Feb18-03 ADAS Bulletin

I must firstly apologise for the delay in this release. As you will recall, we held the intensive four-week 'Winter School' on ADAS and Atomic Calculations at Strathclyde University from 18 Nov. – 13 Dec. This had the two effects of giving us a large number of corrections to implement in ADAS codes and running me into my heavy examining amd marking schedule. The Winter School was nonetheless very beneficial since it was the most concentrated examination of the ADAS package we have ever had.

I had hoped to go with a comprehensive release of all the heavy species handling codes together some little time ago. However, these codes are pretty complicated and are taking a long time to verify, adjust and get working compatibly. Handling heavy species means revising upwards virtually all decisions made many years ago – maximum angular momenta, fields allocated to statistical weights, lengths of configuration strings, translation tables etc. etc. But we are nearly there now and I feel it is best to release some of them now as 'beta' versions so that we get them under more general test. Also, we have already introduced some of the codes to participants at the Winter School, who wish to continue working with them immediately. So this time, we have included ADAS510 for interrogating and displaying envelope feature emissivity coefficients, ADAS808 for previewing complex species spectral emission in selected spectral intervals and setting up appropriate driver data sets for off-line execution and ADAS810 for calculating feature emissivity coefficients. First versions of two other utilities in series 8 are also included, namely, ADAS804 for simple effective potential Born omega and Upsilon calculation, ADAS809 for conversion of an adf04-type 1 file to an adf04-type 3 file. We shall upgrade ADAS809 in the near future to full non-Maxwellian handling.

You will be aware of the gradual shift in the ADAS Project to making available some of our fundamental atomic structure and collision calculation capability. Parts of this are suitable for interactive ADAS (see series 7 and 8) but main calculations need to be done off-line on powerful machines. With the introduction of heavy species modelling to ADAS, the link to off-line calculation becomes essential and we are trying to make this as smooth as possible. Working with off-line structure and collision codes was one of the themes of the Winter School. I have made the complete set of lecture notes, presentations and tutorial exercises available in the ADAS documentation release (see */…/adas/docs/adas-and-atomic-calculations-course/** . I would recommend however that those who wish to use the off-lines codes should try to come to at least to the second part of the Winter School (next occasion Nov 2003) at some stage. Working on a specific example with the experts is worth a lot of words.

You will notice (amongst many others) two new ADAS data formats, *adf38* and *adf39*. These are for photo-excitation and photo-ionisation cross-sections and reflect on-going work of Nigel Badnell and Mike Seaton. This extends and revises some bits of the Opacity Project. I hope this will lead onto a capability for handling photo-ionised plasmas in ADAS sometime in the future. For the moment, the specifications of *ad38* and *adf39* have been added to the IDL-ADAS User Manual (*appxa-38.pdf*, *appxa-39.pdf*).

A final word concerning the ADAS User Manual. It has of course become very large and needs frequent updating, especially when new codes are being brought on stream and the ADAS data formats are being extended to cope with new situtations. I have therefore decided to align the manual version with the ADAS release and enter chapters on new codes in it as they are released. This means that the up-to-date manual is really the computer version (in the */docs/* directory or accessible via http://adas/phys.strath.ac.uk). Also, the manual is now more of a 'road map'. That is it includes entries for codes which we have working in preliminary version, but have not yet had the time to bring-up fully into IDL-ADAS, and data formats which are now necessary, but have not been filled yet with significant amounts of central ADAS data yet.

Corrections and additions to codes (ADAS v2.5.6 to ADAS v2.6)

C.1 There are problems in using ADAS811 particularly on true 64 bit (DEC/Compag/HP) machines. It arises when making call_external IDL routines just using fortran. This was tried with *r8necip.for* as no string passing was involved. However it proved necessary to introduce C glue code.

*** Removed *r8necip_if.for* and replaced with *r8necip_calc.for* and *r8necip_if.c*.

C.2 There are some further issues with ADAS211. The recombining ion charge (iz1) is calculated from the atomic number and isoelectronic sequence. However the test to find the number of electrons in the isoelectronic was case sensitive. Unfortunately ADAS807 produced adf08 files with mixed case. Rather than failing, unfortunately ADAS211 calculated silly quantum defects and defaulted to hydrogenic values. The fix is to do the test having converted to an upper case sequence string. We are attempting to put active string conversion into all codes at key places. Note the conversion subroutine *xxcase.for* in */…/fortran/adaslib*.

C.3 The *adf08* files produced automatically by ADAS807 caused more than just the problem of C.2. In the Li-like case the level configuration strings dropped the full 1s2 shell. The parsing routine in ADAS211 (*bbprs3.for*) did not cope very well. As it does not know the number of electrons, full shells below the currently open one are assumed filled. Therefore 4p1 was taken as 1s2 2s2 2p6 3s3 3p6 3d10 4p1. At least this time nothing was produced so the problem could be traced. The 'solution' is to modify ADAS807 to put in the 1s2 for the Li-like sequence.

Yet another problem is with the seq string. It looks human readable but is fixed format. IDL writes single character sequences as ' C' via A2 format. However this is incorrectly interpreted in adas211.for. We have changed *prop_adf08.pro* to write out 'C '.

Closed shells becomes a bigger issue for heavy complex ions – which is the trend of our development at the moment. The configuration field in the standard adf04 file format is insufficiently long to put the complete configuration for a heavy ion, nor is it helpful for most purposes to see the occupancies of inactive inner shells. We have more advanced versions of the configuration handling, parsing, detection & conversion between forms (Eissner and Standard) subroutines. These include *xxpars.for, xxprs1.for, xxprs3.for, xxcftr.for, xxdtes.for* and so on. These will deal with arbitrarily complex systems and verify inner shell (undeclared) occupancy by examing the ground state configuration of the ion in the *adf00* look-up tables. We are introducing them into the ADAS releases as and when we have checked through all their dependencies.

C.4 A missing utility subroutine for ADAS811 has been added to the IDL library - *i4indf.pro*. This is a complement to the fortran *i4indf.for* subroutine, but in this case, since it is simple, a version has written directly in IDL.

Some new functionality has also added. A *'Print All'* button, which prints all transitions (of a single type) to a file, is included. Also a new information field, which gives the value of x,y (in data units) under the cursor on the graph, is provided.

Ambiguities in labelling on the file selection screen have been fixed. Thus '*Browse'* is replaced by '*Select'* for choosing files. Another *IDL 5.5 array/scalar* problem has been fixed. This was a most tiresome alteration in IDL5.5 which has caused a lot of extra work.

Note incidintally that ADAS801 can also handle the special case of H-like configurations - which are labelled n=2 etc (that is with the bundling notation) in the light ion GCR Project.

C.5 A subtle logic flaw in *read_adf04.pro* has been picked up. When overwriting ionisation rate data from S lines, the level and parent indices were occasionally incorrect.

C.6 Some of the files produced by ADAS204 are obsolete, in particular the *adf10* files. These should now be generated using ADAS208. Some other formatted output files are also not necessary. The output screen has been remodelled into necessary and optional sections. The only mandatory one, required to run, are *adas204_adf17.pass* and/or *paper.txt*. The others are optional. Note that *paper.txt* has re-instated - in the previous IDL-ADAS version, printing to it was suppressed.

Further changes affect both the fortran and IDL. More logic variables have been added to *adas204.for* and the method of specifing a *passdir*, which was used to construct the output file names, has been replaced. Now an array of names is passed in together with an array indicating whether output is required or not.

b4spf1.pro is no longer necessary as its functionality has been replaced by an updated *adas204_out.pro*. This output widget does not require the *cw_adas204_out* compound widget.

*** Removed *b4spf1.pro* and *cw_adas204_out.pro*.

C.7 Yet another missed *IDL 5.5 array/scalar* problem in ADAS402 has been fixed. Also the polynomial fit tolerance query in *cw_adas402_proc.pro* has been fixed.

C.8 There was a logic flaw when cycling between range boxes in explicit scaling of output graphs - if no z range is present, then pressing <return> in y-max caused a crash as the program tries to give input focus to z-min. This bug affects all widgets which use cw_adas_ranges.

C.9 ADAS209 did not include bundling of S-lines. This has proved necessary for H-like lithium. The approach taken is to calculate the rates from the data in the *adf04* file and then take the statistical sum of rates. This sum is then divided by the new, bundled, exponential factor in order to generate valid *adf04* S-lines. Also we have added the name of producer to the output (bundled) *adf04* file automatically via *xxname.for* subroutine.

C.10 There is an odd problem with *adas_in_v2.pro* for IDLv5.4 on DEC machines. It looks like the array of one vs. scalar problem and has the same solution, but it appears to be specific to this version/machine combination. Adding a [0] is harmless to other machines, so we have done so.

C.11 A problem appeared in ADAS703 which failed to produce ordinary dipole transitions between doubly excited states. The program relied on parsing AUTOSTRUCTURE output. Unfortunately, the output formatting changed significantly between v16.5 and 16.10 9 - the current ADAS version). We have to apologise about a failure in our own group's internal communication system.

C.12 A new *read_adf00.pro* routine has been prepared to retrieve data from the adf00 reference atomic data files, that is ionisation potentials and ground configurations of the ionis of all elements.

C.13 We have made many changes to ADAS801 as we tested it to destruction at the Winter School. These are all to do with learning tocope with very heavy species. The main changes are:

- Algorithm deficiency in *rcg* which did not properly allocate unlabeled levels among the multiply labeled ones. This shows up in particular in highly mixed ions.
- Purity of levels is now written to IC *adf04* file.
- Indication in comment section whether a level (or a term within a level) has been re-labeled in *rcg* (*sprnadd.for*).
- Ionisation potentials can now be retrieved from the central ADAS *adf00* collection. Typing in the correct value is still possible.
- Type 1 *adf04* files can now be written directly by ADAS801.
- To accommodate *adf04* files with large level and transition lists the output format of the transition indices and Upsilons is now adjusted according to the number of levels. This fits in with the new flexible *adf04* reading codes. The new complete general purpose *adf04* reading subroutine is *xxdata_04.for* and it resides in the highest level */…/fortran/adaslib* sub-directory.
- *paper.txt* now holds a record of the temporary files used in the calculation.

C.14 Dimension updates have been made in ADAS201, ADAS205 and ADAS207 so as to cope with xenon. This meant that *xxminv.for* also had to be re-dimensioned.

C.15. ADAS403 did not work correctly on SUN hardware. The IDL spawn command requires the */sh* parameter in that case. The addition has no effect on other operating systems.

C.16. ADAS207 had a problem with the neutral density and recombining fractional abundance ratios (the vectors *ratha* and *ratia*). These can change in size between runs but the size stored in the defaults file was fixed. Their values are not stored but the structure assignment in IDL does not allow for re-dimensioning of vectors or arrays.

C.17. ADAS402 had a lingering IDL v5.5 'array of one' bug. A more serious problem was a peculiar logic flaw when using the search button – the central year was not searched for if a default year was present. This has been corrected.

C.18. The IDL version of the *xxdtes* routinewas machine specific. This arose by trying to pass FORTRAN logicals, through C to IDL. A more robust way is to pass integers, but this requires an interfacing FORTRAN program. Keeping with convention, this is called *xxdtes_calc.for* and is stored in *wrapper/adaslib* along with the *xxdtes_if.c* code.

C.19. In ADAS807, the passing files (and internal naming of variables and routines) for the mapping of *adf09* files onto the *adf04* levels hada name reversal. Rather than *a09_a04* which reflects the *adf18/a09_a04* convention, *a04_a09* was used. This has been altered.

C.20. There was an incorrectly named external function declaration in the *xxcftr* interface code, *xxcftr_if.c*. This could have caused problems on some versions of UNIX.

C.21. ADAS312 would process *adf26* files for beam emission, but not beam stopping. This was due to a faulty design which applied an error flag for unavailable transition information in beam emission to the beam stopping case also. This has been corrected.

It was convenient at the same time to tidy up the comments at the end of the *adf21/adf22* output files and change the default pass file name to *adas312_out.pass* (from *default.txt*).

ADAS312 has an unfortunate way of determining species and donor information which are used purely for information on the precessing screen. The adf26 input filename is parsed for this information which effectively restricts it to central ADAS data or correctly named user data. A trap has been inserted to se whether the input file conforms to this pattern and if not, a message is displayed rather than random looking strings as at present.

C.22. ADAS801. A fault has been corrected in the translation of the configuration representation of Cowan to that of Eissner by the subroutine *eissner.for*. The problem arose with occupation numbers greater than 9 and gave incorrect configuration strings in the output *adf04* file.

C.23 Extensions have been made to several subroutines in */../adas/idl_adas/fortran/adaslib/* to allow us to handle very heavy species. These routines are *cstrgrp.for, ceigrp.for, i4eiss.for, i4jgrp.for, i4lgrp.for, i4ndec.for, i4ngrp.for, i4pgrp.for, i4schr.for, xxcftr.for* and *xxdtes.for*. It is only the latter two which might have some impact. xxdtes.for is a substantial extension. It does require the other revised subroutines. Please let us know if you have any unexpected stops from *xxcftr.for* or *xxdtes.for.*

C.24 ADAS407. The subroutine *d7auts.for* checks that the number of entries in the orbital energy list of an adf04 files equals the number of orbitals identified in the configuration lists of the file. For heavy species with empty inner shells, this is overstringent and can cause unnecessary program termination. It is sufficient for the identified orbitals to be a subset.

Corrections and updates to data (ADAS v2.5.6 to ADAS v2.6)

D.1 Manuel Bautista's adf09/27/28 have been changed again. Some files may remain the same but the entire directories have been updated from his files. Twice before release - latest update Jan 2003.

adf09/mb00#he/*
adf27/helike/mb00#he/*
adf28/helike/mb00#he/*

D.2 New Li-like adf04 data for Ar and Fe from Allan. The reference is A D Whiteford et al, J Phys B 35 3729-3740 (2002).

adf04/lilike/lilike_adw02#ar15.dat
adf04/lilike/lilike_adw02#fe23.dat

D.3 PECs and SXBs from relatively high n in the hydrogen like low Z elements have been added. These are generated with the off-line v2bndl code. Datasets for He were added in the 2.5.6 release but Carbon was omitted. These have now been added to the adf13/adf15 96 directories with the bnd extension.

adf13/sxb96#c/sxb96#c_bnd#c5.dat
adf15/pec96#c/pec96#c_bnd#c5.dat

D.4 Lithium has been added from the GCR Project. Many files are required - adf03/4/7/8/10/11/13/15/17/18/25 - approximately 10Mb of data in total.

- New fundamental data for excitation from Connor and Don Griffin, with ionisation from the Auburn group - Stuart and Mitch Pindzola.
- The DR data came from the DR project from Nigel.
- All other data and manipulation from ADAS.
- GCR adf11 sets for ionisation, recombination and power have the year/token/designation 96 in keeping with the other light elements.
- A baseline 89 dataset has also been included which adds CX recombination and power and a specific line power dataset for compatability.

adf03/atompars/atompars_mm#li.dat

adf04/adas#3/cpb02_ls#li0.dat
adf04/adas#3/cpb02_ls#li1.dat
adf04/adas#3/cpb02_ls#li2.dat
adf04/adas#3/cpb02_n#li2.dat
adf04/copmm#3/ls#li0.dat
adf04/copmm#3/ls#li1.dat
adf04/copmm#3/ls#li2.dat
adf04/copmm#3/ls#li3.dat
adf04/lilike/lilike_cpb02#li0.dat
adf04/helike/helike_cpb02#li1.dat
adf04/hlike/hlike_cpb02#li2.dat

adf07/szd02#li/szd02#li_li2.dat
adf07/szd02#li/szd02#li_li1.dat
adf07/szd02#li/szd02#li_li0.dat

adf08/rrc98#h/rrc98#h_li2.dat
adf08/rrc98##/rrc98##_li3.dat
adf08/rrc98#he/rrc98#he_li1.dat

adf10/acd96/pj#acd96_h11.dat
adf10/acd96/pj#acd96_he11.dat
adf10/acd96/pj#acd96_he12.dat
adf10/acd96/pj#acd96_li11.dat

```
adf10/acd96/pj#acd96_li21.dat
adf10/met96/pj#met96_h##.dat
adf10/met96/pj#met96_he##.dat
adf10/met96/pj#met96_li##.dat
adf10/plt96/pj#plt96_h##.dat
adf10/plt96/pj#plt96_he##.dat
adf10/plt96/pj#plt96_li##.dat
adf10/prb96/pj#prb96_h10.dat
adf10/prb96/pj#prb96_he10.dat
adf10/prb96/pj#prb96_li10.dat
adf10/prb96/pj#prb96_li20.dat
adf10/qcd96/pj#qcd96_he12.dat
adf10/qcd96/pj#qcd96_he21.dat
adf10/scd96/pj#scd96_h11.dat
adf10/scd96/pj#scd96_he11.dat
adf10/scd96/pj#scd96_he12.dat
adf10/scd96/pj#scd96_li11.dat
adf10/scd96/pj#scd96_li21.dat
adf10/xcd96/pj#xcd96_li12.dat
adf10/xcd96/pj#xcd96_li21.dat

adf11/acd96/acd96_li.dat
adf11/acd96r/acd96r_li.dat
adf11/scd96/scd96_li.dat
adf11/scd96r/scd96r_li.dat
adf11/prb96/prb96_li.dat
adf11/prb96r/prb96r_li.dat
adf11/plt96/plt96_li.dat
adf11/plt96r/plt96r_li.dat
adf11/qcd96r/qcd96r_li.dat
adf11/xcd96r/xcd96r_li.dat
adf11/acd89/acd89_li.dat
adf11/scd89/scd89_li.dat
adf11/ccd89/ccd89_li.dat
adf11/prb89/prb89_li.dat
adf11/plt89/plt89_li.dat
adf11/prc89/prc89_li.dat
adf11/pls89/pls89_li.dat

adf13/sxb96#li/sxb96#li_pjr#li0.dat
adf13/sxb96#li/sxb96#li_pjr#li1.dat
adf13/sxb96#li/sxb96#li_pju#li1.dat
adf13/sxb96#li/sxb96#li_pju#li0.dat
adf13/sxb96#li/sxb96#li_pjr#li2.dat
adf13/sxb96#li/sxb96#li_pju#li2.dat

adf15/pec96#li/pec96#li_pjr#li0.dat
adf15/pec96#li/pec96#li_pjr#li1.dat
adf15/pec96#li/pec96#li_pju#li1.dat
adf15/pec96#li/pec96#li_pju#li0.dat
adf15/pec96#li/pec96#li_pjr#li2.dat
adf15/pec96#li/pec96#li_pju#li2.dat

adf17/cbnm96#li/cbnm96#li_li0ls.dat
adf17/cbnm96#he/cbnm96#he_li1ls.dat
adf17/cbnm96#h/cbnm96#h_li2ls.dat

adf18/a09_a04/drm96#he/drm96#he_li1.dat
```

adf18/a09_a04/drm96#li/drm96#li_li0.dat
adf18/a17_p208/exp96#h/exp96#h_li2ls.dat
adf18/a17_p208/exp96#h/exp96#h_li2n.dat
adf18/a17_p208/exp96#he/exp96#he_li1ls.dat
adf18/a17_p208/exp96#li/exp96#li_li0ls.dat
adf18/a09_p204/drm96#h/drm96#h_li2n.dat
adf18/a09_p204/drm96#he/drm96#he_li1n.dat
adf18/a09_p204/drm96#li/drm96#li_li0n.dat

adf25/bns96#h/bns96#h_li2.dat
adf25/bns96#he/bns96#he_li1.dat
adf25/bns96#li/bns96#li_li0.dat

D.5 Add the *adf00* directory which holds configuration and ionisation potential data. Note the *ga.dat* file was incorrectly formatted. Incorrect ionisation potentials (missing exponents) in Rb, Tc and Pd.

adf00

D.6 Correction to A-value in OV IC file (Peter Young, RAL).

adf04/adas#8/cop98#8_ic#o4.dat

D.7. The ADAS405 and ADAS406 example scripts atStrathclyde were out of data and so (embarassingly) did not work.

D.8 David Elder pointed out that the '96' neutral carbon *pec* and *sxb* datasets did not include transitions that were present in the '93' set. This is an old problem arising from the rather crude algorithm in ADAS208 for restricting the total number of pecs. A new set of unresolved and resolved files keyed to the visible spectrometer range (*vsu* and *vsr* files) – just as for CII and CIII – have been added for CI as follow:

adf15/pec96#c/pec96#c_vsu#c0.dat
adf15/pec96#c/pec96#c_vsr#c0.dat
adf13/sxb96#c/sxb96#c_vsu#c0.dat
adf13/sxb96#c/sxb96#c_vsr#c0.dat

D.9. New adf38 and adf39 photo-excitation and photo-ionisation data. These have been prepared by Nigel Badnell and Mike Seaton. H-like, hHe-like and Li-like ion s of carbon, oxygen, sulphur and iron ions have been included on this occasion. Note that there are both LS and IC versions. Further data sets are in preparation.

adf38/nrb02#h/<ion>ls<n>l,r.dat
adf38/nrb02#he/<ion>ls<n>l,r.dat
adf38/nrb02#li/<ion>ls<n>l,r.dat

H. P. Summers
07 Feb. 2003

ADAS510: F-PEC - graph envelope feature photon emissivity coefficients

The program interrogates enevelope feature photon emissivity ($\mathscr{F}\_\mathscr{PEC}$) files of type ADF40. The coefficient is extracted for a selected wavelength range of an ion. The coefficient may be displayed in a three dimensional plot.

Background theory:

An envelope feature photon emissivity coefficient, denoted by $\mathscr{F}\_\mathscr{PEC}$, is defined on a wavelength interval and is a composite feature arising from very many lines from a single ionisation stage. The $\mathscr{F}\_\mathscr{PEC}$ 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 ($\mathscr{PEC}$ s). Following Chap 3.8, the emissivity of an individual line is specified as

$$\varepsilon_{j\to k} = A_{j\to k}(\sum_{\sigma=1}^{M}\mathscr{F}_{j\sigma}^{(exc)}N_e N_\sigma + \sum_{\upsilon'=1}^{M_{z+1}}\mathscr{F}_{j\upsilon'}^{(rec)}N_e N_{\upsilon'}^{+}). \qquad 6.10.1$$

This allows specification of the *excitation* photon emissivity coefficient

$$\mathscr{PEC}_{\sigma,j\to k}^{(exc)} = A_{j\to k}\mathscr{F}_{j\sigma}^{(exc)} \qquad 6.10.2$$

and the *recombination* photon emissivity coefficient

$$\mathscr{PEC}_{\upsilon',j\to k}^{(rec)} = A_{j\to k}\mathscr{F}_{j\upsilon'}^{(rec)}. \qquad 6.10.3$$

Each of these coefficients is associated with a particular metastable σ or υ' of the X^{+z}, or X^{+z+1} ions respectively.

Consider a spectral interval, $[\lambda_0,\lambda_1]$, subdivided into N_{pix} intervals as $\{\Delta\lambda_i^{[0,1]} \equiv [\lambda_0 + i(\lambda_1-\lambda_0)/N_{pix}, \lambda_0+(i+1)(\lambda_1-\lambda_0)/N_{pix}] : i=0,..,N_{pix}-1\}$Also suppose that the $j \to k$ spectrum line has a normalised emission profile $\varphi_{j\to k}(\lambda)$. In general, such a profile is a convolution of Doppler and instrumental functions. Then the envelope feature photon emissivity coefficient vector is defined as

$$\mathscr{F}\_\mathscr{PEC}_{\sigma,i}^{(exc)[0,1]} = \sum_{\substack{j,k\\ \lambda_{j\to k}\in[0,1]}} \mathscr{PEC}_{\sigma,j\to k}^{(exc)}\int_{\lambda_i}^{\lambda_{i+1}}\varphi_{j\to k}(\lambda)d\lambda \qquad 6.10.4$$

$\lambda_{j\to k}$ is the natural wavelength of the $j \to k$ spectrum line. The default broadening assumed is Doppler with a Maxwellian distribution for the emitting ion at temperature, T_{ion}, equal to the electron temperature, T_e, used in the collisional–radiative modelling of the $\mathscr{PEC}$ s. This consitutes a minimum broadening. The integral in equation 6.10.4 is then expressible in terms of error functions as

$$\begin{aligned}\mathscr{F}\_\mathscr{PEC}_{\sigma,i}^{(exc)[0,1]} = & \sum_{\substack{j,k\\ \lambda_{j\to k}\in\Delta\lambda_i^{[0,1]}}}\mathscr{PEC}_{\sigma,j\to k}^{(exc)}\tfrac{1}{2}\{\operatorname{erfc}((\lambda_i-\lambda_{j\to k})/\sigma) \\ & -\operatorname{erfc}((\lambda_{i+1}-\lambda_{j\to k})/\sigma)\}\end{aligned} \qquad 6.10.5$$

where $\sigma = \lambda_{j\to k}\alpha\left(\frac{kT_{ion}}{I_H}\cdot\frac{m_p}{m_X}\cdot\frac{m_e}{m_p}\right)^{1/2}$ and m_X is the emitting ion mass.

In principle, the minimal Doppler broadened $\mathscr{F}\_\mathscr{PEC}$ s can be convolved with effective instrument functions and/or representations of wavelength dependent filters. These are called ‘filtered’ $\mathscr{F}\_\mathscr{PEC}$ s and they are structurally the same as the unfiltered $\mathscr{F}\_\mathscr{PEC}$ s.

$$\mathscr{F}\_\mathscr{PEC}_{\sigma,i}^{(exc)[0,1]_F} = F_i \mathscr{F}\_\mathscr{PEC}_{\sigma,i}^{(exc)[0,1]} \qquad 6.10.6$$

where $\{F_i : i = 1,..,npix\}$ denotes a filter. The archiving is unchanged except for the need for a filter code to be assigned as part of the archive.

$\mathscr{F}\_\mathscr{PEC}$ data are extracted from archived files of type ADF40. They are interpolated by cubic splines in electron temperature and density to provide results at an arbitrary set of temperature/density pairs. The code can select the temperature/density pairs graphically. For this purpose the $\mathscr{F}\_\mathscr{PEC}$ must be contracted over wavelength. The functional used for interactive graphical pair selection is the total photon count over the wavelength interval, namely

$$\overline{\mathscr{F}\_\mathscr{PEC}}_{\sigma}^{(exc)[0,1]} = \sum_i \mathscr{F}\_\mathscr{PEC}_{\sigma,i}^{(exc)[0,1]} \qquad 6.10.7$$

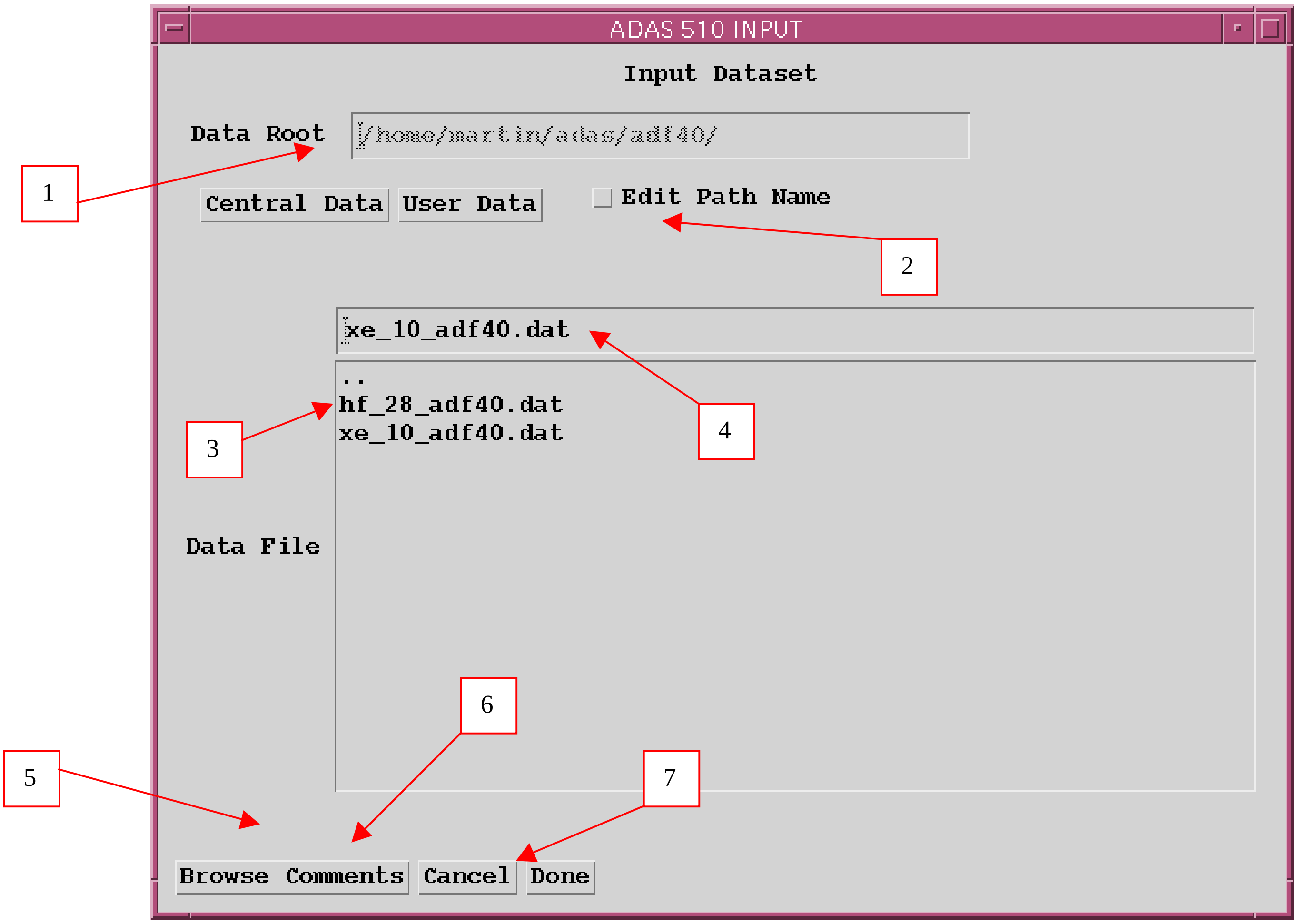
Program steps:

Interactive parameter comments:

Programs of series ADAS5 which make use of data from archived ADAS datasets initiate an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output.

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

1. Data root shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Note that each type of data is stored according to its ADAS data format (*adf* number). 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.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. 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.
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. Datafiles all have the termination *.dat*.
5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
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 is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window



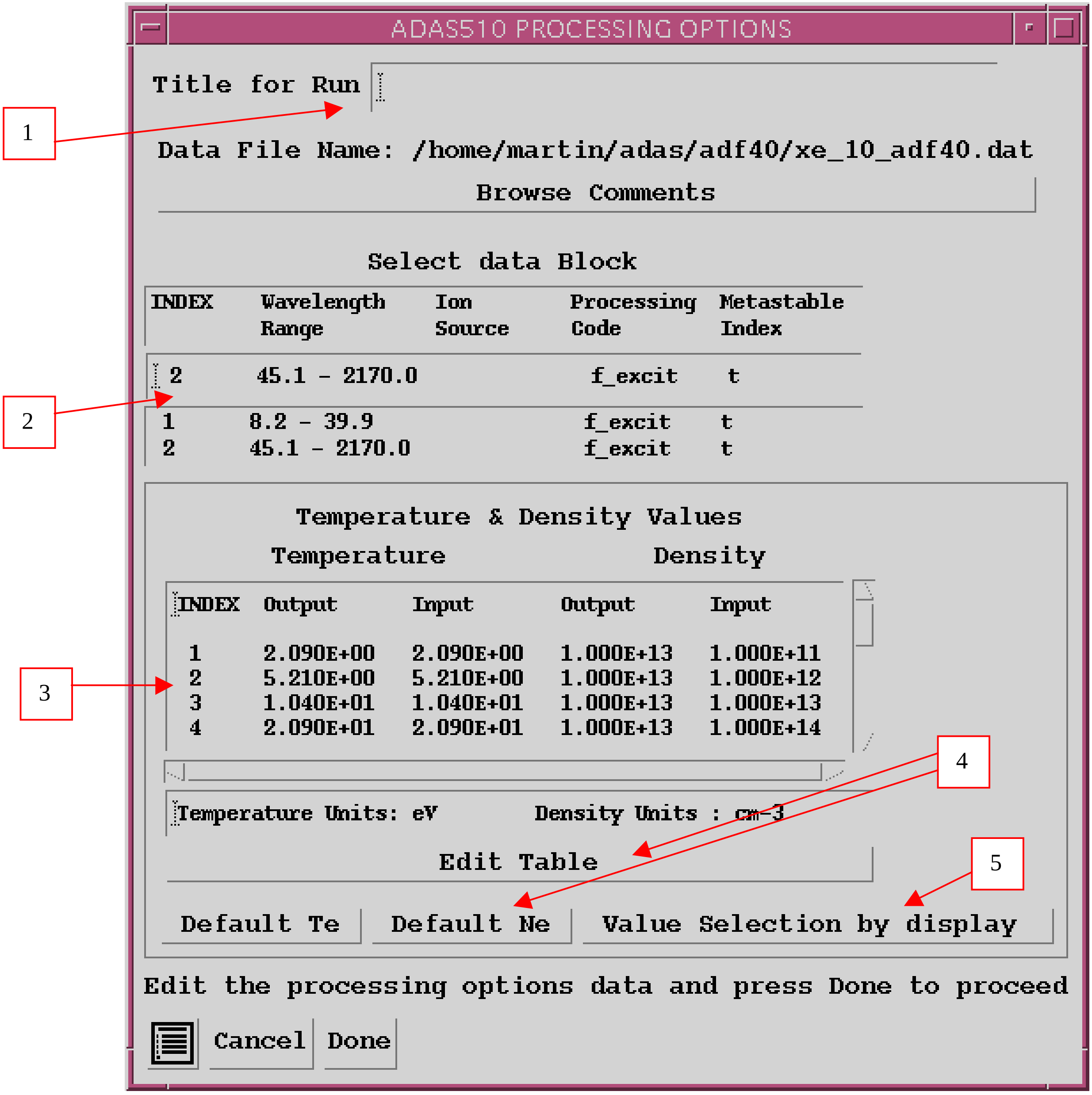
Data Root: /home/martin/adas/adf40/

xe_10_adf40.dat

```
..
hf_28_adf40.dat
xe_10_adf40.dat
```

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

1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
2. Spectral intervals for which envelope feature emissivity coefficients are available in the data set are displayed in the list display window. This is a scrollable window using the scroll bar to the right of the window. Note there is a *Filter* field present for information. Click anywhere on the row for a feature to select it. The selected feature appears in the selection window just above the feature list display window.
3. Your settings of electron temperature/electron density pairs (outputs) are shown in the temperature/density display window. The temperature and density values at which the envelope feature emissivity coefficient is stored in the datafile (inputs) is also shown for information. **Note that you must give temperature/density pairs, ie. the same number of each as for a model.** The underlying datafile has a three-dimensional storage as a function of temperature, density and wavelength.



ADAS510 PROCESSING OPTIONS

Title for Run

Data File Name: /home/martin/adas/adf40/xe_10_adf40.dat

Browse Comments

Select data Block

INDEX	Wavelength Range	Ion Source	Processing Code	Metastable Index
2	45.1 - 2170.0		f_excit	t
1	8.2 - 39.9		f_excit	t
2	45.1 - 2170.0		f_excit	t

Temperature & Density Values

	Temperature		Density	
INDEX	Output	Input	Output	Input
1	2.090E+00	2.090E+00	1.000E+13	1.000E+11
2	5.210E+00	5.210E+00	1.000E+13	1.000E+12
3	1.040E+01	1.040E+01	1.000E+13	1.000E+13
4	2.090E+01	2.090E+01	1.000E+13	1.000E+14

Temperature Units: eV Density Units : cm-3

Edit Table

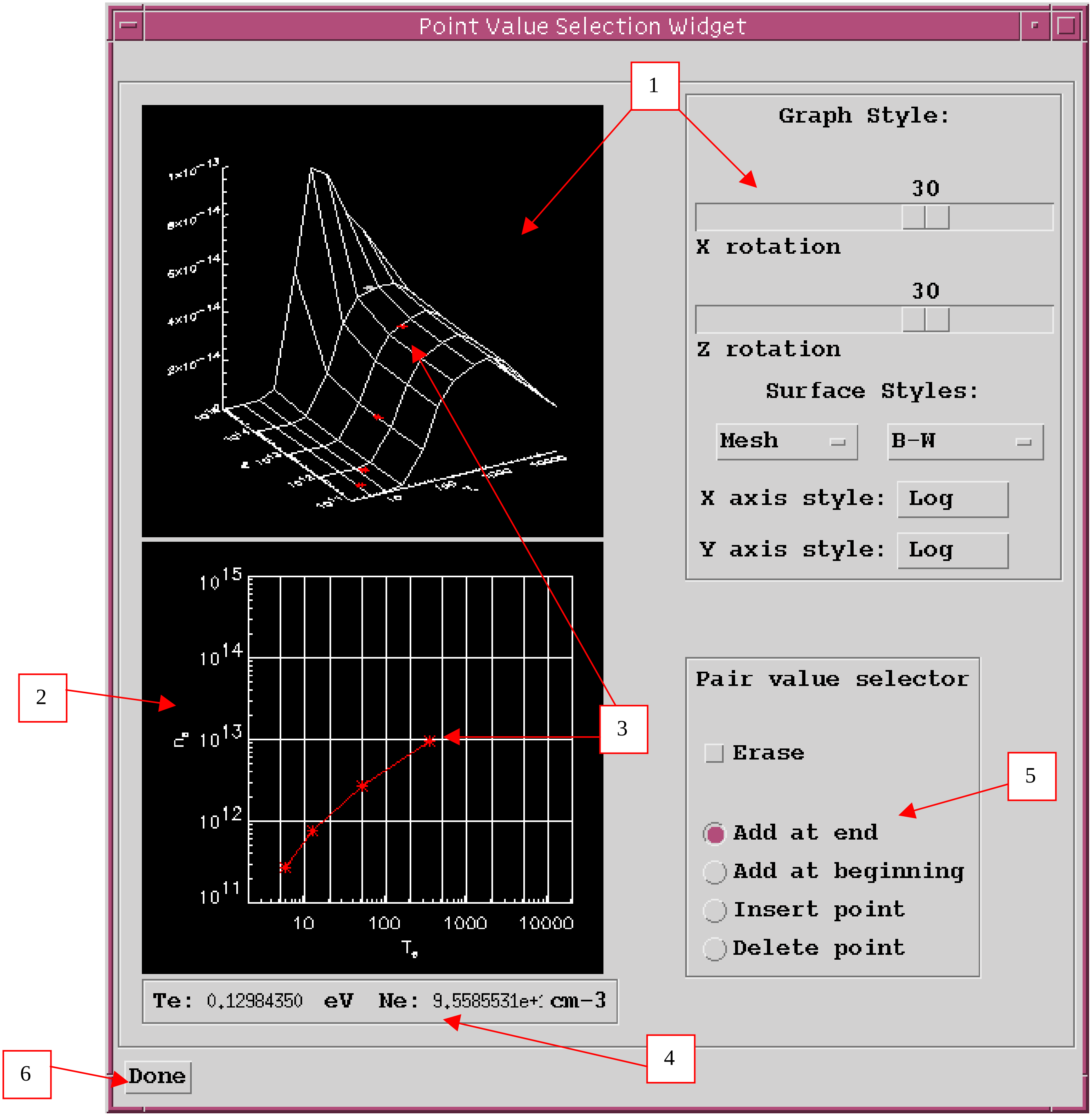
Default Te Default Ne Value Selection by display

Edit the processing options data and press Done to proceed

Cancel Done

4. The program initially recovers the output temperature/density pairs you used when last executing the program. The Temperature & Density Values are editable. Click on the *Edit Table* button if you wish to change the values. The usual 'drop-down' window, the ADAS Table Editor window, appears. *Default Te* and *Default Ne* are available. These buttons insert the electron temperature data or electron density data respectively from the input data set as the output values and offers a choice of a fixed electron density or electron temperature respectively to be associated with these.
5. The third button is for *Value Selection by display*. Click to pop-up the *point value selection widget*. It is designed both to provide a display of the actual three-dimensional surface of the density and temperature dependent wavelength interval summed, envelope feature collisional-radiative emissivity coefficient (see equation 6.10.6) and to allow selection of temperature/density pairs for the output graphs visually.

The **point value selection widget** has the appearance shown below



Graph Style:

30
X rotation

30
Z rotation

Surface Styles:

Mesh B-W

X axis style: Log

Y axis style: Log

Pair value selector

□ Erase

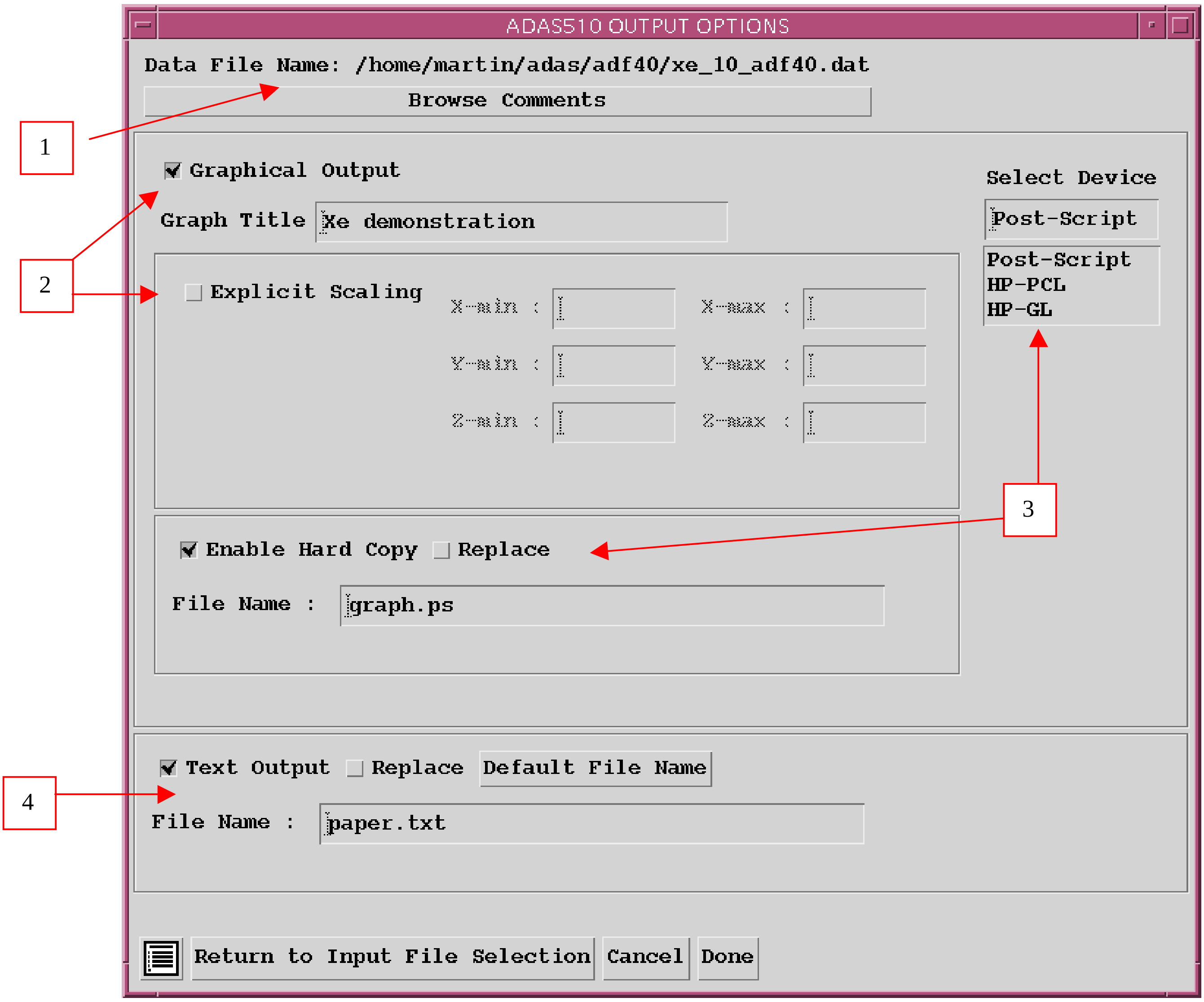
● Add at end
○ Add at beginning
○ Insert point
○ Delete point

Te: 0.12984350 eV Ne: 9.5585531e+ cm-3

1. The summed envelope feature emissivity coefficient surface is shown. Controls are provided to orientate and alter the appearance of the display. Sliders allow rotation about the X-axis and about the Y-axis so that the whole surface can be examined. The surface styles can be altered by selecting from drop-down menus. The styles include continuous or mesh surfaces and the colour of the surface. Finally the form of the axes, that is logarithmic or linear can be chosen from drop-down menus.
2. A two dimensional projection on the Te/Ne plane is displayed. Note that the grid lines are those of the actual data in the source file. The code provides a sophisticated method for selecting Te/Ne pairs by mouse click which allows the user to track over interesting parts of the surface.

3. Move the mouse cursor over the lower Te/Ne grid. A tracking pointer moves over the surface in the upper display. Click the left mouse button to select a Te/Ne pair. A symbol marks the selection on the Te/Ne grid in the lower display and a marker also appears on the surface in the upper display. Continue to select point pairs as required.
4. Note that the position of the cursor in Te/Ne space is shown numerically for precise positioning
5. Control buttons at allow adjustments to your selection set. Pairs can be added at the beginning or end of the set or inserted between pairs. Also a pair can be deleted. Finally the whole set of pairs can be erased.
6. Click *Done* on completion to return to the processing options window. The pairs selected will be present in the editable table. Note that conventional entry or modification of user data with Table Editor remains an option as before.

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



ADAS510 OUTPUT OPTIONS

Data File Name: /home/martin/adas/adf40/xe_10_adf40.dat

☑ Graphical Output

Graph Title: Xe demonstration

□ Explicit Scaling

Select Device: Post-Script

☑ Enable Hard Copy □ Replace

File Name : graph.ps

☑ Text Output □ Replace

File Name : paper.txt

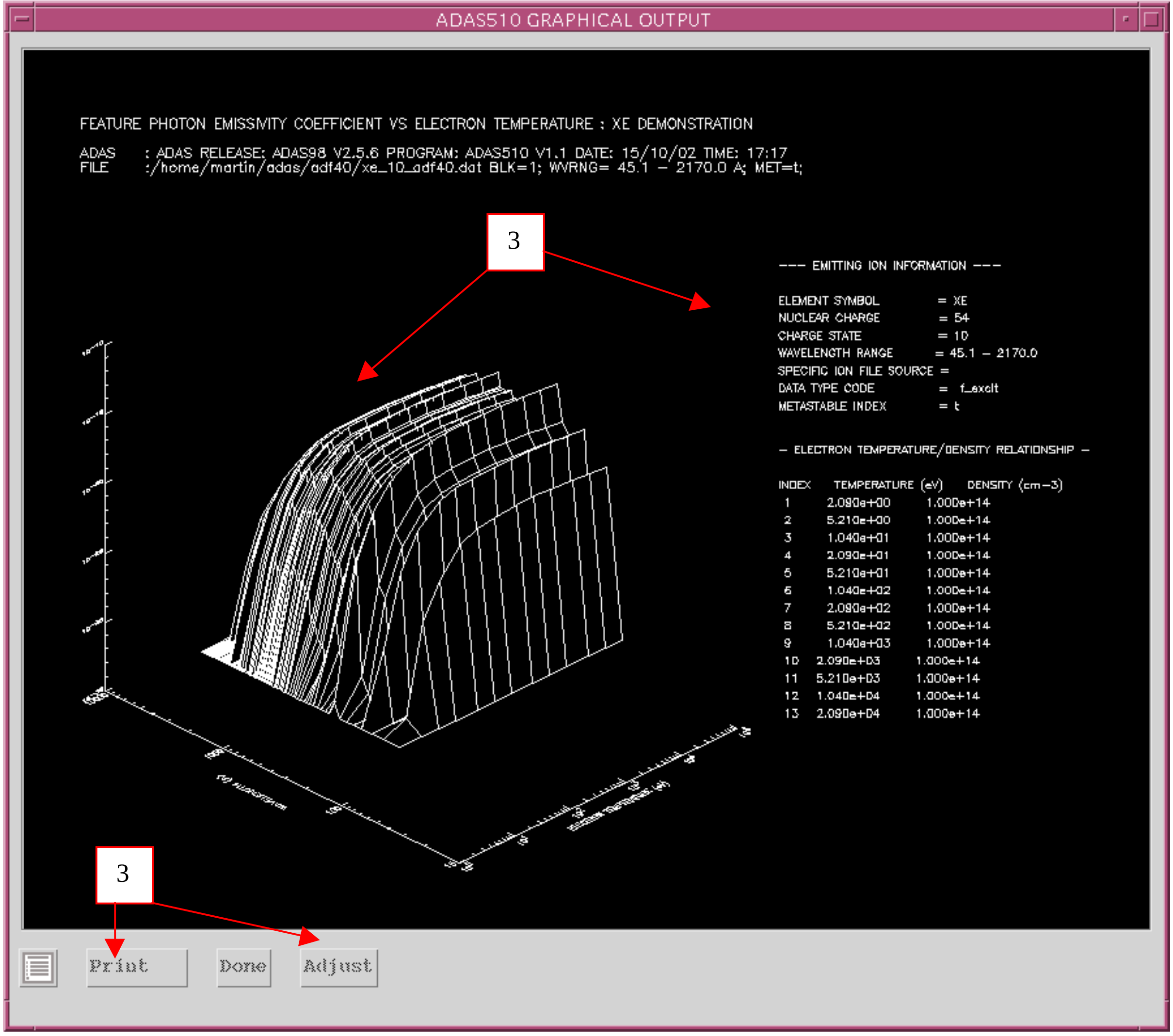
1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
2. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical 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 to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.

3. Hard copy is activated by the *Enable Hard Copy* button . 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. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
4. 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.

The **graphical output** window has the appearance shown below

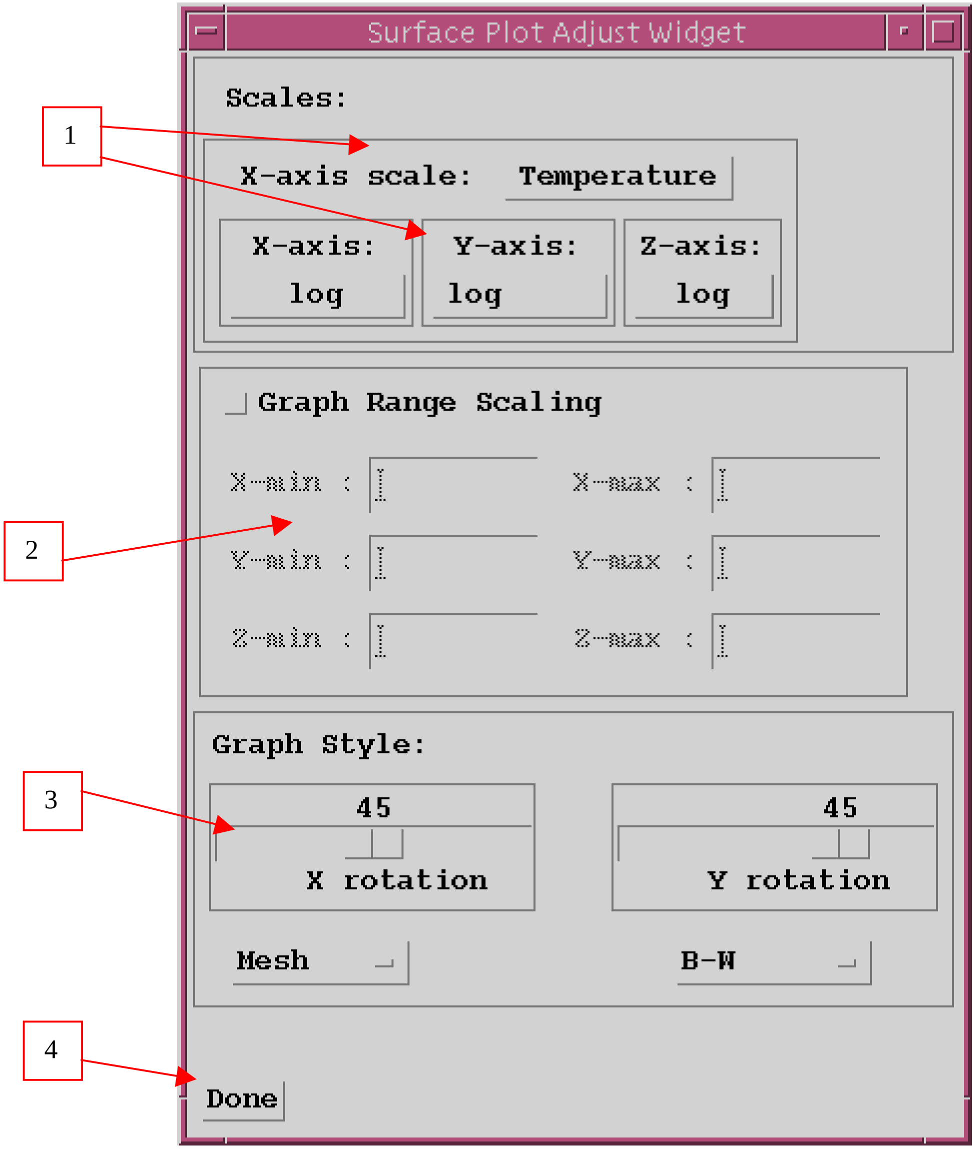
1. The 3-D plot is displayed together with identifying textual annotation.
2. The *Print* button sends the displayed graph to the graphic file. The *Adjust* button pops up the *3-D graph adjustment* widget which allows modification of the graph.



```
FEATURE PHOTON EMISSIVITY COEFFICIENT VS ELECTRON TEMPERATURE : XE DEMONSTRATION

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS510 V1.1 DATE: 15/10/02 TIME: 17:17
FILE    :/home/martin/adas/adf40/xe_10_adf40.dat BLK=1; WVRNG= 45.1 - 2170.0 A; MET=t;

--- EMITTING ION INFORMATION ---

ELEMENT SYMBOL          = XE
NUCLEAR CHARGE          = 54
CHARGE STATE            = 10
WAVELENGTH RANGE       = 45.1 - 2170.0
SPECIFIC ION FILE SOURCE =
DATA TYPE CODE          =  f_exclt
METASTABLE INDEX        = t

- ELECTRON TEMPERATURE/DENSITY RELATIONSHIP -

INDEX    TEMPERATURE (eV)    DENSITY (cm-3)
 1       2.090e+00       1.000e+14
 2       5.210e+00       1.000e+14
 3       1.040e+01       1.000e+14
 4       2.090e+01       1.000e+14
 5       5.210e+01       1.000e+14
 6       1.040e+02       1.000e+14
 7       2.090e+02       1.000e+14
 8       5.210e+02       1.000e+14
 9       1.040e+03       1.000e+14
 10   2.090e+03       1.000e+14
 11   5.210e+03       1.000e+14
 12   1.040e+04       1.000e+14
 13   2.090e+04       1.000e+14
```

The **3-D graph adjustment** widget has the appearance shown below

1. Control is provided to alter the axes. A choice for the X-axis (temperature or density) is provided. Note that the X-axis is representing the variation with both temperature and density, since model pairs are being used. The Y-axis is assigned to wavelength. The style (logarithmic or linear) for each of the axes may be varied.
2. Explicit scaling may be activated and then the usual manual entry of minima and maxima for each of the three axis scales is supported.
3. Control of the orientation of the 3-D display is provided. Also, the appearance of the surface (mesh or surface) and colour of the surface may be chosen.
4. Note that the widget remains present and active for convenience so that a sequence of adjustments may be made. Click *Done* to close the widget..



Scales:

X-axis scale: Temperature

X-axis: log

Y-axis: log

Z-axis: log

□ Graph Range Scaling

X-min :

X-max :

Y-min :

Y-max :

Z-min :

Z-max :

Graph Style:

X rotation: 45

Y rotation: 45

Mesh

B-W

Notes:

ADAS804: Calculate cross-sections & rate coefficients

The code calculates electron impact excitation cross-sections in a one electron distorted wave Born approximation using an optimised Slater type or Jucys screening potential and observed level energies.

Background theory:

For a free electron colliding with a z times ionised ion A^{+z} in the state γ

$$A^{+z}(\gamma)+e(E)\rightarrow A^{+z}(\gamma')+e(E')$$

9.4.1

E and E' are the initial and final electron energies with $E>E'$ and $\Delta E=E-E'$ is the transition energy. The Born collision strength takes the form

$$\Omega_{\gamma,\gamma'}(E,E')=\omega_\gamma 8\frac{\sqrt{EE'}}{I_H}\sum_\lambda Q^{(\lambda)}_{\gamma,\gamma'}R^{(\lambda)}(E,E') \qquad 9.4.2$$

where the sum is over the various multipoles λ. $Q^{(\lambda)}_{\gamma,\gamma'}$ comprises the angular factors and $R^{(\lambda)}(E,E')$ the momentum and radial integrals. The Ochkur extension allows the application tto spin change transitions, but with different $Q^{(\lambda)}_{\gamma,\gamma'}$ and $R^{(\lambda)}(E,E')$. In term coupling the formulae are

No spin change: $\gamma\equiv(S_pL_p)nlSL$; $\gamma'\equiv(S_pL_p)n'l'SL'$.

$$Q^{(\lambda)}_{\gamma,\gamma'}=(2l+1)(2l'+1)(2l'+1)(2\lambda+1)\begin{Bmatrix} l & L & L_p \\ L' & l' & \lambda \end{Bmatrix}^2\begin{pmatrix} l & l' & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2$$

$$R^{(\lambda)}(E,E')=\int_{-1}^{1}\frac{\left|\langle nl|j_\lambda(qr)|n'l'\rangle\right|^2}{a_0^4q^4}d(\cos\theta) \qquad 9.4.3$$

Spin change: $\gamma\equiv(S_pL_p)nlSL$; $\gamma'\equiv(S_pL_p)n'l'S'L'$.

$$Q^{(\lambda)}_{\gamma,\gamma'}=(2l+1)(2l'+1)(2l'+1)(2\lambda+1).$$

$$\frac{(2S'+1)}{2(2S_p+1)}\begin{Bmatrix} l & L & L_p \\ L' & l' & \lambda \end{Bmatrix}^2\begin{pmatrix} l & l' & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2$$

$$R^{(\lambda)}(E,E')=\int_{-1}^{1}\frac{\left|\langle nl|j_\lambda(qr)|n'l'\rangle\right|^2}{a_0^4q^4}\left(\frac{q}{k}\right)^4 d(\cos\theta) \qquad 9.4.4$$

q is the momentum transfer at scattering angle q and q is the initial momentum. Other notation is conventional. The radial integrals are evaluated from numerical wave functions as follows.

Effective potential non-hydrogenic radial integrals: Let z_0 be the nuclear charge of ions A^{+z} and write $z_1=z+1$. A parameterized effective central potential is adopted here as the basis for calculating these wave functions. The central potential is established by defining an effective screening configuration

$$n_1l_1^{q_1}n_2l_2^{q_2}....n_sl_s^{q_s} \text{ such that } q_1+q_2+....+q_s=z_0-z_1. \qquad 9.4.5$$

The electron in shell i is supposed to be screened from the nucleus by the electrons in shells $<i$ and partially screened by the other electrons in shell i itself. So the effective charge for the ith shell electron is

$$z_i=z_0-\sum_{j=1}^{i-1}q_j-\tfrac{1}{2}q_i. \qquad 9.4.6$$

The adopted (Slater type) potential is then

$$V(r) = \frac{z_0}{r} - \sum_{i=1}^{s} \frac{q_i}{r} \exp(-\alpha_i z_i r / n_i) \left(\sum_{k=0}^{n_i} a_{ik} r^{-k} \right) \qquad 9.4.7$$

The α_i are adjustable parameters chosen so that the one electron wave function satisfies the one electron Schrodinger equation with potential $V(r)$ and the observed eigenenergy ε and quantum defect μ. In practice, we set $\alpha_i = \overline{\alpha_i}\alpha$ with $\overline{\alpha_i}$ specified so that only the overall scaling parameter α is varied to match the observed quantum defect. The radial integrals are evaluated by numerical quadratures.

Program steps:

Interactive parameter comments:

The **archive selection window** appears first. It is slightly different in operation than the usual file selection window.

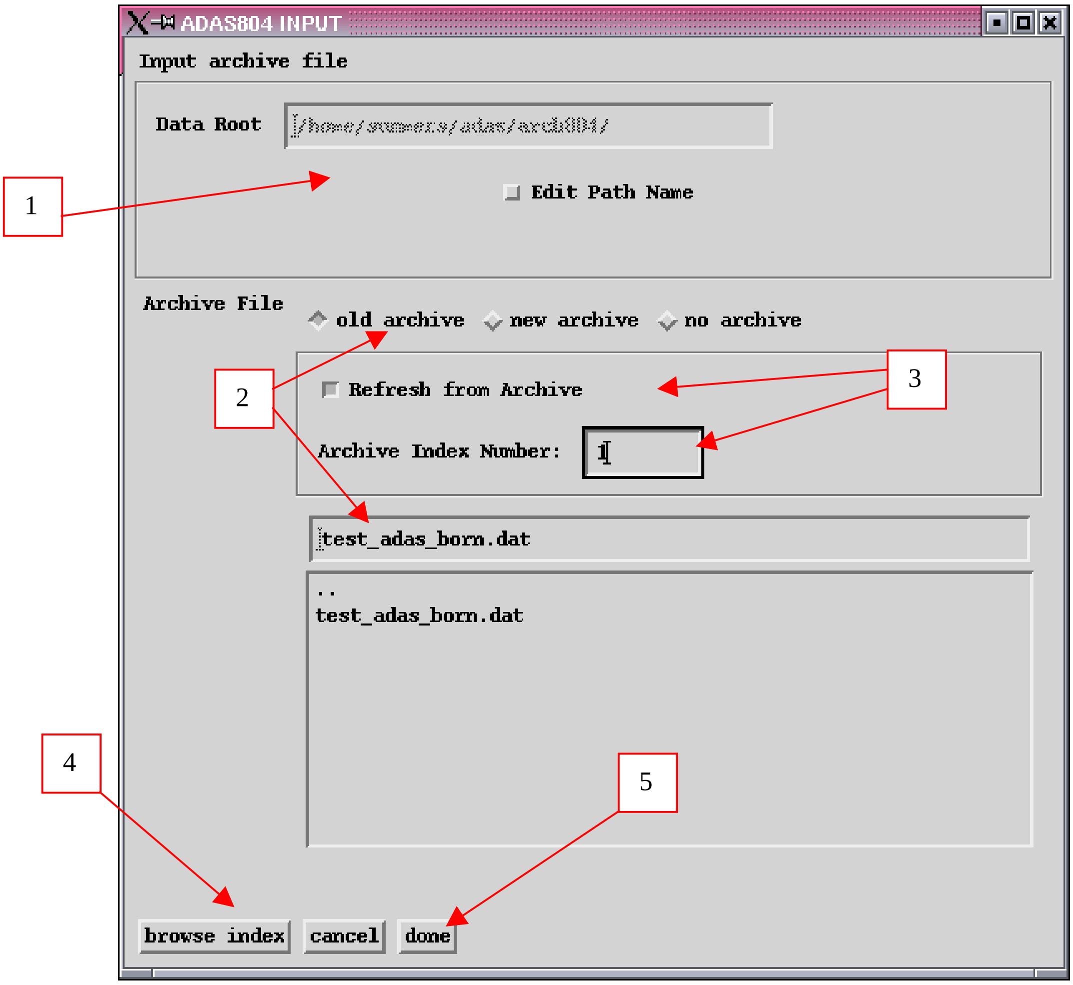
1. The recommended root path for user archiving for ADAS804 analysis is

   .../uid/adas/arch804/

   which may be edited in the usual manner.
2. Click the appropriate button 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**.
3. The capability is given for reworking or re-displaying the results of an earlier analysis stored in an archive file. 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.
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.
5. 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** appearance is shown below

1. An arbitrary title for the run may be set. If an archive is in use, then its name is given. Also the index of the archive can be browsed.
2. The nuclear and ionic charges should be specified along with Zeff, the effective ion charge. Normally, Zeff is set equal to the ion charge+1.
3. Specify the parent term or level. Note that the code can deal with LS-coupled terms or levels and with J-resolved parents in Jp-j coupling. If the parent is a term, leave the Jp field bank.



Input archive file

Data Root /home/summers/adas/arch804/

□ Edit Path Name

Archive File ◇ old archive ◇ new archive ◇ no archive

□ Refresh from Archive

Archive Index Number: 1

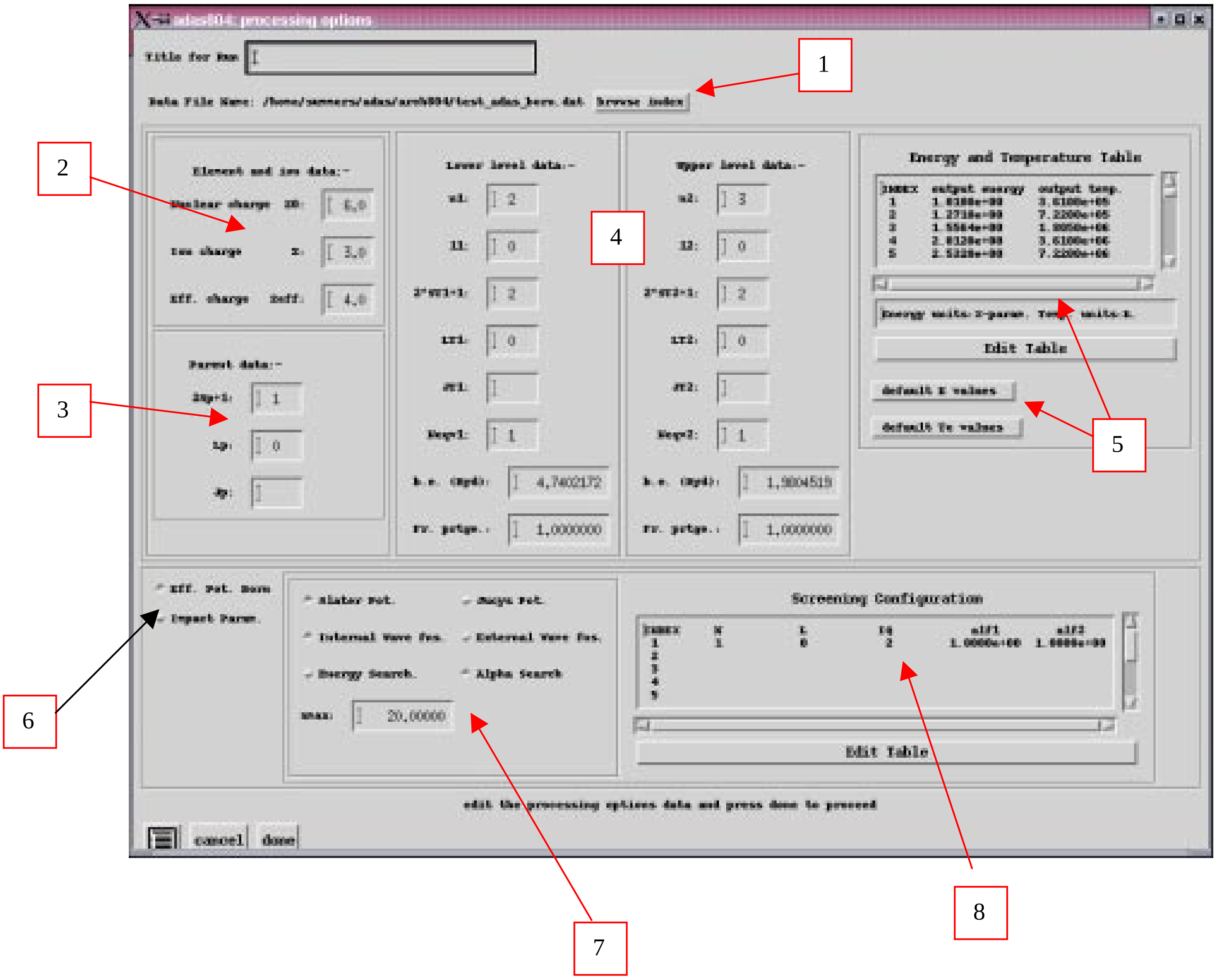
test_adas_born.dat

..
test_adas_born.dat

4. Specify the details of the lower and upper levels of the transition. For a transition between terms, leave the fields JT1 and JT2 blank. Note that the number of equivalent electrons are required for the initial and final shell of the active electron together with fractional paranetages associated with the identified parent. The binding energy is the energy (rydbergs) required to remove the active electron leaving the residual ion in the identified parent state.
5. Select required energies at which the collision strength should be calculated and temperatures at which the Upsilons should be calculated. The table is editable and there are default buttons for both the energies and temperatures. The default values are the standard ADAS sets.
6. At the present time, only the effective potential Born calculation is provided. The option for an impact parameter calculation (of dipole allowed transitions only) will be provided in the future.
7. A choice of Slater and Jucys forms for the effective potential is provided. The current trend of our work is to prefer the Slate form. At this time only internal (calculation) of wavefunctions is permitted. The option of reading in numerical radial wavefunctions may nbe made available at a later stage. Adjustable (alpha) parameters in the potential may be varied so that the wavefunction eigenenergy corresponds to the input energy. There is another option, whereby the potential parameters are locked and the

eigenenergy sought. This is a less useful option in the present context.

8. The potential form is established by specification of a ‘screening configuration’. Typically this is the distribution of the electrons amongst their various nl-shells in the initial state, excluding the active electron (that is the parent ion). Also, initial values of the adjustable parameters may be set. Usually both are set to 1.0 initially.



adas804: processing options

Title for Run

Data File Name: /home/summers/adas/arch804/test_adas_born.dat

browse index

Element and ion data:-

Nuclear charge Z0: 6.0

Ion charge Z: 3.0

Eff. charge Zeff: 4.0

Parent data:-

2Sp+1: 1

Lp: 0

Jp:

Lower level data:-

n1: 2

l1: 0

2*S1+1: 2

L1: 0

J1:

Negp1: 1

b.e. (Ryd): 4.7402172

rv. prtge.: 1.0000000

Upper level data:-

n2: 3

l2: 0

2*S2+1: 2

L2: 0

J2:

Negp2: 1

b.e. (Ryd): 1.9804519

rv. prtge.: 1.0000000

Energy and Temperature Table

INDEX	output energy	output temp.
1	1.0180e+00	3.6100e+05
2	1.2718e+00	7.2200e+05
3	1.5584e+00	1.0850e+06
4	2.0120e+00	3.6100e+06
5	2.5220e+00	7.2200e+06

Energy units: X-param. Temp. units: K.

Edit Table

default X values

default Te values

○ Eff. Pot. Born

○ Impact Param.

○ Slater Pot. ○ Nagy Pot.

○ Internal Wave fns. ○ External Wave fns.

○ Energy Search. ○ Alpha Search

amax: 20.00000

Screening Configuration

INDEX	N	L	IQ	alf1	alf2
1	1	0	2	1.0000e+00	1.0000e+00
2					
3					
4					
5					

Edit Table

edit the processing options data and press done to proceed

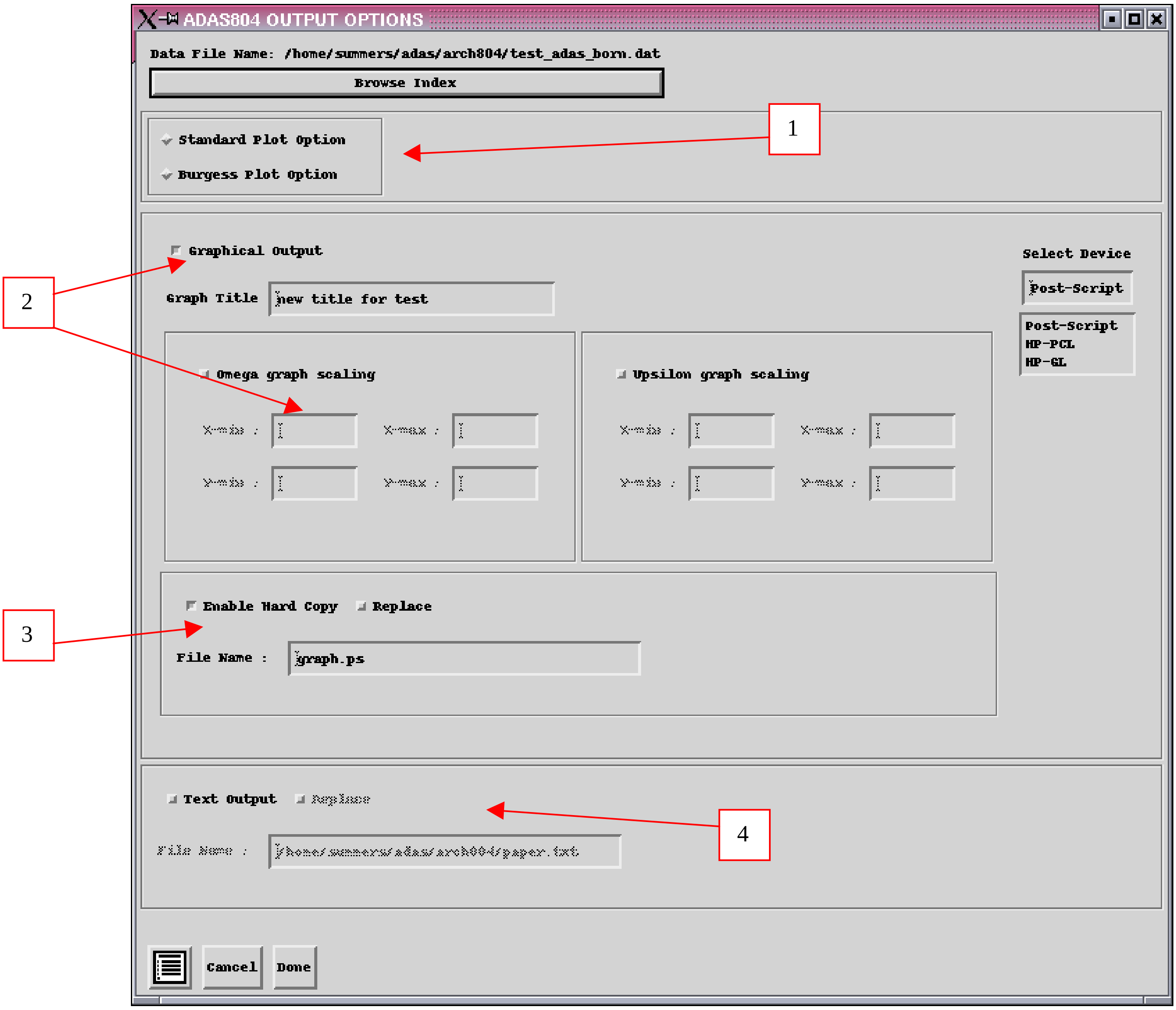
cancel done

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

1. There is a choice of method for examination and display of the results data. Click either the *Standard Plot Option* of the *Burgess Plot Option*. The sub-window varies depending on this choice.
2. Graphical display is activated by the *Graphical Output* button. This will cause the graphs 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 to allow separate explicit minima and maxima for the graph axes of the omega and Upsilon plots to be inserted.
3. Hard copy is activated by the *Enable Hard Copy* button . 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.

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

4. 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.



ADAS804 OUTPUT OPTIONS

Data File Name: /home/summers/adas/arch804/test_adas_born.dat

◇ Standard Plot Option
◇ Burgess Plot Option

☐ Graphical Output

Graph Title: new title for test

☐ Omega graph scaling
X-min : X-max :
Y-min : Y-max :

☐ Upsilon graph scaling
X-min : X-max :
Y-min : Y-max :

Select Device: Post-Script
Post-Script
HP-PCL
HP-GL

☐ Enable Hard Copy ☐ Replace

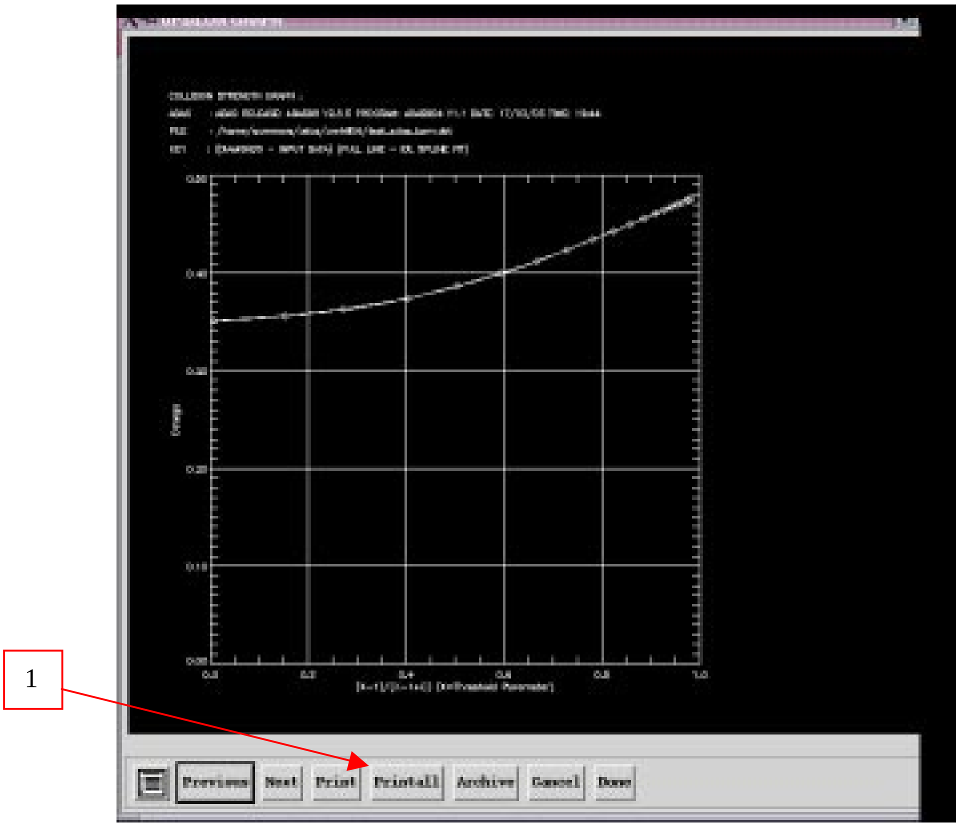
File Name : graph.ps

☐ Text Output ☐ Replace

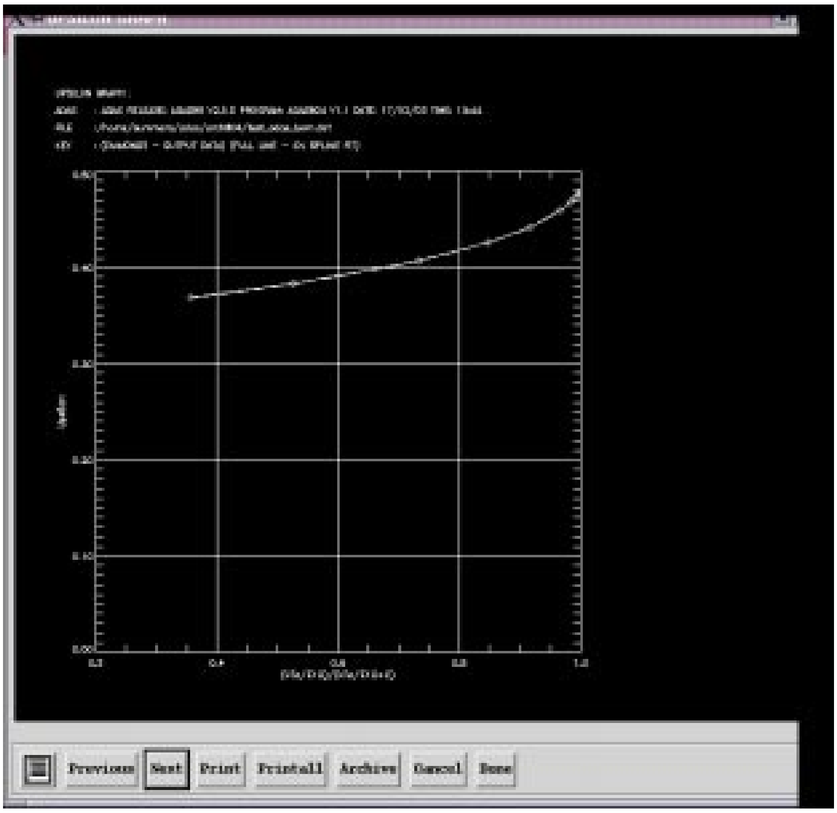
File Name : /home/summers/adas/arch804/paper.txt

The **output graph windows** are shown below

1. The *Previous* and *Next* buttons allow switching between the Upsilon and Omega plots. *Print* and *Printall* send the graphs to the hard copy unit. Click *Archive* to add the complete set of results for the case analyses to the end of the archive selected on input and assign the next sequence number to it.



COLLISION STRENGTH GRAPH :
ADAS : ADAS RELEASED: ADAS99 V2.5.3 PROGRAM: ADAS804 V1.1 DATE: 17/10/00 TIME: 15:44
FILE : /home/summers/adas/[illegible]/test_adas_[illegible].dat
KEY : (DIAMONDS - INPUT DATA) (FULL LINE - 3D SPLINE FIT)



UPSILON GRAPH :
ADAS : ADAS RELEASED: ADAS99 V2.5.3 PROGRAM: ADAS804 V1.1 DATE: 17/10/00 TIME: 15:44
FILE : /home/summers/adas/[illegible]/test_adas_[illegible].dat
KEY : (DIAMONDS - OUTPUT DATA) (FULL LINE - 3D SPLINE FIT)

Notes:

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 automaticaaly 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, $\mathcal{F}\_\mathcal{PEC}$, is introduced (analogous to the emissivity coefficient, $\mathcal{PEC}$) is intrdoduced to describe these envelope features. The associated code, ADAS810, calculates such $\mathcal{F}\_\mathcal{PEC}$ 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

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

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 ≡

‘a’, 11 ≡ ‘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 ≡ ‘1’, 2p ≡ ‘2’, 4f ≡ ‘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 $\{\mathscr{A}^{+z} : z = z_{min},...,z_{max}\}$ of the element $\mathscr{A}$. 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 nl 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 shellcase 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 $\lambda_{IJ}^{(av)} = hc / \left| E_J^{(av)} - E_I^{(av)} \right|_{E_J^{(av)} < E_I^{(av)}}$. 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 $\mathscr{D}_{min}^{2(av)}$ on the reduced dipole matrix elements, $\left| \left\langle I \| \mathscr{D} \| J \right\rangle \right|^2$ 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 $\mathscr{F}\_\mathscr{PEC}$, is defined on a wavelength interval and is a composite feature arising from very many lines from a single ionisation stage. The $\mathscr{F}\_\mathscr{PEC}$ 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 ($\mathscr{PEC}$ 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 $\mathscr{F}\_\mathscr{PEC}$ calculations – see ADAS810 for more details.

Program steps:

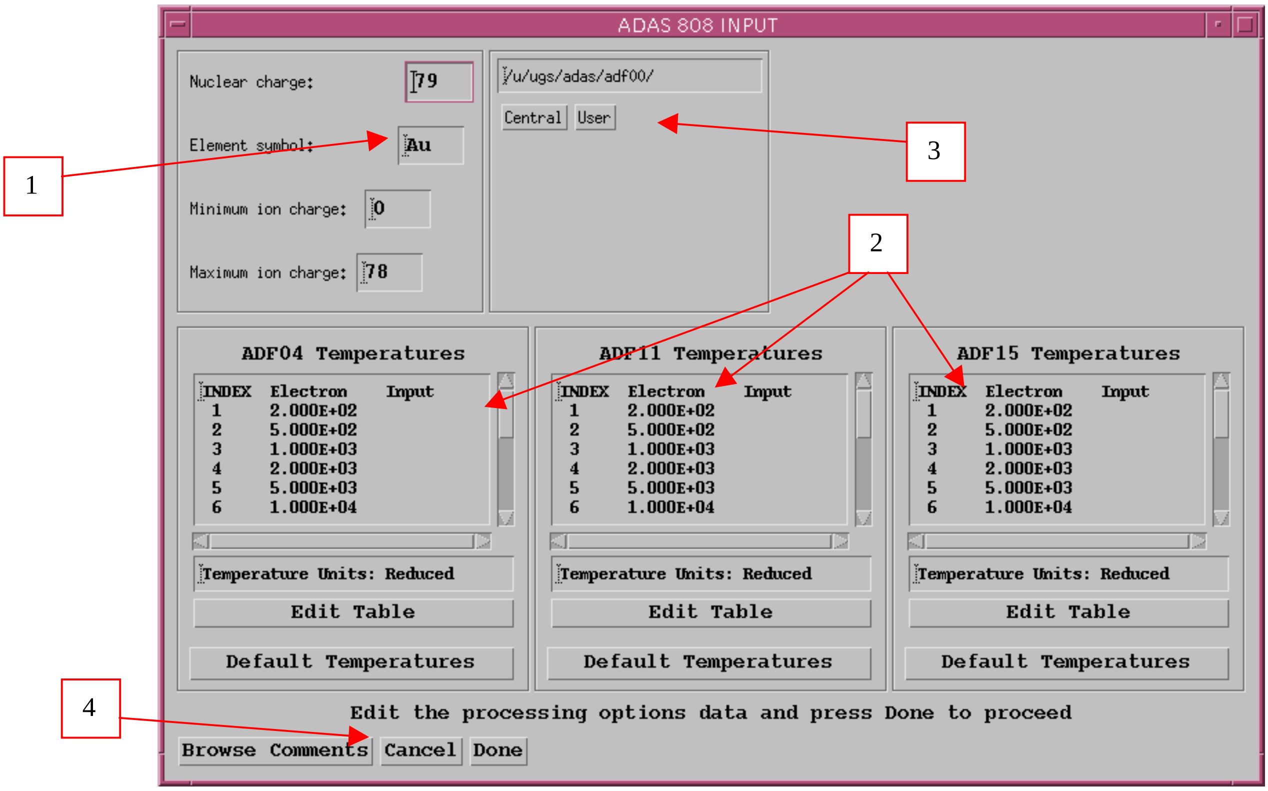
Interactive parameter comments:

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/* .



Nuclear charge: 79

Element symbol: Au

Minimum ion charge: 0

Maximum ion charge: 78

/u/ugs/adas/adf00/

ADF04 Temperatures

INDEX	Electron	Input
1	2.000E+02	
2	5.000E+02	
3	1.000E+03	
4	2.000E+03	
5	5.000E+03	
6	1.000E+04	

Temperature Units: Reduced

ADF11 Temperatures

INDEX	Electron	Input
1	2.000E+02	
2	5.000E+02	
3	1.000E+03	
4	2.000E+03	
5	5.000E+03	
6	1.000E+04	

Temperature Units: Reduced

ADF15 Temperatures

INDEX	Electron	Input
1	2.000E+02	
2	5.000E+02	
3	1.000E+03	
4	2.000E+03	
5	5.000E+03	
6	1.000E+04	

Temperature Units: Reduced

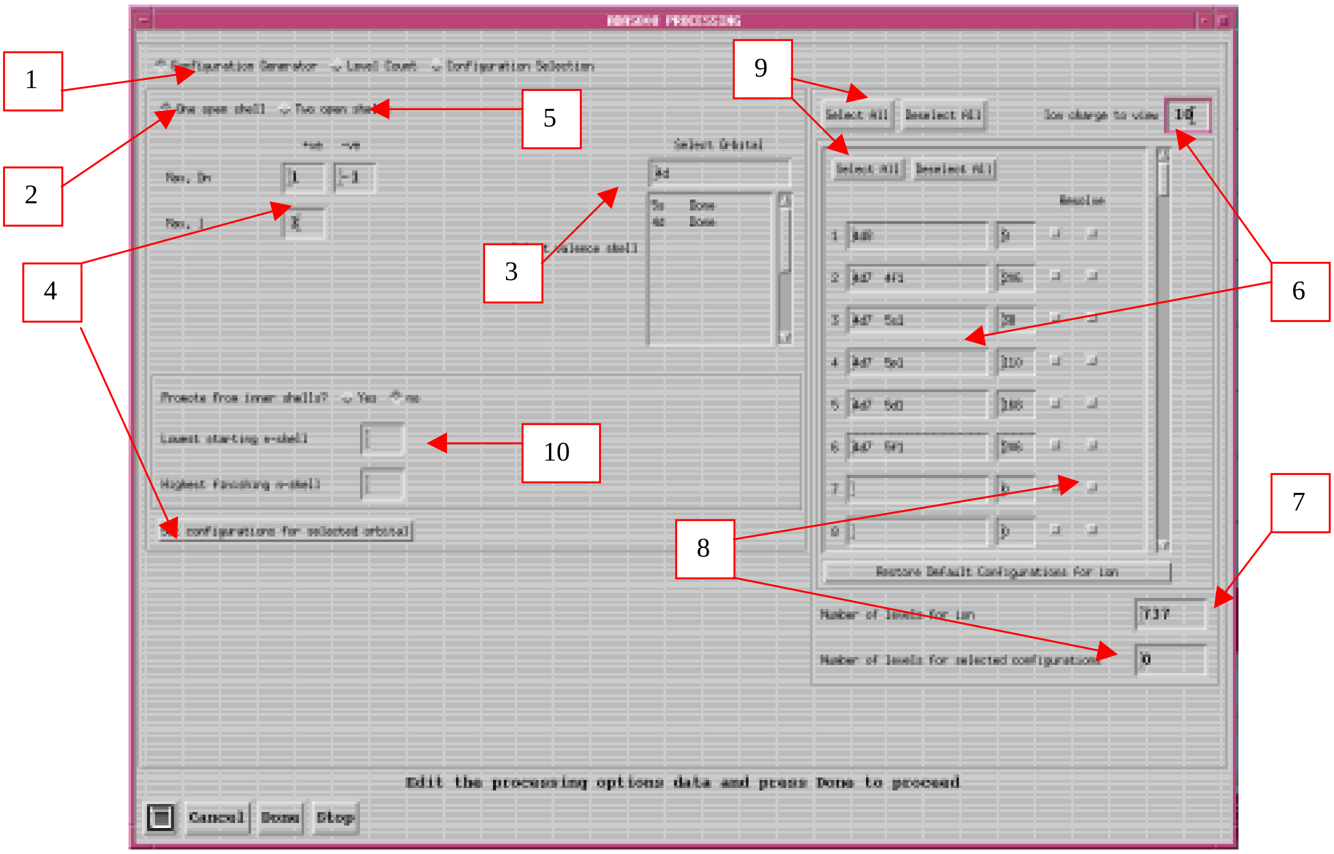
Edit the processing options data and press Done to proceed

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.


ADAS208 PROCESSING
1
2
3
4
5
6
7
8
9
10
○ Configuration Generator
○ Level Count
○ Configuration Selection
○ One open shell
○ Two open shell
Select Orbital
Select valence shell
Promote from inner shells? ○ Yes ○ no
Lowest starting n-shell
Highest finishing n-shell
Set configurations for selected orbital
Select All
Deselect All
Select All
Deselect All
Resolve
Restore Default Configurations for ion
Edit the processing options data and press Done to proceed
Cancel
Done
Stop

	+ve	-ve
Max. Dn	1	-1
Max. l	2	

4d

5s	Done
4d	Done

Ion charge to view 10

			Resolve
1	4d8	9	□ □
2	4d7 4f1	296	□ □
3	4d7 5s1	38	□ □
4	4d7 5p1	110	□ □
5	4d7 5d1	180	□ □
6	4d7 5f1	296	□ □
7		0	□ □
8		0	□ □

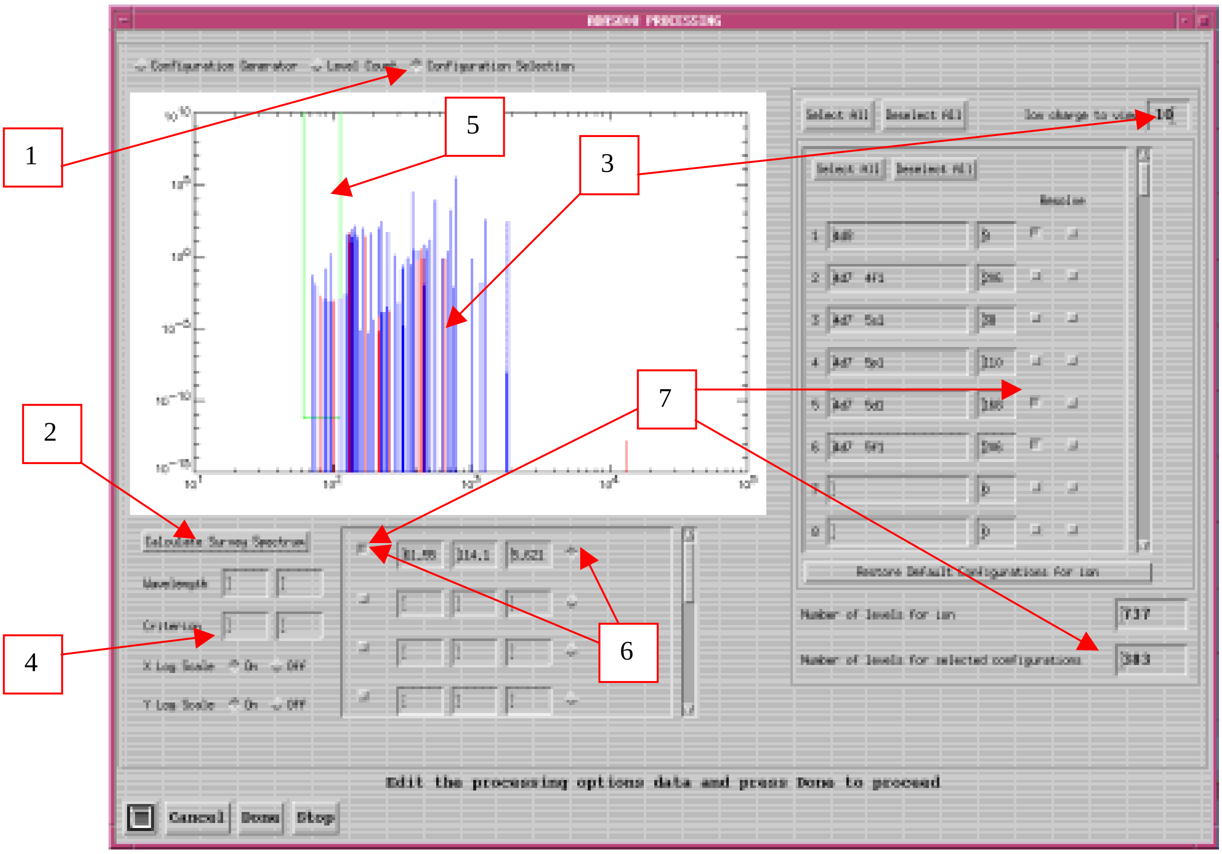
Number of levels for ion 737

Number of levels for selected configurations 0

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. **In the present ‘beta’ version, this button is omitted**

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 a stick spectrum of the various transition arrays.



Edit the processing options data and press Done to proceed

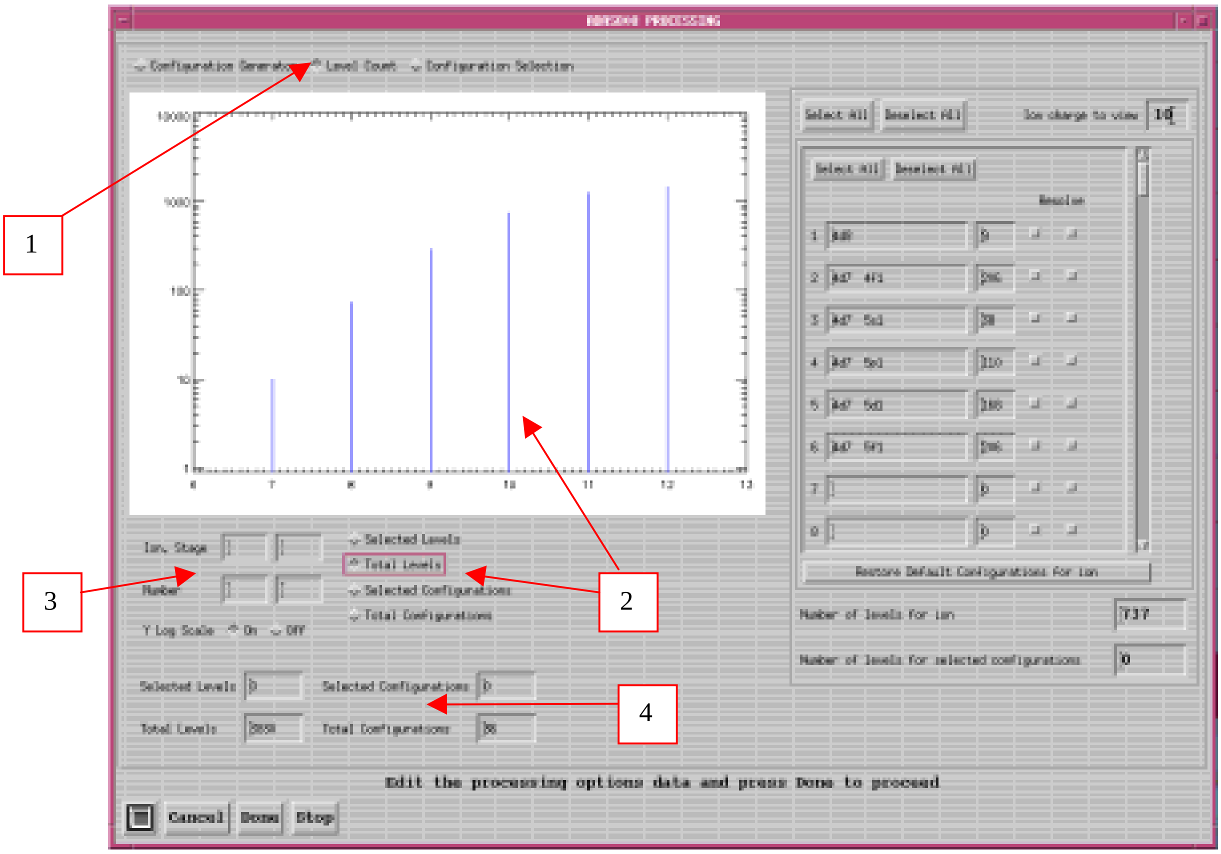
2. Clicking the *Calculate Survey Spectrum* button spawns the calculation of the first stage of the Cowan code to obtain the necessary parameters. The calculation may take a few minutes, but then all information is available the stick plot is displayed. Any further selections operate rapidly.
3. The 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, ($\lambda_{min}, \lambda_{max}, \mathcal{D}^2_{min}$) 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



Ion charge to view: 10

1	4d8	9	□ □
2	4d7 4f1	296	□ □
3	4d7 5s1	38	□ □
4	4d7 5p1	110	□ □
5	4d7 5d1	180	□ □
6	4d7 5f1	296	□ □
7		0	□ □
8		0	□ □

Number of levels for ion: 737

Number of levels for selected configurations: 0

Ion. Stage: 1 1

Number: 1 1

Y Log Scale ● On ○ Off

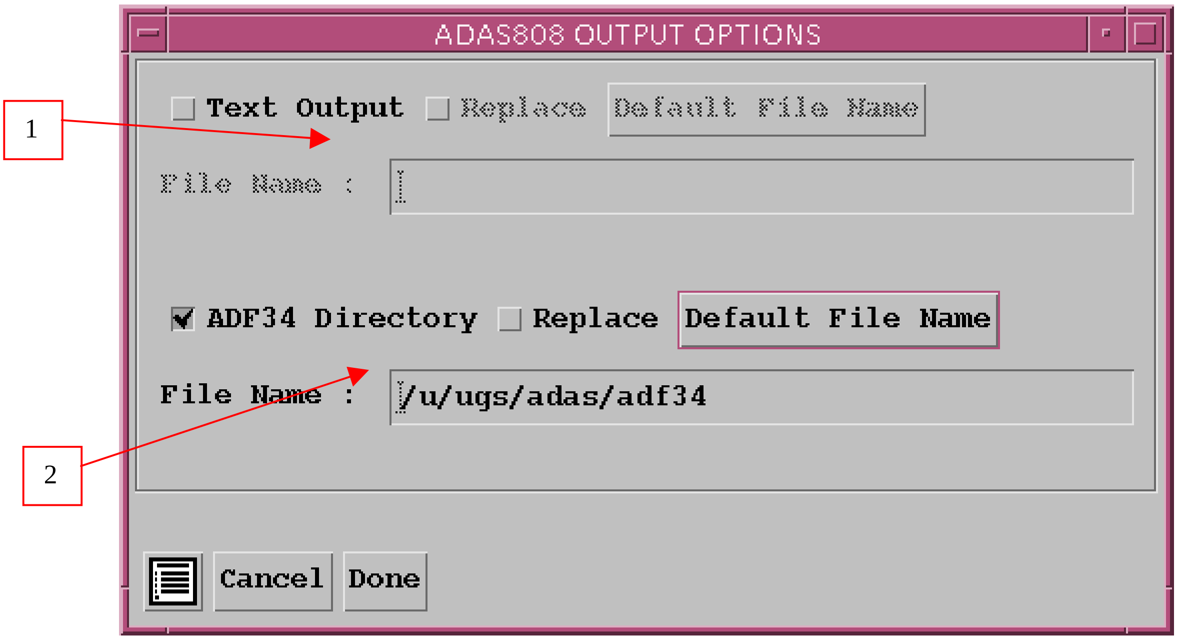
○ Selected Levels
● Total Levels
○ Selected Configurations
○ Total Configurations

Selected Levels: 0
Selected Configurations: 0
Total Levels: 2859
Total Configurations: 38

Edit the processing options data and press Done to proceed

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.



ADAS808 OUTPUT OPTIONS

□ Text Output □ Replace Default File Name

File Name :

☑ ADF34 Directory □ Replace Default File Name

File Name : /u/ugs/adas/adf34

Cancel Done

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:

ADAS809: Non-Maxwellian modelling - change adf04 file type

The program converts an ADF04 – type 1 file to a standard ADF04 – type 3 file. That is an ADF04 file with collision strength data is converted to an ADF04 file with Maxwell averaged collision strengths.

Background theory:

The tabulation of the electron impact excitation and ionisation data in an ADF04 – type 1 file is of collision strength Ω versus threshold parameter X. $X = \varepsilon_i / \Delta E_{ij}$ where ΔE_{ij} is the energy of the transition $i \rightarrow j$ and ε_i is the incident electron energy with the target in the lower energy state i. At the finest energy resolution, collision strengths display detailed resonance structure. It is assumed that the tabulated collisions strengths in the ADF04 – type 1 file are smoothly varying, that is they have been subject to some averaging over resonant structure. It is evident that if the 'width' of the averaging interval above is $\Delta E_{res-avge}$, then the generation of Maxwell averaged collision strengths at temperature T_e is meaningful only if $kT_e >> \Delta E_{res-avge}$. The numerical quadrature procedure takes account of dipole, non-dipole and spin change forms for excitation. The behaviours for transition $i \rightarrow j$ are as

$$\begin{aligned} &\textit{dipole}: && \Omega_{ij} \approx F_3 S_{ij} \log(X + F_2) \\ &\textit{non-dipole}: && \Omega_{ij} \approx F_3 + F_2 / X \qquad\qquad 9.9.1 \\ &\textit{spin change}: && \Omega_{ij} \approx F_3 / (X + F_2)^2 \end{aligned}$$

where F_2 and F_3 are constants. In the dipole case, asymptotically $F_3 = 4/3$. S_{ij} is the *line strength* for the transition. For ionisation, the dipole form with $F_3 S_{ij}$ replaced by the single constant F_3' is appropriate. For electron impact excitation of ions, the collision strength tends to a finite value at threshold. In contrast, for neutral atom excitation and ionisation, the collision strength tends to zero at theshold, with the threshold behaviour $\Omega \sim aX^{\alpha}$. Usually $\alpha = 1/2$ for neutral atom excitation and $\alpha \sim 1$ for ionisation of both atoms and ions.

For the tabulation $\{(X_k, \Omega_k) : k = 1,...,n\}$, the quadrature

$$\Upsilon_{ij} = \int_0^{\infty} \Omega_{ij}(\varepsilon_j) \exp(-\varepsilon_j / kT_e) d(\varepsilon_j / kT_e) \qquad 9.9.2$$

is expressed as

$$\Upsilon_{ij} = (\Delta E_{ij} / kT_e) exp(\Delta E_{ij} / kT_e)$$

$$\int_1^{\infty} \Omega_{ij}(X) exp[-X(\Delta E_{ij} / kT_e))] dX \qquad 9.9.2$$

and the integral divided into the ranges $\int_1^{X_1}$, $\int_{X_1}^{X_n}$ and $\int_{X_n}^{\infty}$. The asymptotic behaviours extrapolating from the first and last two tabular points are used in the evaluation of the first and last integrals respectively. The second integral is evaluated piece-wise in each tabular interval with the integrand locally fitted to a quadratic in either a linear scale (ie. $\Omega = c_1 + c_2 X + c_3 X^2$) or logarithmic scale picture (ie. $\ln\Omega = c_1 + c_2 \ln X + c_3 \ln X^2$).

Quadrature precision is checked from the exact integrals of the approximate forms, namely,

$$\begin{aligned} &dipole: && \Upsilon_{ij} \approx F_3 S_{ij} [ln(1+F_2) + EEI((1+F_2)\Delta E_{ij} / kT_e)] \\ &non-dipole: && \Upsilon_{ij} \approx F_3 + F_2(\Delta E_{ij} / kT_e) EEI(\Delta E_{ij} / kT_e) \qquad 9. \\ &spin\ change: && \Upsilon_{ij} \approx \frac{F_3(\Delta E_{ij} / kT_e)}{1+F_2} EE2((1+F_2)\Delta E_{ij} / kT_e) \end{aligned}$$

9.3

where $EEI(x) = \exp(x) E_1(x)$ and $EE2(x) = \exp(x) E_2(x)$ with E_1 and E_2 the first and second exponential integrals. A further verification on the quadratures is from the exact integrals for $\Omega =$ constant, $\Omega = X - 1$ and $\Omega = (X-1)^2$ which are exact for the quadratic fit, linear scale option.

The program has a capability for comparison and display. In addition to the input ADF04 – type 1 file for conversion, it can accept a second ADF04 – type 3 file. The temperature set for output is copied from the latter reference file. Additionally, the collision data for a selected single transition may be graphed along with the corresponding data from the reference file if it exists. The usual display and output routing facilities are provided.

Program steps:

Interactive parameter comments:

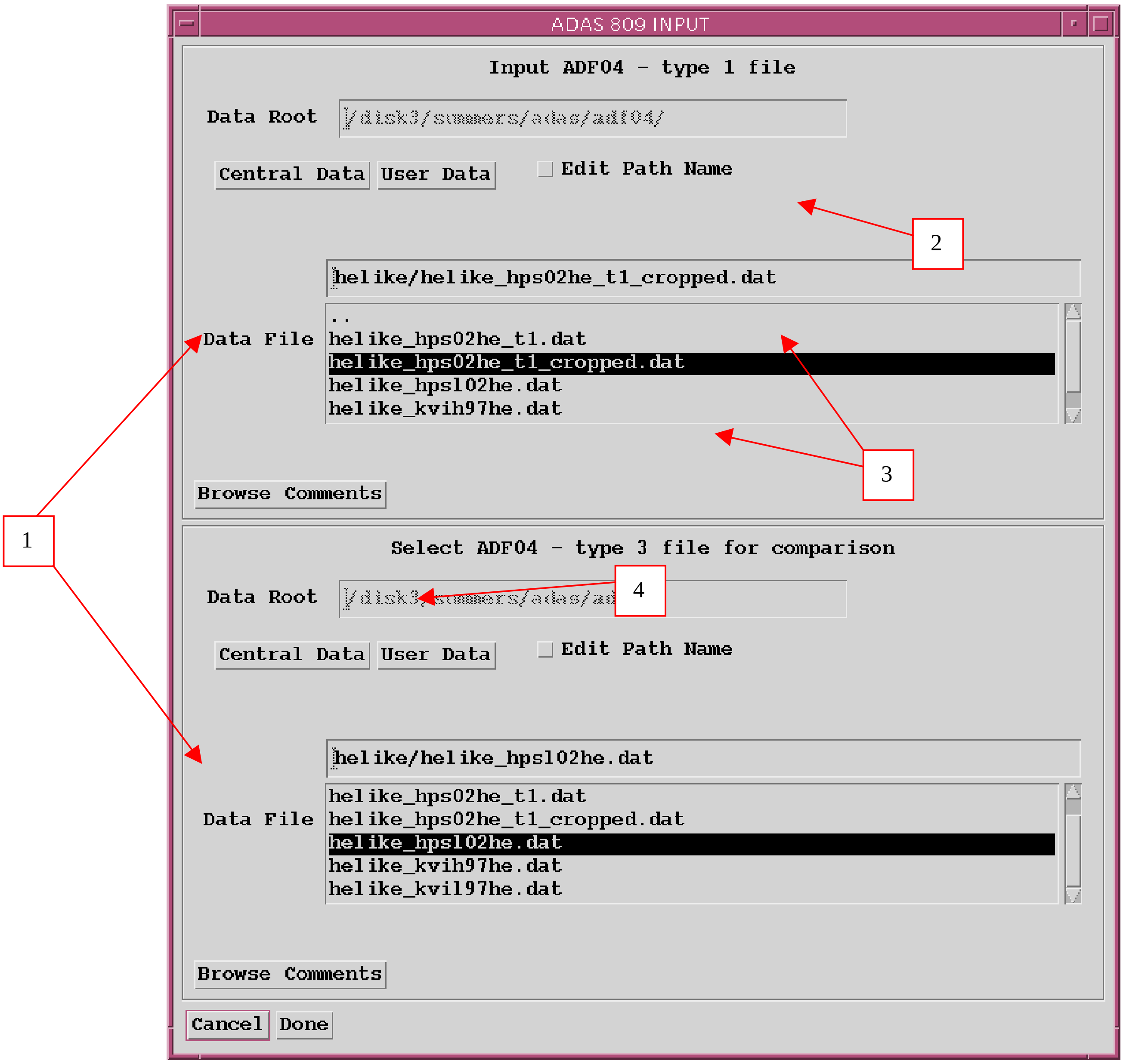
Remember to ensure you have a defaults directory allocated. This should have the pathway

/..../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. 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). Initiate ADAS, move to the series 2 menu and click on the first button to activate ADAS201.

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

1. Selection of two adf04 files is permitted. The first selected in the upper sub-window is of *adf04 – type1* and is mandatory. The second optional file, selected in the lower sub-window is of adf04-type3. It provides a temperature grid for the conversion. Selection of the *adf04* files follows the standard ADAS.
2. Data root shows the full pathway to the appropriate *adf04* data subdirectories. 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. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. 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. 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. Datafiles all have the termination *.dat*.
4. Once the *adf04* files are selected, the set of buttons at the bottom of the main window become active. Clicking on the *Browse Comments* button displays the comment line information stored with the *adf04* 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.



Data Root: /disk3/summers/adas/adf04/

Data File: helike/helike_hps02he_t1_cropped.dat

```
..
helike_hps02he_t1.dat
helike_hps02he_t1_cropped.dat
helike_hpsl02he.dat
helike_kvih97he.dat
```

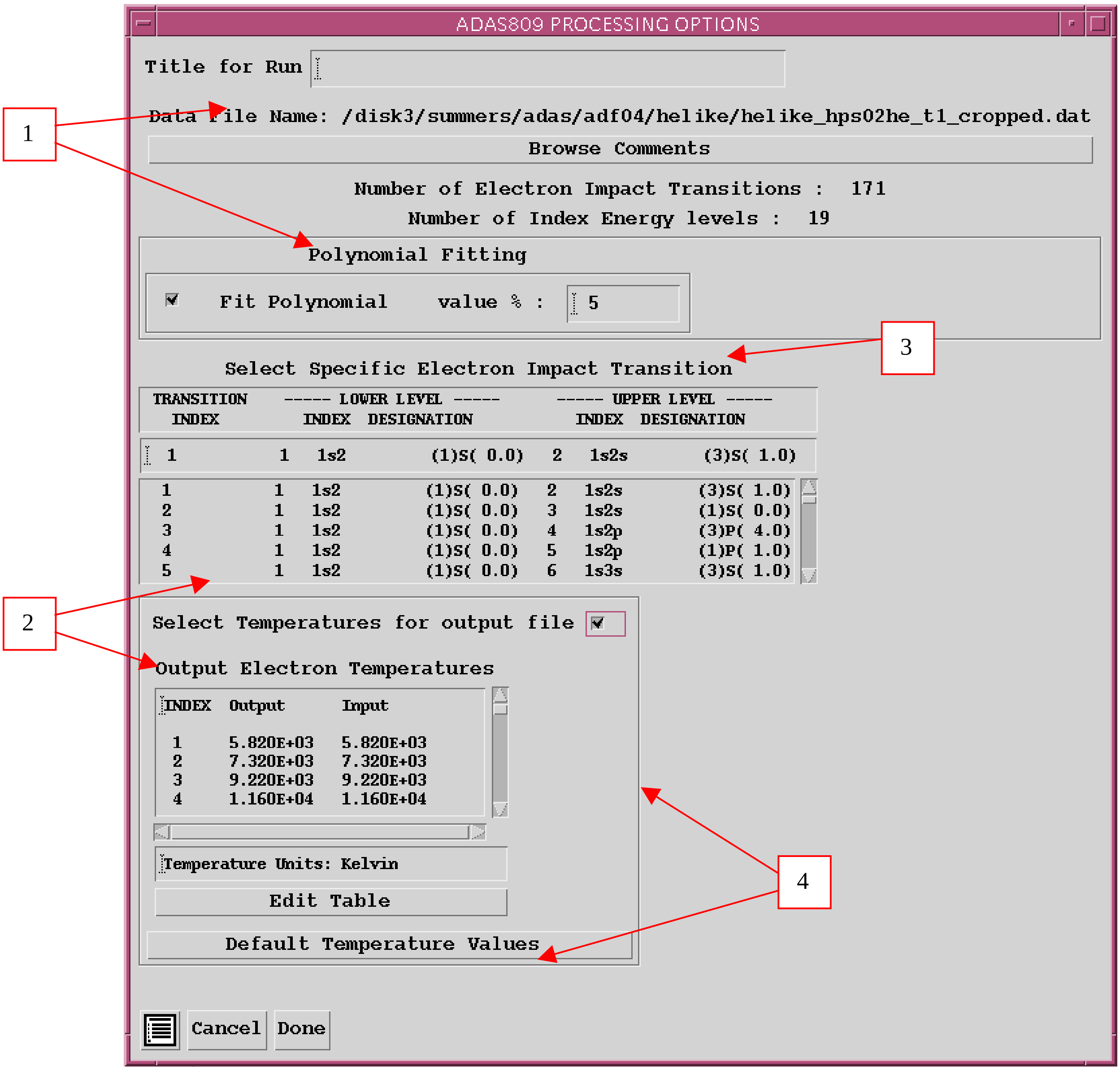
Data Root: /disk3/summers/adas/ad

Data File: helike/helike_hpsl02he.dat

```
helike_hps02he_t1.dat
helike_hps02he_t1_cropped.dat
helike_hpsl02he.dat
helike_kvih97he.dat
helike_kvil97he.dat
```

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

1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists. A summary of the number of electronic transitions and energy levels is also given.
2. Transitions for which electron impact excitation data are available in the data set are displayed in the line list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a line to select it. The selected transition appears in the selection window just above the line list display window. This single transition will displayed.
3. The output rate coefficient for the selected transition may be fitted with a polynomial. This is as a function of temperature. Clicking the *Fit Polynomial* button activates this. The accuracy of the fitting required may be specified in the editable box. The value in the box is editable only if the *Fit Polynomial* button is active.



Title for Run

Data File Name: /disk3/summers/adas/adf04/helike/helike_hps02he_t1_cropped.dat

Number of Electron Impact Transitions : 171

Number of Index Energy levels : 19

Polynomial Fitting

☑ Fit Polynomial   value % : 5

Select Specific Electron Impact Transition

TRANSITION INDEX	----- LOWER LEVEL ----- INDEX	DESIGNATION		----- UPPER LEVEL ----- INDEX	DESIGNATION	
1	1	1s2	(1)S(0.0)	2	1s2s	(3)S(1.0)
1	1	1s2	(1)S(0.0)	2	1s2s	(3)S(1.0)
2	1	1s2	(1)S(0.0)	3	1s2s	(1)S(0.0)
3	1	1s2	(1)S(0.0)	4	1s2p	(3)P(4.0)
4	1	1s2	(1)S(0.0)	5	1s2p	(1)P(1.0)
5	1	1s2	(1)S(0.0)	6	1s3s	(3)S(1.0)

Select Temperatures for output file ☑

Output Electron Temperatures

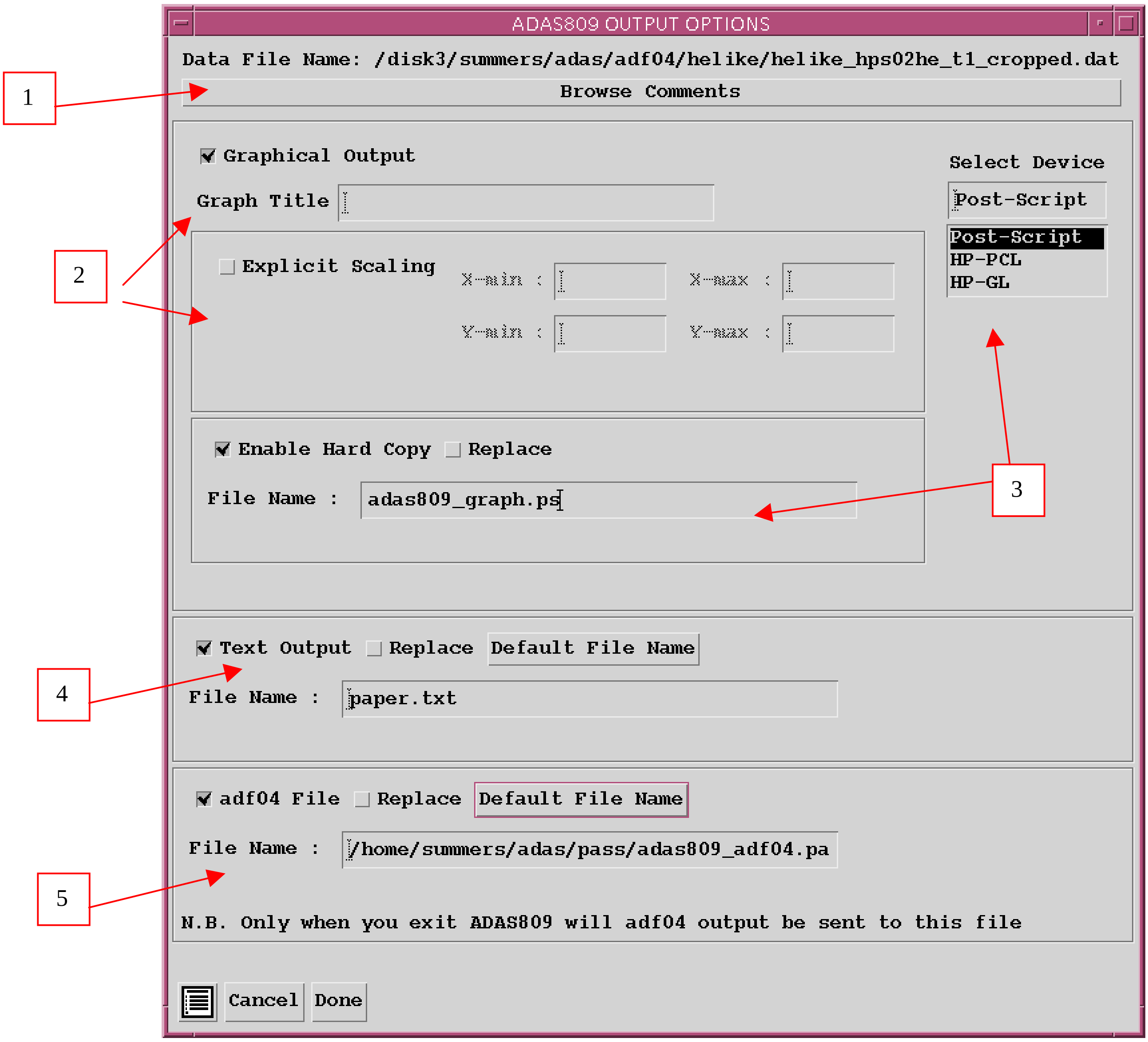
INDEX	Output	Input
1	5.820E+03	5.820E+03
2	7.320E+03	7.320E+03
3	9.220E+03	9.220E+03
4	1.160E+04	1.160E+04

Temperature Units: Kelvin

4. To obtain an output *adf04-type3* file output temperatures must be selected. If a comparative *adf04-type3* file was selected, the Input temperatures are taken from that file. Otherwise temperatures from the Defaults file are used. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures
5. The Temperature Values are editable. Click on the *Edit Table* button if you wish to change the values. A ‘drop-down’ window, the ADAS Table Editor window: It follows the same pattern of operation as described in bulletin.

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

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.



ADAS809 OUTPUT OPTIONS

Data File Name: /disk3/summers/adas/adf04/helike/helike_hps02he_t1_cropped.dat

☑ Graphical Output

Graph Title :

□ Explicit Scaling

X-min : X-max : Y-min : Y-max :

☑ Enable Hard Copy □ Replace

File Name : adas809_graph.ps

Select Device: Post-Script

☑ Text Output □ Replace

File Name : paper.txt

☑ adf04 File □ Replace

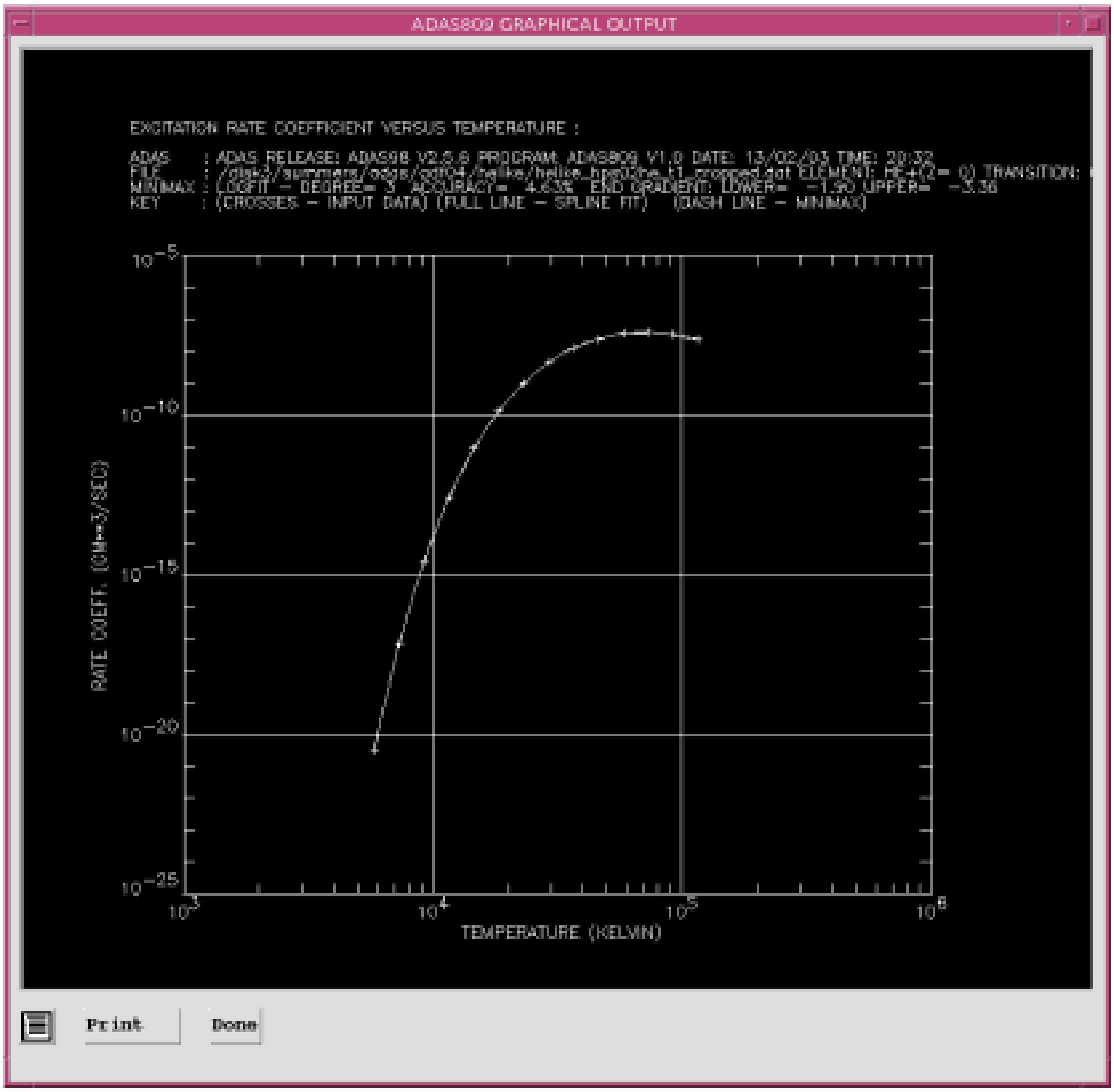
File Name : /home/summers/adas/pass/adas809_adf04.pa

N.B. Only when you exit ADAS809 will adf04 output be sent to this file

2. Graphical display is activated by the *Graphical Output* button. 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 to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.
3. Hard copy is activated by the *Enable Hard Copy* button. 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. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
4. 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.
5. The *adf04 File* button activates writing of the full configured adf04-type 3 dataset to an output file. The file name may be entered in the editable File name box. The default file name '…/pass/adas809_adf04.pass' 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.

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



```
EXCITATION RATE COEFFICIENT VERSUS TEMPERATURE :

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS809 V1.0 DATE: 13/02/03 TIME: 20:32
FILE    : /disk2/summers/adas/adf04/helike/helike_hpg02he_t1_cropped.dat ELEMENT: HE+(Z= 0) TRANSITION:
MINIMAX : (LOGFIT - DEGREE= 3  ACCURACY=  4.63%  END GRADIENT: LOWER=  -1.90 UPPER=  -3.36
KEY     : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT)   (DASH LINE - MINIMAX)
```

ADAS810: Generate envelope feature photon emissivity coefficient

The program calculates envelope feature emissivities of type ADF40 for an ion of a complex element. The program is a foreground, interactive, version of the mass production, parallised background code ADAS810_offline. The interactive version is designed for restricted sample testing and result display prior to large scale excution. It requires the same driver data file types as the offline version, but allows the user to modify some driver parameters. The interactive code can initiate the background code although the usual practice is for launch of ADAS810_offline from the command line, independently of IDL-ADAS, via a PERL script [see **NOTES:** below]

Background theory:

An envelope feature photon emissivity coefficient, denoted by $\mathcal{F}\_\mathcal{PEC}$, is defined on a wavelength interval and is a composite feature arising from very many lines from a single ionisation stage. The $\mathcal{F}\_\mathcal{PEC}$ 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 ($\mathcal{PEC}$ s). Following Chap 3.8, the emissivity of an individual line is specified as

$$\varepsilon_{j\to k} = A_{j\to k}\Big(\sum_{\sigma=1}^{M}\mathcal{F}_{j\sigma}^{(exc)}N_e N_\sigma + \sum_{\upsilon'=1}^{M_{z+1}}\mathcal{F}_{j\upsilon'}^{(rec)}N_e N_{\upsilon'}^{+}\Big). \qquad 9.10.1$$

This allows specification of the *excitation* photon emissivity coefficient

$$\mathcal{PEC}_{\sigma,j\to k}^{(exc)} = A_{j\to k}\mathcal{F}_{j\sigma}^{(exc)} \qquad 9.10.2$$

and the *recombination* photon emissivity coefficient

$$\mathcal{PEC}_{\upsilon',j\to k}^{(rec)} = A_{j\to k}\mathcal{F}_{j\upsilon'}^{(rec)}. \qquad 9.10.3$$

There are similar coefficients, namely, the *charge exchange* photon emissivity coefficient and the *ionisation* photon emissivity coefficient, which are of less relevance here. Each of these coefficients is associated with a particular metastable σ or υ' of the X^{+z}, or X^{+z+1} ions respectively.

Consider a spectral interval, $[\lambda_0,\lambda_1]$, subdivided into N_{pix} intervals as $\{\Delta\lambda_i^{[0,1]} \equiv [\lambda_0 + i(\lambda_1-\lambda_0)/N_{pix}, \lambda_0 + (i+1)(\lambda_1-\lambda_0)/N_{pix}] : i = 0,..,N_{pix}-1\}$Also suppose that the $j \to k$ spectrum line has a normalised emission profile $\varphi_{j\to k}(\lambda)$. In general, such a profile is a convolution of Doppler and instrumental functions. Then the envelope feature photon emissivity coefficient vector is defined as

$$\mathcal{F}\_\mathcal{PEC}_{\sigma,i}^{(exc)[0,1]} = \sum_{\substack{j,k\\ \lambda_{j\to k}\in[0,1]}} \mathcal{PEC}_{\sigma,j\to k}^{(exc)}\int_{\lambda_i}^{\lambda_{i+1}}\varphi_{j\to k}(\lambda)d\lambda \qquad 9.10.4$$

$\lambda_{j\to k}$ is the natural wavelength of the $j \to k$ spectrum line. The default broadening assumed is Doppler with a Maxwellian distribution for the emitting ion at temperature, T_{ion}, equal to the electron temperature, T_e, used in the collisional–radiative modelling of the $\mathcal{PEC}$ s. This consitutes a minimum broadening. The integral in equation 9.10.4 is then expressible in terms of error functions as

$$\begin{aligned}\mathcal{F}\_\mathcal{PEC}_{\sigma,i}^{(exc)[0,1]} = \sum_{\substack{j,k\\ \lambda_{j\to k}\in\Delta\lambda_i^{[0,1]}}} \mathcal{PEC}_{\sigma,j\to k}^{(exc)}\tfrac{1}{2}\{&\operatorname{erfc}((\lambda_i-\lambda_{j\to k})/\sigma) \\ &-\operatorname{erfc}((\lambda_{i+1}-\lambda_{j\to k})/\sigma)\}\end{aligned} \qquad 9.10.5$$

where $\sigma = \lambda_{j\to k}\alpha\left(\dfrac{kT_{ion}}{I_H}\cdot\dfrac{m_p}{m_X}\cdot\dfrac{m_e}{m_p}\right)^{1/2}$ and m_X is the emitting ion mass.

In actual spectral analysis involving complex heavy species, individual strong spectrum lines may be distinguishable from the envelope. It is therefore appropriate to archive a restricted number of the strongest individual $\mathcal{PEC}$ s and these can be identified and ordered as processing for the $\mathcal{F}\_\mathcal{PEC}$ s takes place. Again, while passing through the complete set of radiative transitions for assignment to excitation $\mathcal{F}_\mathcal{PEC}^{(exc)}$s, the line radiative power coefficient for the ion, $P_{LT}^{(z)}$, can be totalled. This total line power coefficient (archived in the data class ADF11, subcategory $\mathcal{PLT}$), which is the part driven by excitation for the ground or metastable levels of the ion, is a more precise estimate that than computed by the code ADAS408 and so is a preferred substitute for that data. For application to actual measurements of total radiation emission, it is normally necessary to calculate $P_{LT}^{(z)}$ as modified by appropriate soft x-ray and /or bolometer filter transmission functions. Such modification can not be done retrospectively on the unfiltered $P_{LT}^{(z)}$. In contrast, the $\mathcal{F}\_\mathcal{PEC}^{(exc)}$ is suited to further processing which can include imposition of spectrometer instrument functions as well as filtering and integration over extended wavelength regions. Such additional operations on $\mathcal{F}\_\mathcal{PEC}$ s are treated as separate from ADAS810 and are handled in a new interrogation code for $\mathcal{F}\_\mathcal{PEC}$ s, ADAS510, complementing ADAS503. Note that preparation of filters is provided by the codes ADAS414 and ADAS415. It is also assumed that this is the route for preparation of higher precision filtered $P_{LT}^{(z)}$ s and requires the initial creation of appropriate $\mathcal{F}\_\mathcal{PEC}$ s via the present ADAS810 code.

In like manner, $\mathcal{PEC}^{(rec)}$ s can be produced, provided the input data (ADF04) supports this. Note that for ease and consistency in modelling, the same spectral intervals apply to both the $\mathcal{F}\_\mathcal{PEC}^{(exc)}$ s and the $\mathcal{PEC}^{(rec)}$ s and to each of the metastable drivers – if more than one. Also, the selection of the strong individual $\mathcal{PEC}$ s is determined from the whole ground excitation driven set and the selected set is then used for all other metastable drivers and for recombination. The rank ordering of individual $\mathcal{PEC}$ s is from the maximum of each $\mathcal{PEC}$ viewed as a tabular function of T_e and N_e.

Note finally that $\mathcal{F}\_\mathcal{PEC}$ s are tabulated as a function of selected wavelength range, wavelength interval bin, T_e and N_e with $T_i = T_e$.

Program steps:

It is noted again that the code is designed to allow single ion testing of $\mathcal{F}\_\mathcal{PEC}$ production. The primary intent is nonetheless mass production and so the interactive code ADAS810 makes use of the driver data sets and file naming conventions of the mass production codes. Thus, as ADAS810 is in essence a variant of the population code ADAS208, as well as direct selection of an ADF04 file, the data set selected on the INPUT screen may be a driver data. The driver files for this application are of format ADF42. The relevant pathway is */…/adas/adf42/iso_nucl/<element>/.* The primary parameter settings for operation of ADAS810 are contained in the driver, which must be copied to the equivalent user area and edited directly to modify operation. The driver structure is shown in the illustration below.

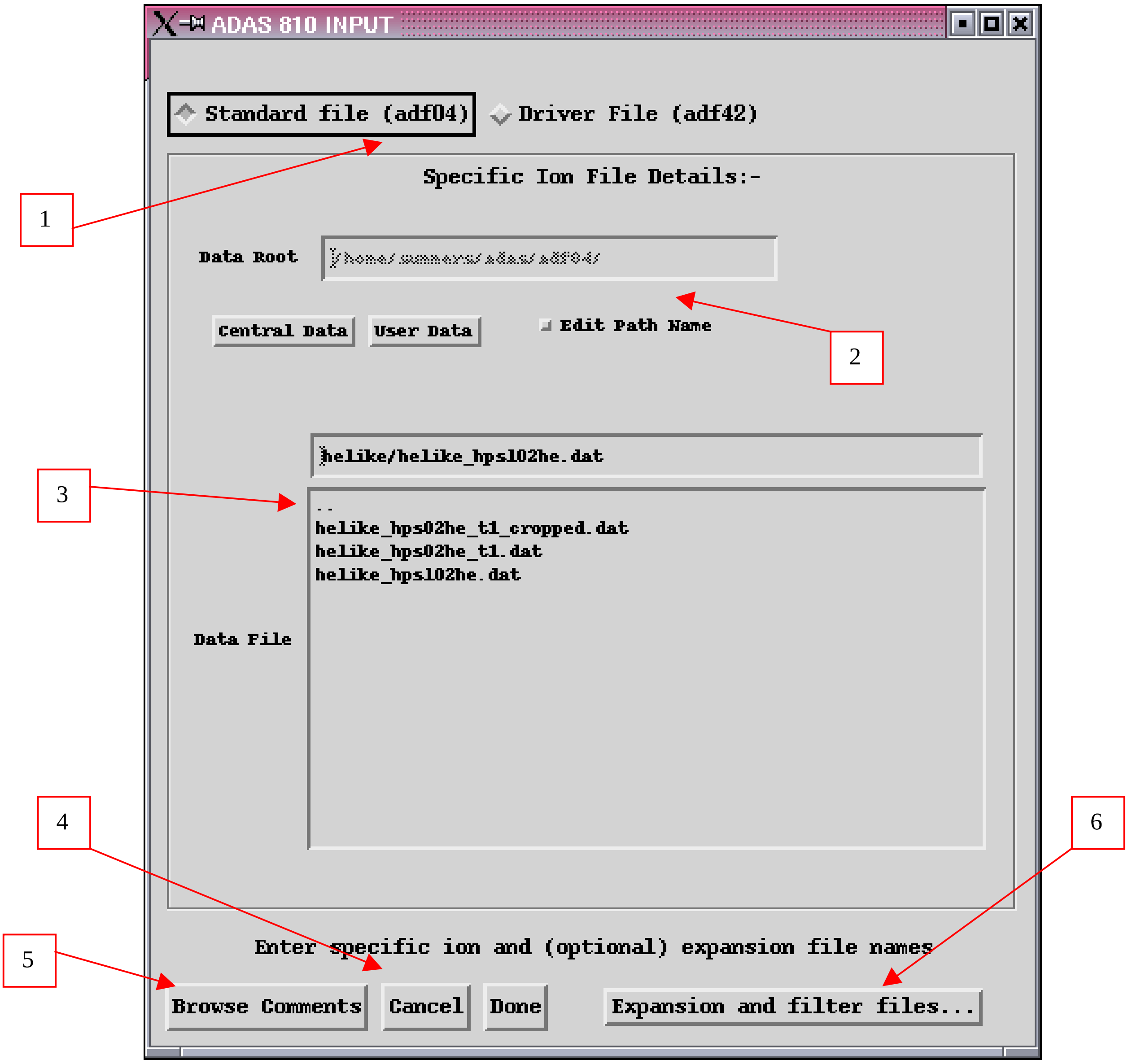
Note the various file pathways (lines 2-4) which include the input ADF04 file and then the output $\mathcal{PLT}$, $\mathcal{PEC}$ and $\mathcal{F}\_\mathcal{PEC}$ files. In interactive operation, ADAS810 allows re-specification of some parameters such as wavelength intervals, temperatures etc. (on the processing screen and of output file routing (on the output screen)) overiding the adf42 driver file. All other parameters are predetermined or set in the driver file. Note the use of namelists where possible in the driver file structure

```
&FILES
   dsn04  = '/home/adas/adas/adf04/adas#6/mom97_ls#c2.dat',
   dsn18  = 'NULL',
   dsn35  = 'NULL',
   dsn15  = 'test_adf15_pec.dat',
   dsn40  = 'test_adf40_fpec.dat',
   dsn11  = 'test_adf11_plt.dat',
   dsn11f = 'test_adf11_plt_filter.dat'
 &END

 &ION
    element = 'C',
    z0      = 6,
    z1      = 2,
    ip      = 386241.0
 &END

 &META
   nmet     = 1,
   imetr(1) = 1
 &END

 &PROCESS
   liosel = .FALSE.,
   lrsel  = .FALSE.,
   lisel  = .FALSE.,
   lnsel  = .FALSE.,
   lpsel  = .FALSE.,
   zeff   = 0.0
 &END

 &OUTPUT
   lmetr   = .FALSE.,
   ltscl   = .FALSE.,
   ldscl   = .FALSE.,
   lbrdi   = .FALSE.,
   numte   = 5,
   numtion = 0,
   numth   = 0,
   numdens = 5,
   numdion = 0,
   numwvl  = 3
 &END

 1.800e+04 4.500e+04 9.000e+04 1.800e+05 4.500e+05

 1.000E+11 1.000E+12 1.000E+13 1.000E+14 1.000E+15

 64 1.500e+00 3.00e+00
 32 1.000e+01 1.00e+02
 32 4.500e+02 8.00e+02
```

Interactive parameter comments:

The **file selection window** is as shown below

5. Two primary files are required, namely an adf04 for the ion whose spectral line and envelope emissivities are required, and a driver file of format adf42. The latter is optional and provides conditions of electron temperature and density, spectral ranges etc. This driver file maintains compatibility of operation of the interactive ADAS810 with the automatic offline mass production codes. Data from the driver fills the editable fields in on the following Processing window. Otherwise they mauts be edited in.
6. Note that each type of data is stored according to its ADAS data format (*adf* number). *adf42* is the appropriate format for use by the program ADAS810. 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.*
7. 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 Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
8. Once a data file is selected, the set of buttons at the bottom of the main window become active.
9. 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. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window.
10. An extra button, *Expansion and filter files,* is present. Click it to pop-up a supplementary file selection window shown below. These supplementary files may be included, if available, to extend the population and emissivity calculation, paralleling the selections available in ADAS208.

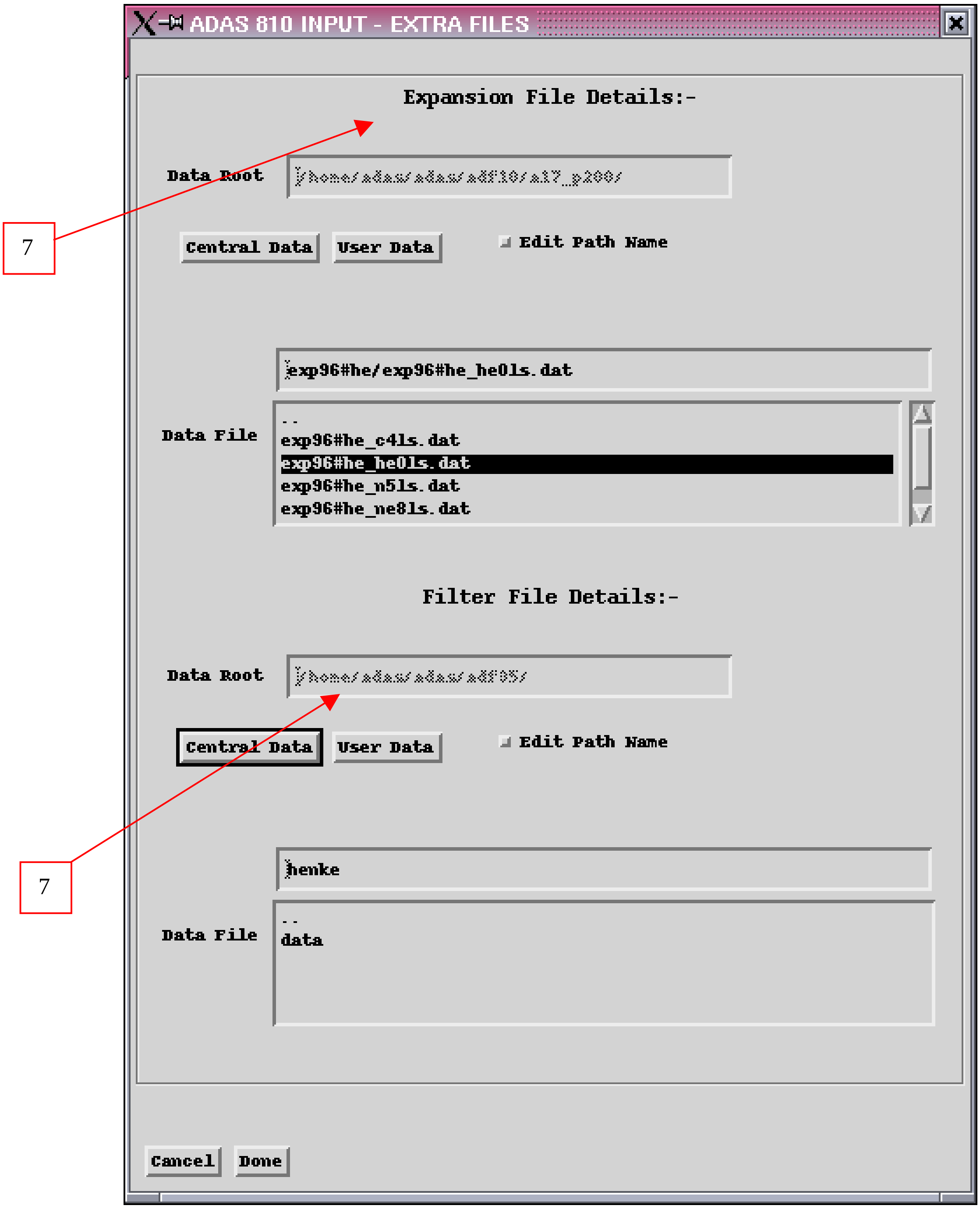


Data Root: /home/summers/adas/adf04/

Data File: helike/helike_hps102he.dat

```
..
helike_hps02he_t1_cropped.dat
helike_hps02he_t1.dat
helike_hps102he.dat
```

11. On the upper sub-window, an expansion file may be selected. This is the same expansion file as used by ADAS208 and is drawn from the cross-referencing file subclass *adf18/a17_p208*.
12. On the lower sub-window, a filter file of format *adf35* may be selected. ADAS810 provides total radiative power and filtered power as well as the line and envelope emisisvities.



Expansion File Details:-

Data Root /home/adas/adas/adf10/a17_p200/

□ Edit Path Name

exp96#he/exp96#he_he0ls.dat

Data File
..
exp96#he_c4ls.dat
exp96#he_he0ls.dat
exp96#he_n5ls.dat
exp96#he_ne8ls.dat

Filter File Details:-

Data Root /home/adas/adas/adf35/

□ Edit Path Name

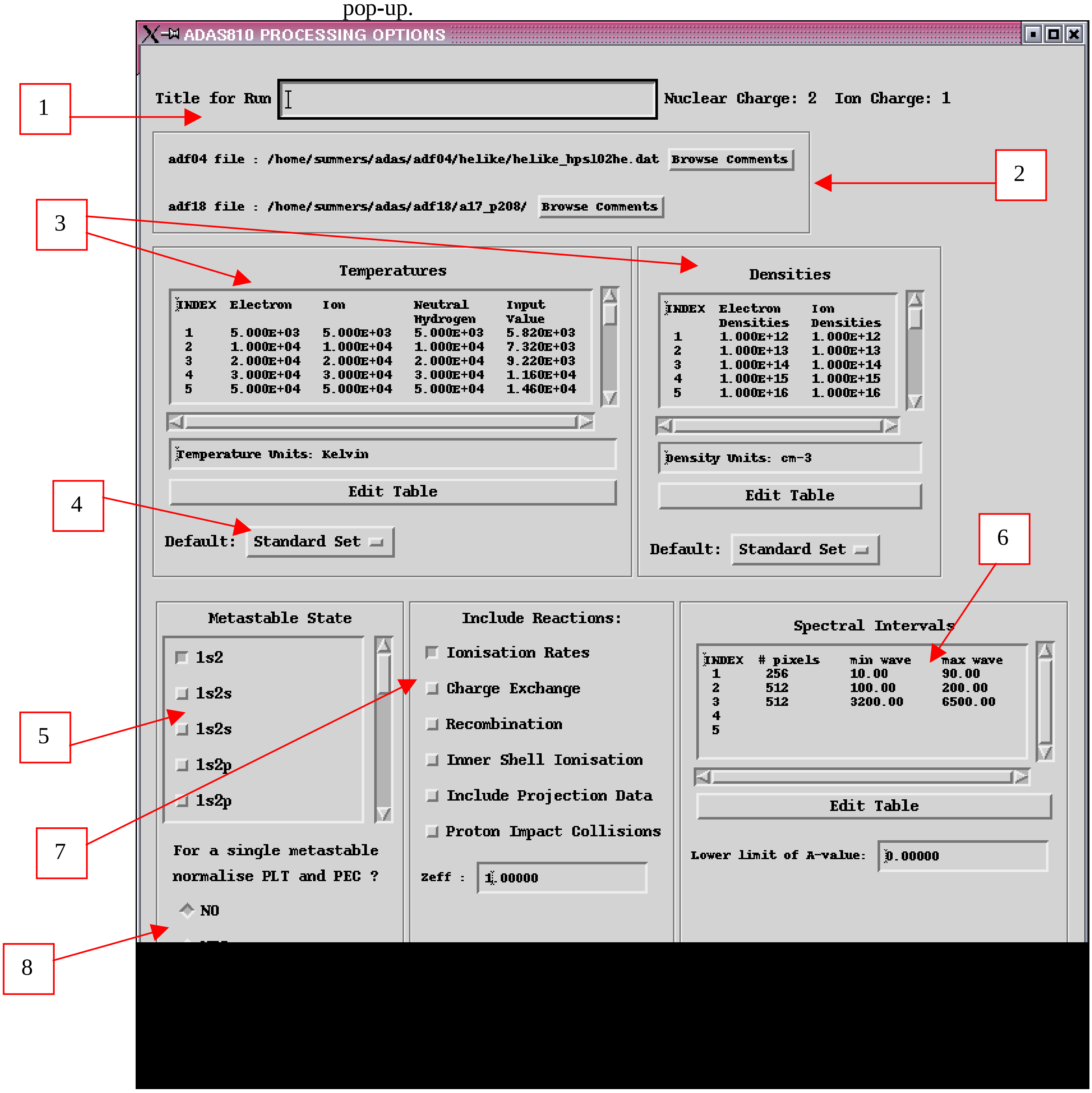
henke

Data File
..
data

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

1. An arbitrary title may be given for the case being processed.
2. For information the full pathways to the datasets being processsed are also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
3. The main inputs follow that those of ADAS208. Your settings of electron temperature, ion temperature and neutral hydrogen temperature are shown in the temperature display window. The temperature values at which the excitation rate coefficients (in fact ‘upsilons’) are stored in the selected adf04 (input) are also shown for information. The program obtains the output from the adf42 driver file if available. A similar pattern is shown in the Density sub-window although there is no ‘Input’ from the adf04 file.

4. Selection of *Default* temperatures is somewhat different from the usual ADAS pattern. A drop-down menu allows choice from a number of favoured sets, such as the GCR Standard set
5. Selection of metastables is done from a scrollable button list rather than a pop-up.



ADAS810 PROCESSING OPTIONS

Title for Run [ ] Nuclear Charge: 2 Ion Charge: 1

adf04 file : /home/summers/adas/adf04/helike/helike_hps102he.dat Browse Comments

adf18 file : /home/summers/adas/adf18/a17_p208/ Browse Comments

Temperatures

INDEX	Electron	Ion	Neutral Hydrogen	Input Value
1	5.000E+03	5.000E+03	5.000E+03	5.820E+03
2	1.000E+04	1.000E+04	1.000E+04	7.320E+03
3	2.000E+04	2.000E+04	2.000E+04	9.220E+03
4	3.000E+04	3.000E+04	3.000E+04	1.160E+04
5	5.000E+04	5.000E+04	5.000E+04	1.460E+04

Temperature Units: Kelvin

Edit Table

Default: Standard Set

Densities

INDEX	Electron Densities	Ion Densities
1	1.000E+12	1.000E+12
2	1.000E+13	1.000E+13
3	1.000E+14	1.000E+14
4	1.000E+15	1.000E+15
5	1.000E+16	1.000E+16

Density Units: cm-3

Edit Table

Default: Standard Set

Metastable State

☑ 1s2
□ 1s2s
□ 1s2s
□ 1s2p
□ 1s2p

For a single metastable normalise PLT and PEC ?

◇ NO

Include Reactions:

☑ Ionisation Rates
□ Charge Exchange
□ Recombination
□ Inner Shell Ionisation
□ Include Projection Data
□ Proton Impact Collisions

zeff : 1.00000

Spectral Intervals

INDEX	# pixels	min wave	max wave
1	256	10.00	90.00
2	512	100.00	200.00
3	512	3200.00	6500.00
4			
5			

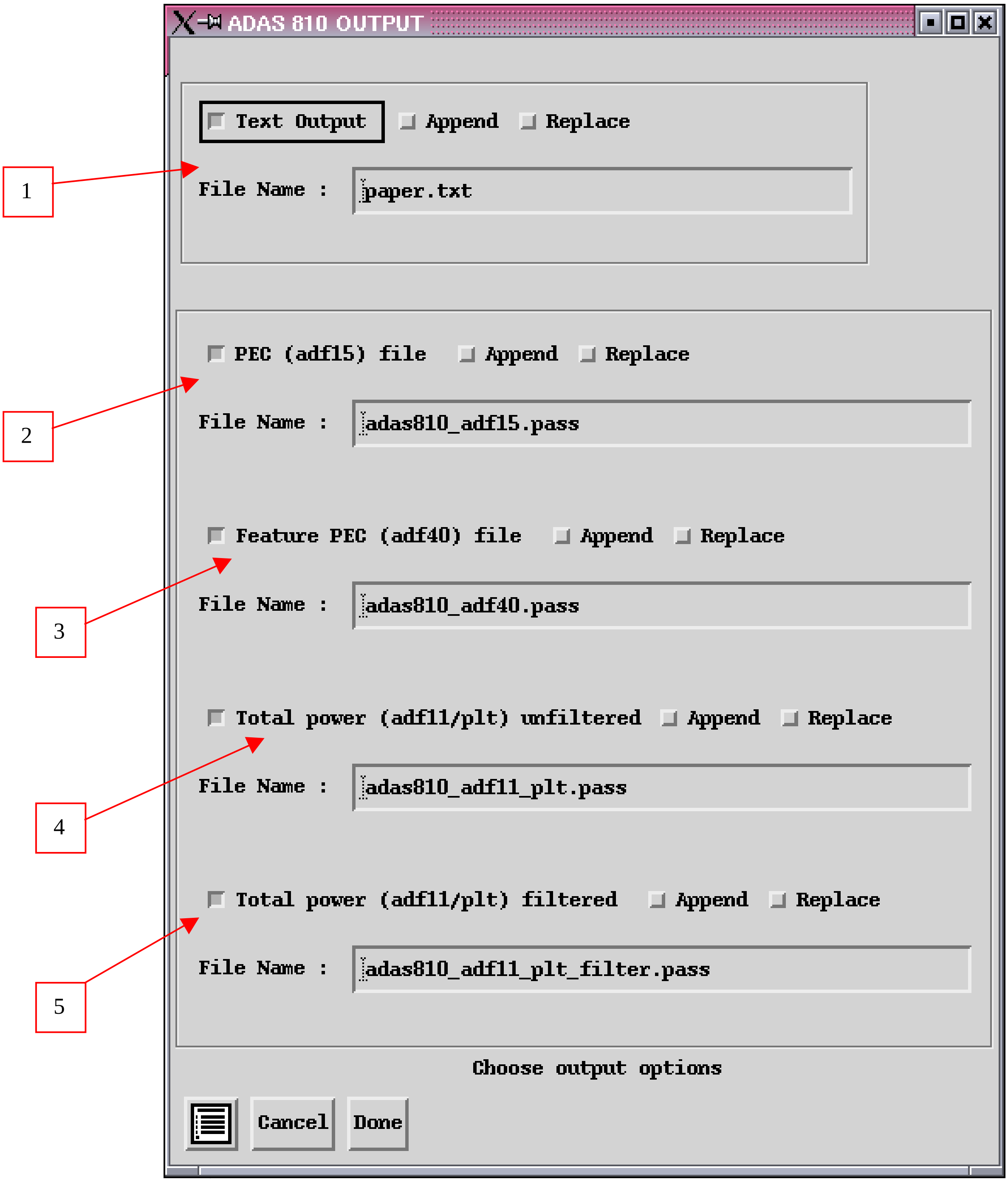
Edit Table

Lower limit of A-value: 0.00000

6. Wavelength ranges and associated pixels are specified in an editable table.
7. The set of control parameters for the calculation follows ADAS208.
8. The Normalisation option should be chosen when there is only a single metastable..

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. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.
2. The *PEC (adf15)* file comprises the set of individual line emissivity coefficients.



□ Text Output □ Append □ Replace

File Name : paper.txt

□ PEC (adf15) file □ Append □ Replace

File Name : adas810_adf15.pass

□ Feature PEC (adf40) file □ Append □ Replace

File Name : adas810_adf40.pass

□ Total power (adf11/plt) unfiltered □ Append □ Replace

File Name : adas810_adf11_plt.pass

□ Total power (adf11/plt) filtered □ Append □ Replace

File Name : adas810_adf11_plt_filter.pass

Choose output options

3. The *Feature PEC (adf40)* file comprises the envelope feature data for each selected wavelength interval and each metastable, tabulated in pixel space as a function of temperature and density .
4. The *Total power (adf11/plt) unfiltered* file comprises the total radiated power in the spectral intervals.
5. The *Total power (adf11/plt) filtered* file comprises the radiated power in the spectral intervals as transmitted by the filter specified in the input filter file – if selected.

Notes: