a feature photon emissivity coefficient, \mathcal{F}_{PEC} , is introduced (analogous to the emissivity coefficient, PEC) is introduced to describe these envelope features. The associated code, ADAS810, calculates such \mathcal{F}_{PEC} s and it is convenient for ADAS808 to prepare the drivers for offline execution of ADAS810 also. Following interactive execution of ADAS808, all subsequent calculations and assembly of the complete *ADAS Baseline Atomic Data* are achieved by launching an integrated *PERL* script to the target high performance parallel computer system. No further user intervention is required.

Configuration definition The set of working configuration for the atomic structure calculation is obtained by an electron promotional strategy starting from the ground configuration

$$\Gamma_g = n_1 l_1^{q_1} n_2 l_2^{q_2} \dots n_m l_m^{q_m} \text{ where } q_i > 0 \text{ for } i = 1, \dots, m \text{ and } \sum_{i=1}^m q_i = N$$

For complex systems, there may be empty inner shells and multiple open shells. Elements up to uranium are within the scope of ADAS808. The ground configurations for every ion of every element up to uranium are provided in the ADAS data format for general constants ADF00 as `./../adas/adas/adf00/ground_configs/<element symbol>.dat`. An equivalent data set provides both the ground configurations and the ionisation potentials as `./../adas/adas/adf00/ground_ionpots/<element symbol>.dat`. It is helpful to maintain a consistent pattern for configurations. In ADAS two conventions are use, namely the *Standard form* and *Eissner form*. *Standard form* represents each shell with three characters with a space separating shells in the whole configuration as '1s2 2s2 2p1' representing $1s^2 2s^2 2p^1$. For certain calculations, principal quantum numbers greater than 9 may be required and for complex element ion, shell occupancies greater than 9 also may occur. To maintain the three character shell notation, the integers beyond nine are represented alphabetically, that is 10 \equiv 'a', 11 \equiv 'b' etc. Thus in *Standard form*, $2p^6 6f^{11} 11s^1$ is represented by '2p6 6fb bs1'. In *Eissner form*, each orbital, starting from 1s is indexed. The index is an integer up to 9, but continues through

the upper case alphabet and then through the lower case alphabet. Thus 1s \equiv '1', 2p \equiv '2', 4f \equiv 'A'. A portion of the conversion table is

Orbital	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f
Eissner	1	2	3	4	5	6	7	8	9	A
Orbital	5s	5p	5d	5f	5g	6s	6p	6d	6f	6g
Eissner	B	C	D	E	F	G	H	I	J	K

The shell occupancy is represented as a two digit integer as 50+q and this precedes the shell index character. Thus again the shell is represented by a three character field but is written with no separation between the fields in the whole configuration. Thus in *Eissner form* $1s^2 2s^2 2p^6 6g^{11}$ is represented by '52152256361K'. ADAS works freely with both notations and subroutines in the ADAS library transform from one to the other. *Eissner form* is the preferred form in ADAS series 7 codes since structure calculations there use the *Autostructure* code. Standard form is the preferred form in ADAS series 8 codes since structure calculations there use the *Cowan/O'Mullane* code. *Eissner form* is the most compact and is generally adopted with very complex configurations.

A promotional strategy Consider a group of ions $\{e\mathcal{A}^{+z} : z = z_{min}, \dots, z_{max}\}$ of the element \mathcal{A} . A set of configurations targetted on a structure calculation is established by promoting electrons from the ground configurations of the ions. The criteria for promotion are shell-based and not set up ion by ion - rather they are for the group of ions of the element. For complex ions, it is possible to have ground configurations with more than one partially filled shell, which are called valence shells. By reviewing the ground configurations of the ion group, a list of single valence shells present is identified - likewise for double valence shells and in principal on to triple valence shells. The promotional strategy depends on whether there is a single or double valence shell. At this time, ADAS808 has no strategy for triple and higher valence shells.

1. In the single valence shell case, we progress through each of the identified valence shell orbitals in turn. Consider valence orbital $n_v l_v$. Distinguish promotions upward in principal quantum number, that is to $n l$ shells such that $\Delta n = n - n_v > 0$ from promotions downward (in normal shell ordering) with $\Delta n < 0$. Principal quantum shell promotions are determined by the permitted maximum $|\Delta n|$ and by the sign of the promotion. The negative case allows promotions to empty inner shells to be treated. In similar manner, promotions are ranked according to the maximum $|\Delta l|$ allowed with positive and negative Δl handled separately. Note that the valence shells treated in this manner are partially filled. Promotions from inner closed shells excluding the valence shell, which may generate many less important configurations, are preferably restricted by setting the lowest n-shell from which the promotion can occur and the highest n-shell to which the promotion can take place. Again it is single electron promotion which is done. Finally, it is a usual policy in accurate energy level calculations to include all the configurations of a complex if one of the configurations of the complex is present. Such a policy can generate large numbers of configurations in the complex ion case. It is helpful to decide if whole complexes associated with the single electron promotion configurations are to be included.
2. A similar procedure may be applied in the two valence shell case but with the permissions for each electron specified separately.

Configuration partitioning For complex ions, the number of configurations which satisfy even quite restricted promotional rules can be large. Also, since these configurations often include more than one unfilled shell, the level count for each configuration can be very large. Mechanisms beyond the basic promotional rules are required to restrict the total level set to match available computer power. In ADAS808, a second mechanism is introduced based on observational spectral regions of interest. The principle is straightforward. Consider a spectral region of interest $[\lambda_0, \lambda_1]$, which may be the range of a particular spectrometer or an interval of special diagnostic value. For configurations I and J , introduce the configuration average energies $E_I^{(av)}$ and $E_J^{(av)}$, the transition array average energy $\Delta E_{IJ}^{(av)} = E_J^{(av)} - E_I^{(av)}$ and wavelength $\lambda_{IJ}^{(av)} = hc / |E_J^{(av)} - E_I^{(av)}|_{E_J^{(av)} < E_I^{(av)}}$. Configurations

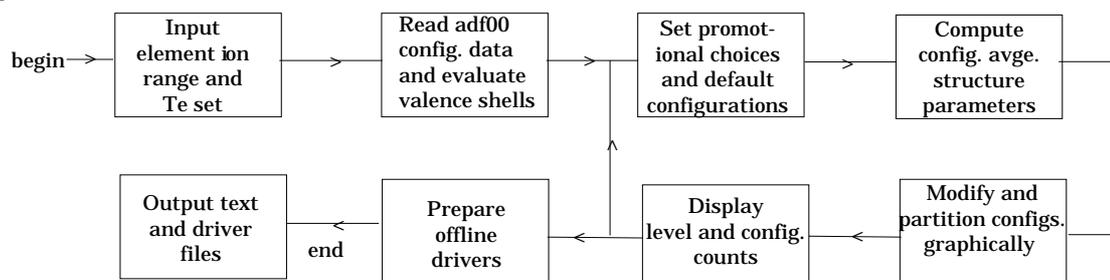
such that the transition wavelength $\lambda_{IJ}^{(av)} \in [\lambda_0, \lambda_1]$ should be handled at high resolution, that is *level resolved*, while configurations such that the transition wavelength $\lambda_{IJ}^{(av)} \notin [\lambda_0, \lambda_1]$ may be handled at low resolution, that is *configuration average*. In general, there may be a set of wavelength intervals of interest and from the total number of configurations, N_C is partitioned into the *level resolved* set, numbering N_{C_R} , and the configuration average set, numbering N_{C_A} , such that $N_C = N_{C_R} + N_{C_A}$. A further constraint may be imposed by setting a lower limit for transition probabilities, thereby excluding very weak lines. At the configuration average level, this means a lower limit $\mathcal{D}_{min}^{2(av)}$ on the reduced dipole matrix elements, $\left\langle \left\| I \mathcal{D} J \right\| \right\rangle^2$ for the transition arrays. A preliminary stage of the Cowan structure code package generates configuration average energies and reduced dipole matrix elements. This stage is rapid and makes low demands on computer resources. It is convenient therefore to provide a *transition array spectrum* display so that the definition of wavelength regions of interest can be done directly in interaction with the display. Immediate information is returned to the user on resolved level counts and on resolved and unresolved configuration counts, so that the size of the subsequent full structure computations may be assessed and regulated. The *transition array spectrum* in which the ordinates are reduced dipole matrix elements provides a relatively crude picture. Transition arrays between excited configurations are on the same footing as those involving the ground configuration. There is no real population information. It is to be noted however that the first stage of the Cowan code package also returns the reduced Born matrix elements. Thus a configuration average population calculation and emissivity production is possible without significant additional computational overhead. The configuration average transition array emissivity coefficients for an ion provides a more realistic footing. On the other hand, at this first stage of structure calculation, no basis for relative weighting of transition array emission functions from different ionisation stages is available. Due to the sensitivity of the spectrum and dominant ionisation stage to electron temperature, a constraint based on temperature is unsound at this point of the data generation exercise. Equal weighting of ionisation stages abundances is the most appropriate choice. ADAS808 presents either a reduced dipole or configuration average emissivity *transition array spectrum* to the user. These details are described in detail below.

Envelope features An envelope feature photon emissivity coefficient, denoted by \mathcal{F}_{PEC} , is defined on a wavelength interval and is a composite feature arising from very many lines from a single ionisation stage. The \mathcal{F}_{PEC} is suitable as a descriptor in wavelength intervals and at spectral resolutions where the individual component lines are unresolved or only partly resolved. This situation occurs with very complex heavy element ions for which it becomes helpful and economical to handle the envelope feature rather than the individual line emissivity coefficients (\mathcal{PES} s). The primary use of ADAS808 is to set up calculations for very heavy species and so the wavelength intervals such as $[\lambda_0, \lambda_1]$ above, introduced as a focus for partitioning configurations, are identified as the spectral intervals over which the envelope features are sought. ADAS808 therefore provides drivers also for the \mathcal{F}_{PEC} calculations – see ADAS810 for more details.

Program steps:

These are summarised in figure 9.08.

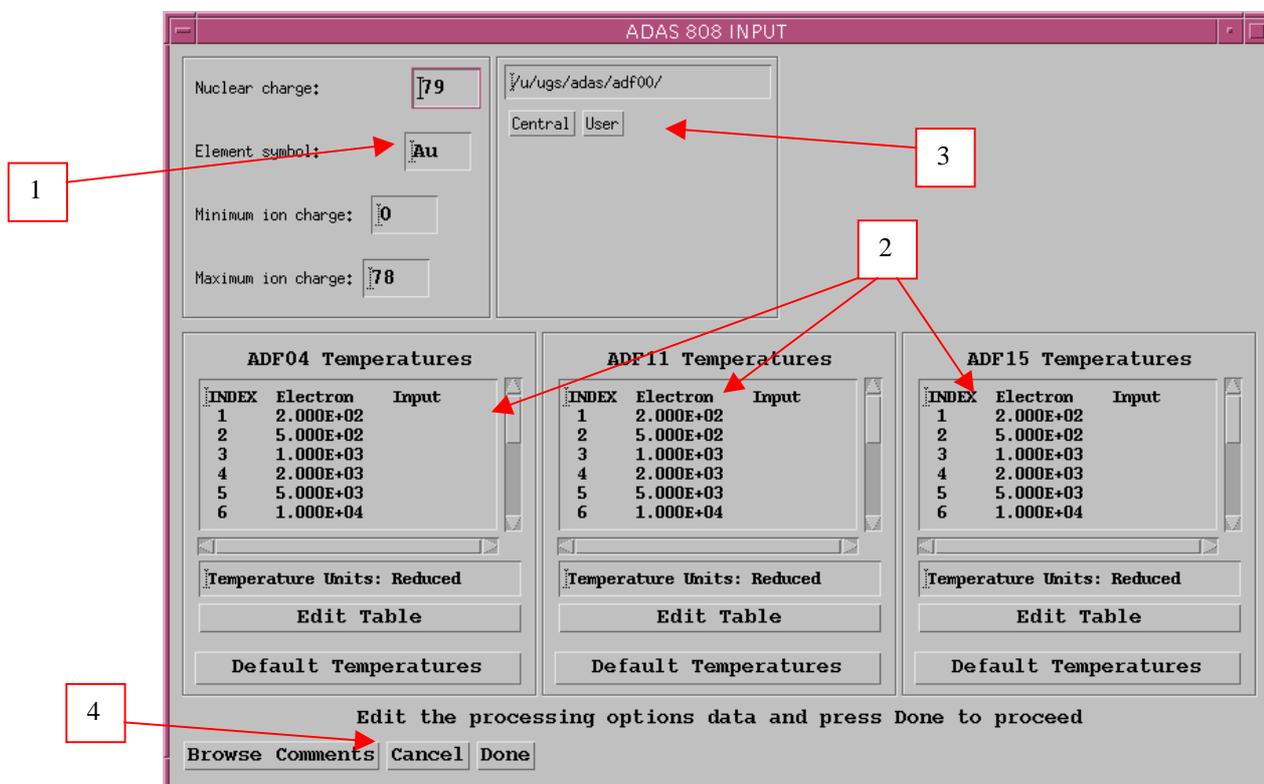
Figure 9.08



Interactive parameter comments:

The **input window** is as shown below

1. Enter the element symbol. Note that the element symbol and nuclear charge number boxes are linked so if one of them is changed, the other is automatically updated. Also, set the minimum and maximum ion charges, noting that the last ion of an element in this context is the hydrogen-like stage with $z = z_0 - 1$ where z_0 is the nuclear charge.
2. Three sets of electron temperatures must be specified. These temperatures are passed through to the final drivers and ultimately are the temperatures used in the ADF04, AD11 and ADF15 files. The *Input* temperatures are usually the ADF standard reduced temperatures. Note that the temperature set is editable and a user's units of choice may be selected.
3. A pathway to ionisation potentials for all elements and their ions is required. These data include the ground configurations and are provided in the Central ADAS archive `/packages/adas/adas/adf00/`.



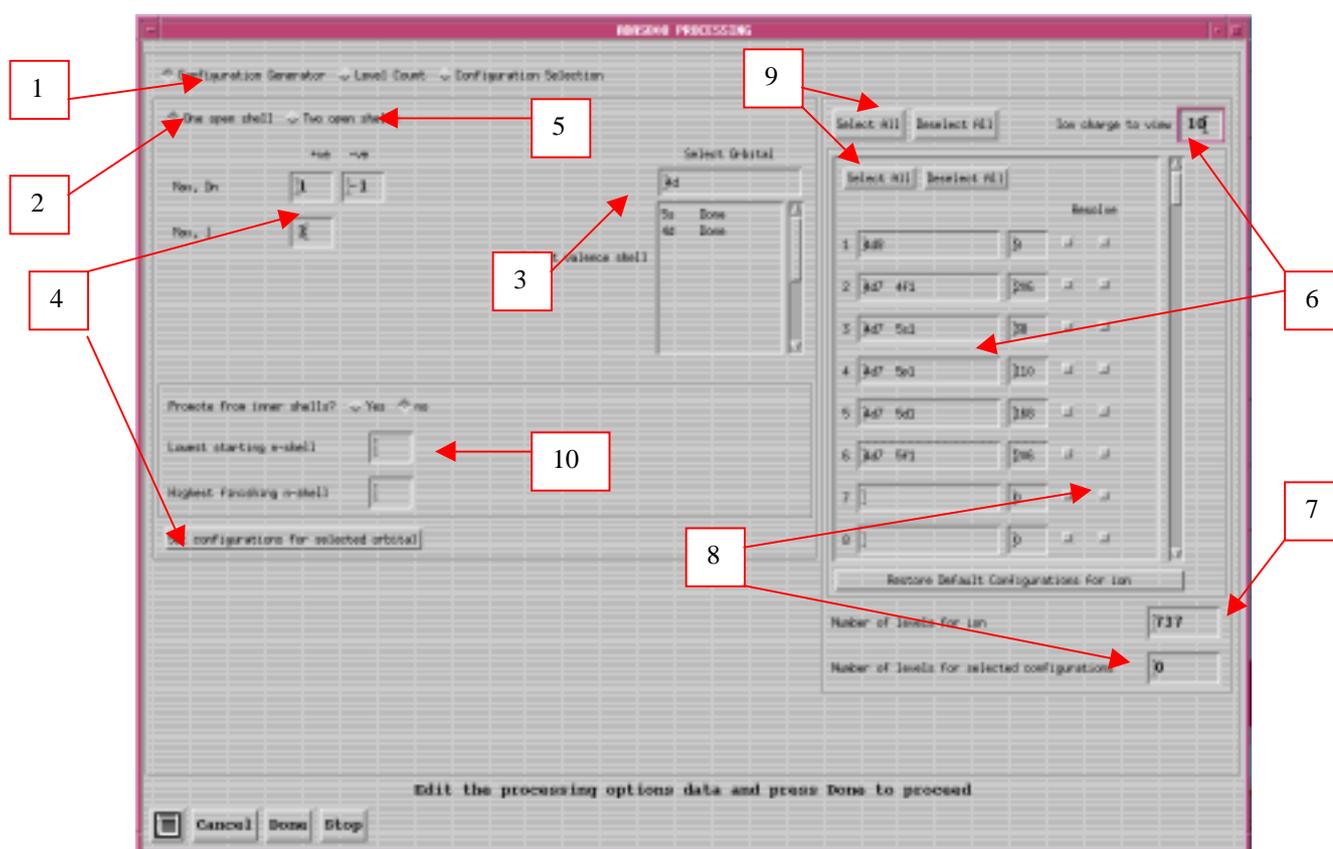
4. The *Browse Comments* button has no effect at this time. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window.

The **processing – configuration generator window** is shown below:

1. The processing window has three separate modes of operation which may be selected. In *Configuration Generator* mode, the window appearance is as shown below. This mode must be completed before the other modes are meaningful and is described below.
2. The sub-window on the left permits the setting up of a promotional strategy for configuration generation. **You must note that this strategy applies to simultaneously to all ions selected on the Input window.** Single and double valence shell cases are chosen as required and the fields which are

presented depends on that selection. The one valence shell case is illustrated below.

3. The valence shells are listed. Clicking on a member of the list causes it to appear in the selection widget. Then the choices made on the left at 4 apply to that valence electron.
4. Make the preferred choices, then click on the *Set Default Configurations* Button. *Done* is appended to the chosen valence shell in the list widget. Work through each shell in the list. Note that a shell may be reworked simply by reselecting it.
5. In like manner select the *Two open shell* button and then work through the two valence shell list.
6. When the promotional strategy is complete, enter an ion charge from the selected range in the text box. The set of default configurations for that ion is presented in the table together with the number of levels, which would result from that configuration. The table is editable to add further configurations which are not entered by the promotional strategy.

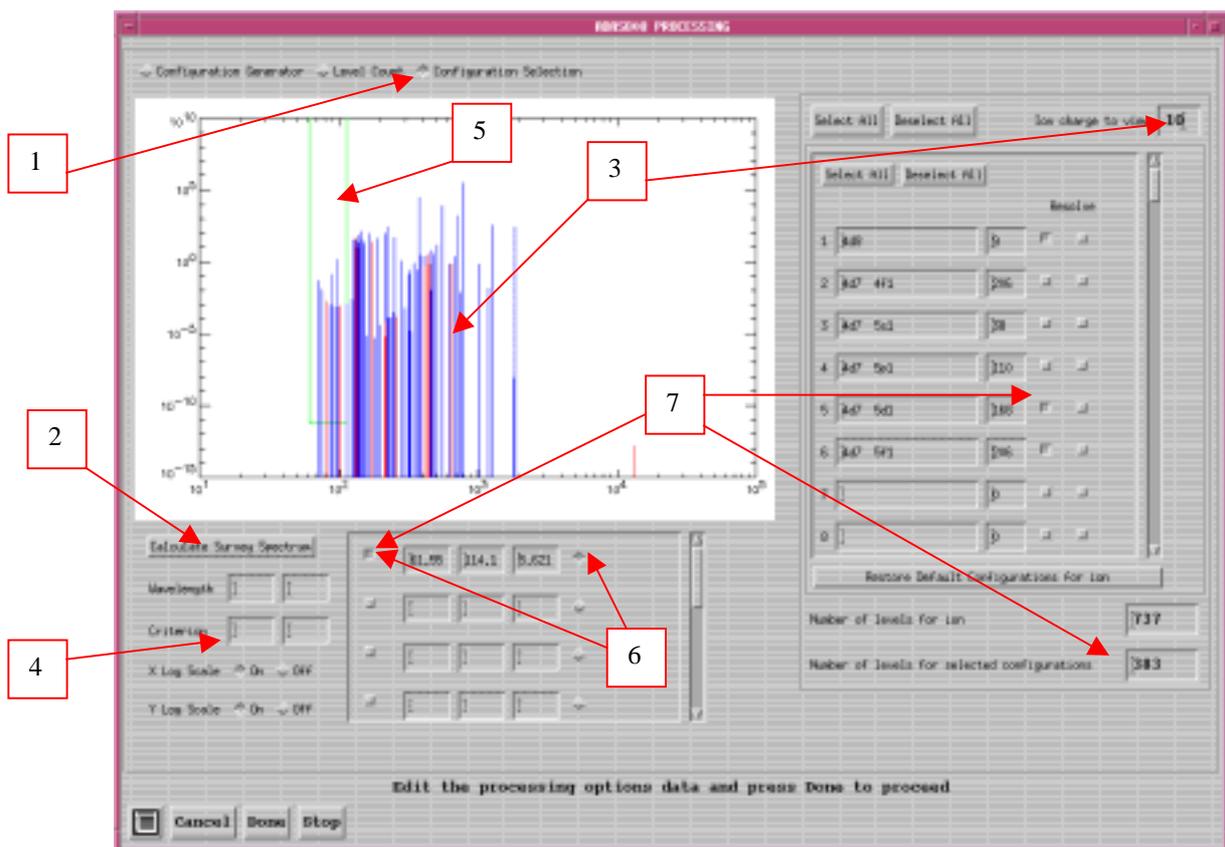


7. The total level count for the ion is shown.
8. It is now possible to select configurations to be treated as *resolved* by activating the right-most buttons. The number of levels in the *resolved* set of configurations is displayed in the lower box.
9. There are two sets of *Select All* and *Deselect All* buttons which apply to the right-most button selectors. The upper pair apply to the lists for every ion in the whole ion range simultaneously. The lower pair apply only to the currently displayed ion.
10. Additional strategies for inner shell promotion are in development and are subject to change.

The **processing - configuration selection** window is shown below

1. Clicking the *Configuration Selection* button presents the window shown below, in which the sub-window on the left is now used to show a stick spectrum of the various transition arrays.

2. Clicking the *Calculate Survey Spectrum* button spawns the calculation of the first stage of the Cowan code to obtain the necessary parameters. The calculation may take a few minutes, but then all information is available the stick plot is displayed. Any further selections operate rapidly.
3. The stick plot shows the transition arrays for every ion in the group. Transition arrays for the ion selected at the right are marked with sticks in a contrasting colour.
4. The wavelength range of the stick plot may be altered and logarithmic or linear axes chosen.
5. The plot area is active. The mouse may be used to delimit rectangular areas which are the spectral intervals of special interest. The base of the rectangle set a minimum value of the reduced dipole matrix element for transition array configurations to be included in the *resolved* set.
6. To mark a rectangle, first activate a square row button on the left of a row of the spectral ranges sub-window, so that it is displayed and the button on the right to make the row active for editing. Drag out a horizontal line on the plot area using the right mouse button and release. The rectangle may be stretched by catching an edge and dragging with the left mouse button. The selections, $(\lambda_{min}, \lambda_{max}, \mathcal{D}_{min}^2)$ are shown in the boxes.
7. The left hand button of a spectral range row defines configurations which contribute to lines in that range as requiring level resolution on the configuration list and that configuration is marked its button indicator light. The selected configurations count is updated accordingly. **Remember to reselect an ion at 3. to update the configuration list sub-window display after each alteration.**

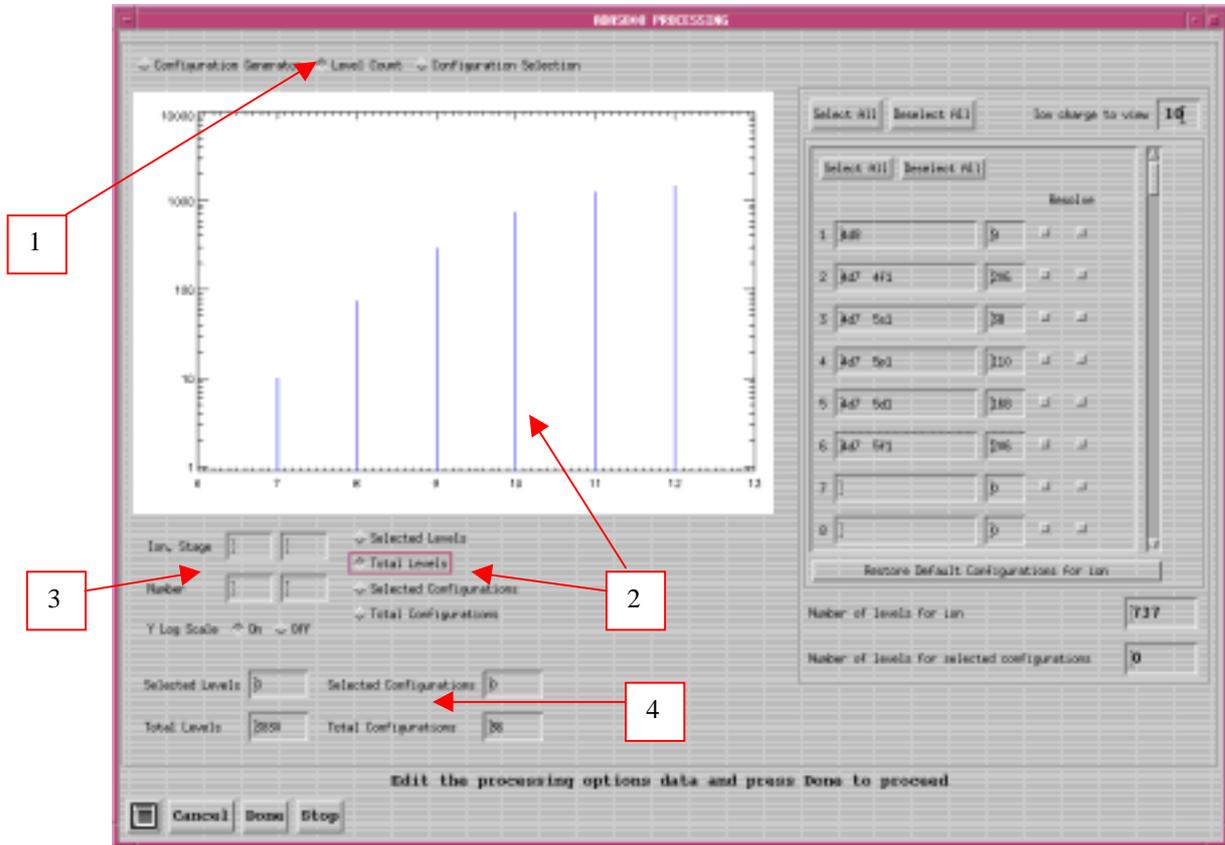


The **processing – level count window** is shown below

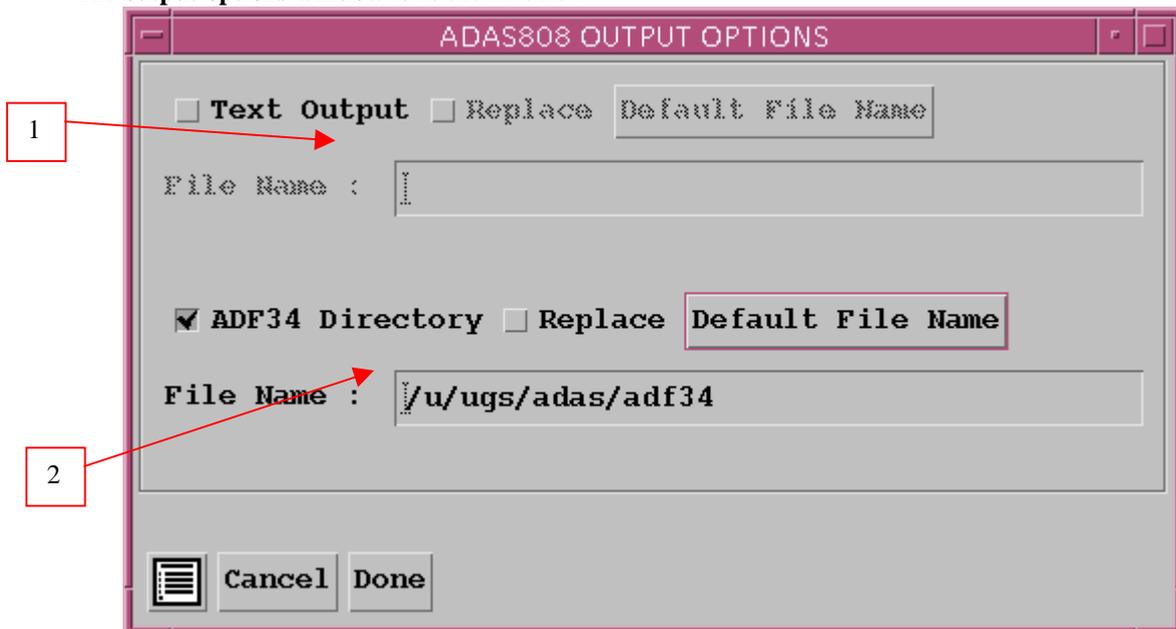
1. Clicking the *Level Count* button presents the window shown below. The sub-window to the left displays a count summary plot.
2. Display of configuration counts and level counts for each ion in the selected ion range may be chosen. Note that the Total Levels and Total

Configurations may be shown prior to the calculating the survey spectrum. Selected Levels and Selected Configurations require the survey spectrum to be calculated first.

3. The graph display scales may be adjusted.
4. Note the summary information



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



1. 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.

2. The primary output is to an *adf34* sub-directory which can be entered and/or selected.

Illustration:

Table 9.08a w_7_adf34.dat

```

2 -5 2 10 1.0 5.d-09 5.d-11-2 0130 1.0 0.65 0.0 0.5
74 8 w 4f13 5s2 0 4f13 5s2 5p6
74 8 w 4f13 5s2 3 4f13 5s2 5p5 6p1
74 8 w 4f12 5s2 7 4f12 5s2 5p6 6p1
74 8 w 4f13 5s2 4f13 5s2 5p5 6s1
74 8 w 4f12 5s2 4f12 5s2 5p6 6s1
74 8 w 4f13 5s2 4f13 5s2 5p5 5d1
74 8 w 4f13 5s2 4f13 5s2 5p5 6d1
74 8 w 4f12 5s2 4f12 5s2 5p6 5d1
74 8 w 4f12 5s2 4f12 5s2 5p6 6d1
-1

```

Table 9.08b w_7_inst.dat

```

z0 74
zi 7
parity-1 3
parity-2 6
E2 3
M1 3
scale 93 99 93 93 93
temperature 25
2.00000E+02 5.00000E+02 1.00000E+03 2.00000E+03 5.00000E+03
1.00000E+04 2.00000E+04 5.00000E+04
1.00000E+05 2.00000E+05 5.00000E+05 1.00000E+06 2.00000E+06
2.20000E+06 2.20000E+06 2.20000E+06
2.20000E+06 2.20000E+06 2.20000E+06 2.20000E+06 2.20000E+06
2.20000E+06 2.20000E+06 2.20000E+06
2.20000E+06

```

Table 9.08c w_7_pp.dat

```

1
Allan Whiteford
15/12/79
1
C Comments are for losers!
&FILES ifgfile = './ifg#w_7_adf34.dat' , outfile = './w_7_adf04.dat'
&END
&OPTIONS ip = 1134988.8, coupling = 'IC' , aval = 'YES' ,
isonuclear = 'NO', lweight = 'NO' , comments = 2, numtemp = 14, &END
1 2 3 4 5 6 7 8 9 10 11 12 13 14

```

Table 9.08d w_7_pec_drv.dat

```

w + 9 74 10 1475969.1

./w_9_adf04.dat # input adf04 file
./w_9_adf11.dat # output plt file
./w_9_adf15.dat # output pec file
./w_9_adf40.dat # output f_pec file

lmetr = false # true to resolve
metastables
ltscl = true # true for z-scaled
temperatures
ldscl = false # true for z-scaled
densiities
lbrdi = true # true for ion temp.
broadening

13 # no. of temperatures
2.000E+02 5.000E+02 1.000E+03 2.000E+03 # temperatures (K)
5.000E+03 1.000E+04 2.000E+04 5.000E+04
1.000E+05 2.000E+05 5.000E+05 1.000E+06

```

2.000E+06	
5	# no. of densities
1.000E+11 1.000E+12 1.000E+13 1.000E+14	# densities (cm-3)
1.000E+15	
2	# no. of wavelength
intervals	
128 2.759e+01 2.112e+03	# pixel no., wvmin, wvmax
triplets	
128 5.890e-01 2.242e+00	(wavelenths in Angstrom)

Notes: