ADAS216: Population and emissivity error analysis

The program allows examination of the sensitivity of populations of excited levels of ions in a plasma to uncertainty in the fundamental collisional rate coefficient and A-value from the ADF04 file upon which the calculation is based. The ADF04 file accessed includes a formatted error specification comment block for the data set. This enables the code to conduct multiple population calculations to explore the influence of the individual errors or to evaluate a statistical cumulative error based on Monte Carlo sampling. If the ADF04 file lacks and error specification block, the program assists in its creation.

Background theory:

In collisional-radiative modelling away from the coronal picture, simple connection between fundamental process and derived population or emissivity is lost. Instead these quantities become dependent on many fundamental processes with unknown weightings. To put values on these weightings and to define and assess a statistical standard error for the derived quantities, the propagation of error through the collisional-radiative model must be computed. The code achieves this numerically by repeated population calculations (of the complete ADAS208 type) on varied ADF04 files. The varied ADF04 files are generated either by individual fundamental rate variation or by variation of the complete set of fundamental rates according to a statistical sampling methodology.

The error comment block: The block is prepared as a set of contiguous lines, initiated and terminated by an 'C+++ERROR' code sequence, in the comments section of the ADF04 file and consists of keywords and values.

```
C-----------------------------------------------------------------------------------------
C
C+++ERROR specification start++++++
C
C Recombination
C
C  * -*  20.0
C  *-1   30.0
C
C Excitation
C *-*  20.0
C 1-*  10.2
C  1-2   15.0
C
C
C+++ERROR specification end+++++++
C
C Notes  : *-* is the default value applied to all
C          1-* is the general for all to level 1
C          2-3 is error applied to this transition
C
C        : precedent applied is – specific transition
C                               - general (lower level has highest precedent)
C                               - default
C        : errors are given as a percentage and will be applied to the
C          rates as a multiplier (1.0+err/100) and (1.0-err/100)
C
C-----------------------------------------------------------------------------------------
```

Keywords: These identify the direct reaction types and match the types recognised in ADF04 files, namely, excitation, recombination, charge transfer, and ionisation. The keyword begins with a capital. It is followed by a set of values on successive lines. Blank lines and redundant spaces are ignored.

Values: These specify the error of the fundamental rate as a triplet (lower level index, upper level index, percentage error). The lower and upper level indices must be separated by a '-'. Codes, used for ranges of levels, include: '*' ⇒ all levels. It is helpful to lay out the errors in default, general and specific categories as shown in the illustration below although these are not keywords.

Detailed assessed errors are only available for a few reactions. Usually, errors adopted are those presented as expected uncertainties from different classes of calculation of the fundamental rate coefficients. Thus electron impact collisional rate coefficients from an R-

matrix calculation might be expected to be ~15%, while those from distorted wave calculations might be expected to be ~ 30%. Further sub-divisions of expectations might be according to n-shell, n-shell jump or dipole, non-dipole, spin-change character. Evidently there is a measure of subjectivity here. Error blocks are being added to system generated ADF04 files but *caveat emptor*.

Individual error propagation: For process class p of total number of transitions I_p and rate coefficients $q_i(T_e)$, let

$$q_i(T_e) = q_i(T_e) \text{ for } i \neq i^*, i \in I_p$$

$$q_{i^*_+}(T_e) = q_i(T_e) + \Delta_i \text{ for } i = i^* \qquad 3.16.1$$

and create the manifold of population solutions

$$N_l^{i^*_+}(T_e, N_e), N_l^{i^*_-}(T_e, N_e) \text{ for } l \in L, i^* \in I_p \qquad 3.16.2$$

where L is the number of levels in the ADF04 file, T_e is the electron temperature and N_e is the electron density. If $N_l(T_e, N_e)$ is the population without error variation, then the errors

$$\Delta N_l^{i^*_+}(T_e, N_e) = (N_l^{i^*_+}(T_e, N_e) - N_l(T_e, N_e)) / N_l(T_e, N_e)$$

$$\Delta N_l^{i^*_-}(T_e, N_e) = (N_l^{i^*_-}(T_e, N_e) - N_l(T_e, N_e)) / N_l(T_e, N_e) \qquad 3.16.3$$

are obtained. The code allows selective display of subsets of the $\Delta N_l^{i^*_+}(T_e, N_e)$ and $\Delta N_l^{i^*_-}(T_e, N_e)$.

Statistically sampled error: For process class p of total number of transitions I_p, let the probability of the i[th] coefficient at temperature taking value x_i be

$$\frac{1}{\sqrt{2\pi\Delta_i}} \exp(-(x_i - q_i(T_e))^2 / \Delta_i^2) \qquad 3.16.4$$

A set of N samples $\{S_n\{x_i : i = 1,..., I_p\} : n = 1,..., N\}$ is created by random number according to the distributions 3.16.4. and a manifold of population solutions

$$N_l^n(T_e, N_e, S_n) \text{ for } l \in L, n = 1,..., N \qquad 3.16.5$$

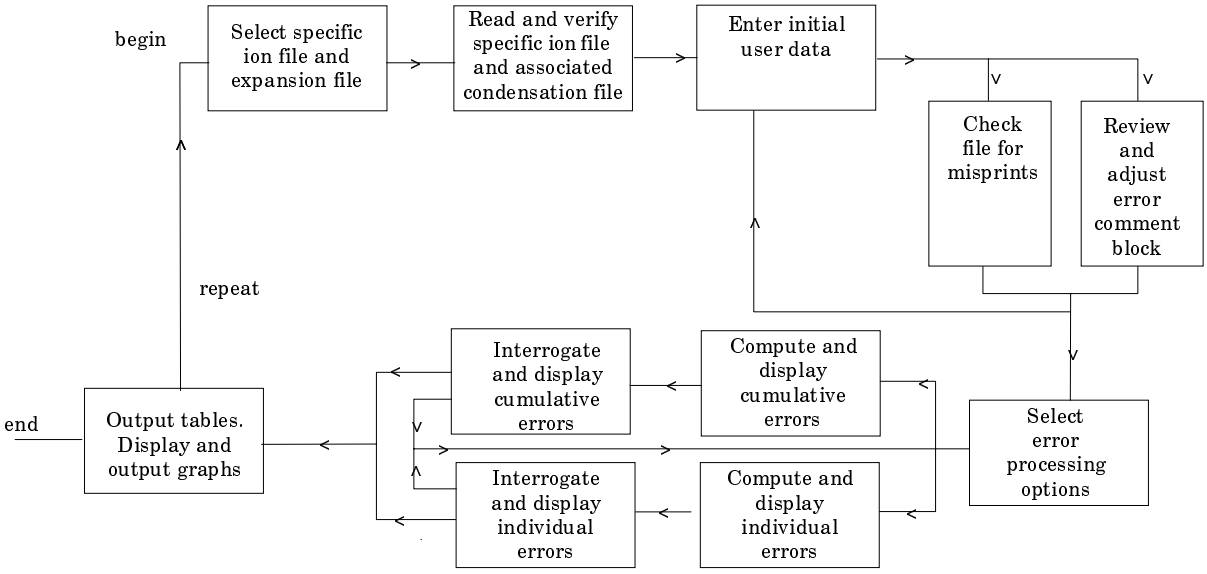
If $N_l(T_e, N_e)$ is the population without error variation, then the $N_l^n(T_e, N_e, S_n)$ should follow a Gaussian distribution of mean $N_l(T_e, N_e)$. A Gaussian shape is fitted to the histogram of sample deviations from the mean to give a half-width error.

User introduced error: There is one further issue. The ADF04 file, which is the starting point for the above analysis, usually includes many transitions from a variety of sources. There is a significant possibility of introduction of typographical and such like errors at this compilation stage. ADAS216 allows a preliminary check for such errors in the collisional excitation rate coefficients. Three criteria are used to identify transitions which should be re-examined. (a) an attempt is made to fit a low order polynomial fit to upsilon Vs temperature for each transition to a specified accuracy. Failure to achieve this is signalled. (b) each upsilon is compared to a local average. Deviation by more than a defined fraction is signalled. (c) large local gradient of upsilon Vs temperature is signalled. A summary of the transitions detected is produced. This is not to say that a transition picked out is in error but merely that re-scrutinising is recommended.

Program steps:

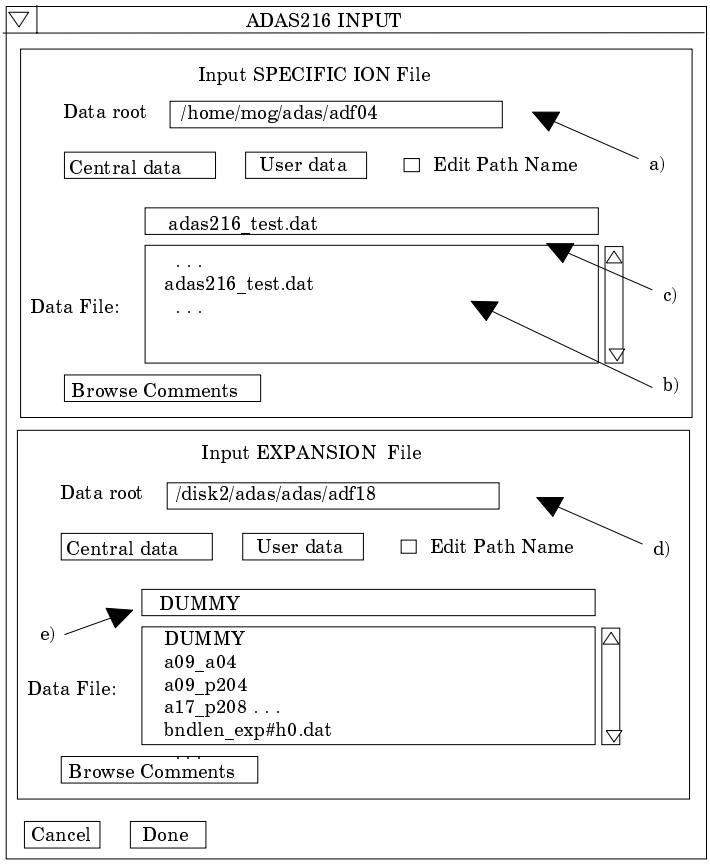
These are summarised in figure 3.16.

Figure 3.16



Interactive parameter comments:

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



1. Data root a) 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. The appropriate ADAS data format for input to this program is ADF04 ('specific ion files'). 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 b). 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 c) 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. A second file selection is given. This is the choice of expansion file of type ADF18 (subdirectory */a17_p208*) which cross-references projection matrices (ADF17) into the specific ion file under examination. The expansion file must be consistent with the specific ion file with which it is linked and in fact contains the specific ion file name. Select DUMMY if no expansion file is to be included.

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

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

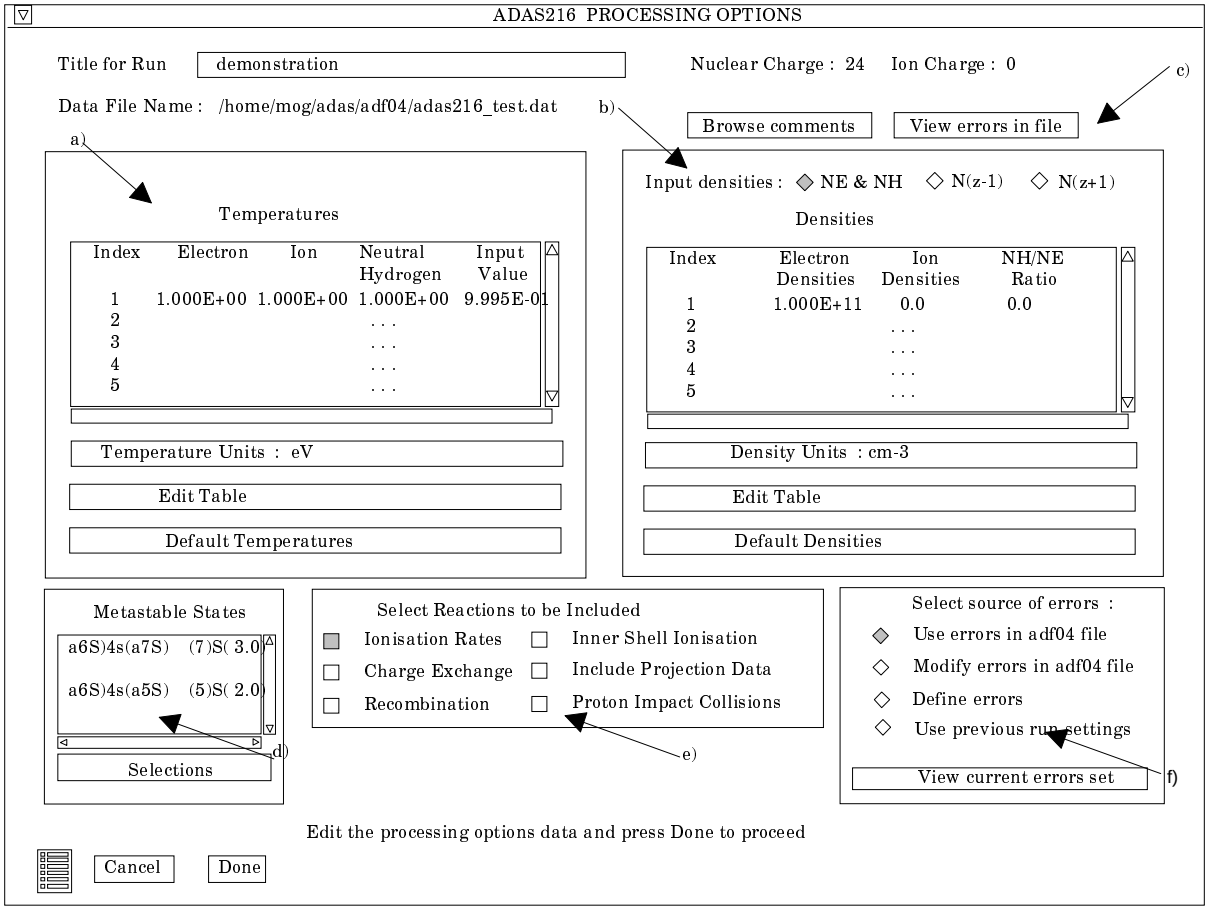
9. There are three 'pop-up' windows for setting temperatures, densities and for designating metastable levels. For the temperature window a), click on the *Edit Table* button to open up the table editor. The editing operations are as described in the introductory chapter. Note that there is a set of input electron temperatures from the selected file. These indicate the safe range of temperatures if extrapolation is to be avoided. Note that altering units (which must be done with the table edit window activated) converts the input values and interprets the output values in the selected units. It **does not convert** output values already typed in. *Default Temperatures* are inserted in the selected units on clicking the appropriate button. Note that the ion and neutral hydrogen temperatures are **only used if** such collisional data is present in the input ADF04 file.

10. There are three choices of densities tables. Click the choice to enter the table in the display window. Thereafter it is handled in like manner to the temperature table. Note that in this case there are no input density values. Thus unit changing only affects the interpretation of the output values created by the user. The N_H/N_e, etc.) **are only used if** the corresponding data are present in input ADF04 file. These vectors are specified at each electron density so the vectors and electron density vector are of the same length. That is a model is specified. By contrast the output electron temperatures are independent so that final calculated populations are obtained at points of a two-dimensional electron temperature/electron density grid.

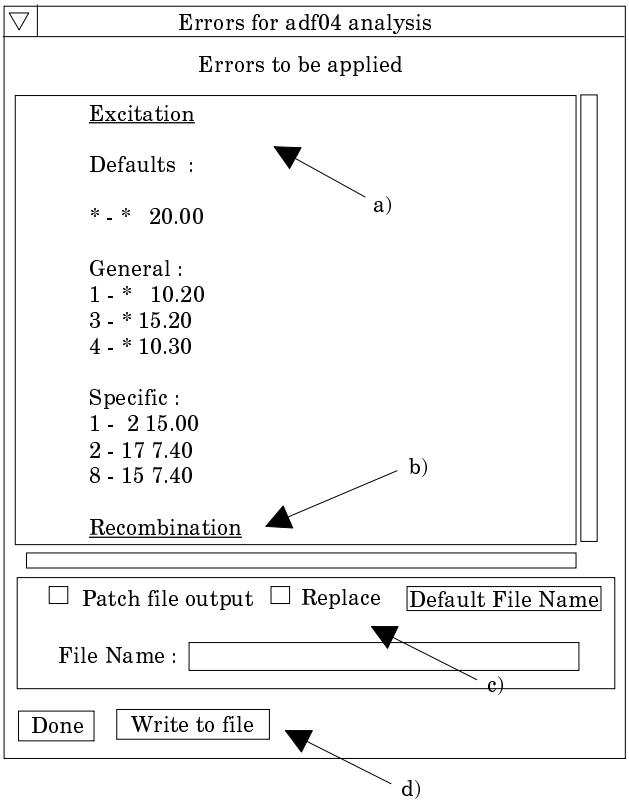
11. At c), the full comments section of the ADF04 file can be browsed. Alternatively only the error block in the comments section can be browsed. A further button at c) initiates the preliminary check for possible user mis-typing in the ADF04 file as described in the background theory.

12. The Metastable State *Selections* button d) pops up a window indexing all the energy levels. Activate the buttons opposite levels which you wish treated as metastables.

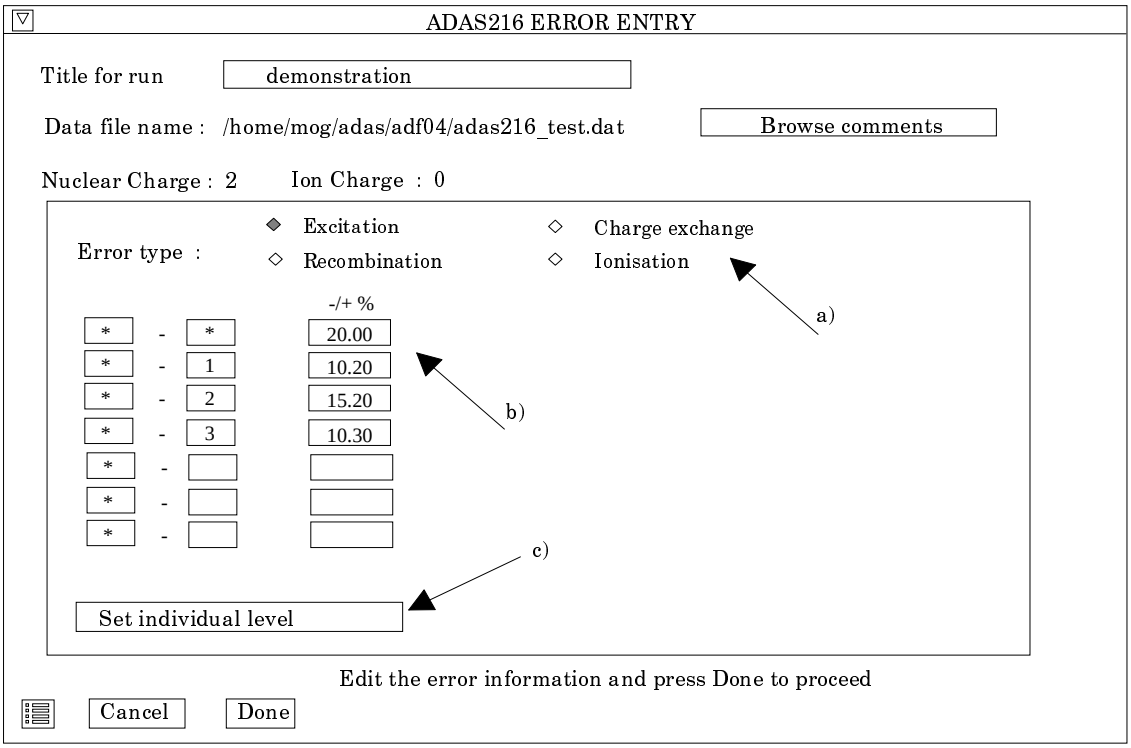
13. Various processes, supplementary to the primary electron excitation collisions and bound-bound radiative transitions, are activated as desired by clicking on the appropriate buttons at e).



14. At f), the user can select or modify the error comment block in the ADF04 file. Choices include using the error block as it is, modifying the errors, defining a error block if one does not already exist and finally using the error block from a previous run. Make the choice at f) and click the *View current errors* set button to examine or adjust the errors. A pop-up widget is displayed as shown below.

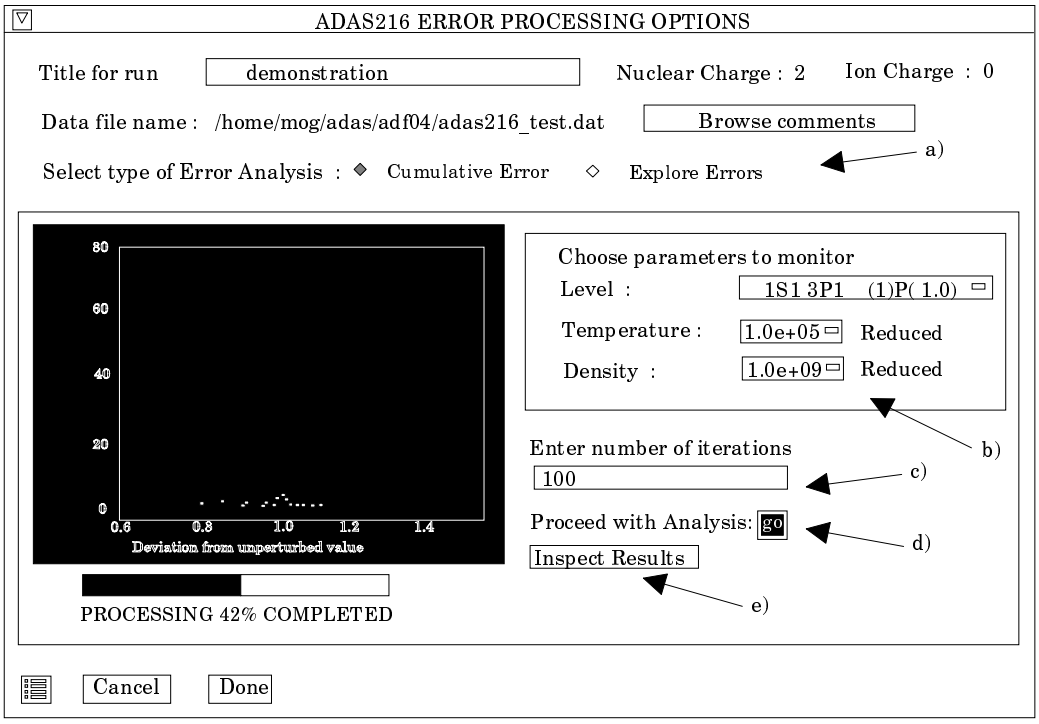


15. Note the format for definition of the error block at a). At the present time the code deals with only the electron impact excitation errors. The other processes such as recombination b) will be introduced in due course. An altered or newly created error block may be written to a patch file output at c) for subsequent addition to the ADF04 file.



16. Click *Done* to return to the main processing widget and again *Done* to proceed to the error analysis.

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



17. At a), the type of error analysis is selected. The *Cumulative error button* is for the Monte Carlo statistical error study. The *Explore error button* is for the individual error propagation study. For the former, the sub-widget is as shown at b).

18. The graphical display window allows monitoring of results for one choice of parameters, that is level, electron temperature and electron density. Make this choice

at b). It is to be noted that results are obtained for all levels, temperatures and densities but only one case is shown in the active display.

19. Enter the number of iterations, that is random samples at c) and click Go at d) to start the sampling. The histogram of number Vs deviation builds actively and the course of the calculation is indicated in the thermometer sub-widget. Visual inspection of the histogram indicates if the number of iterations should be increased

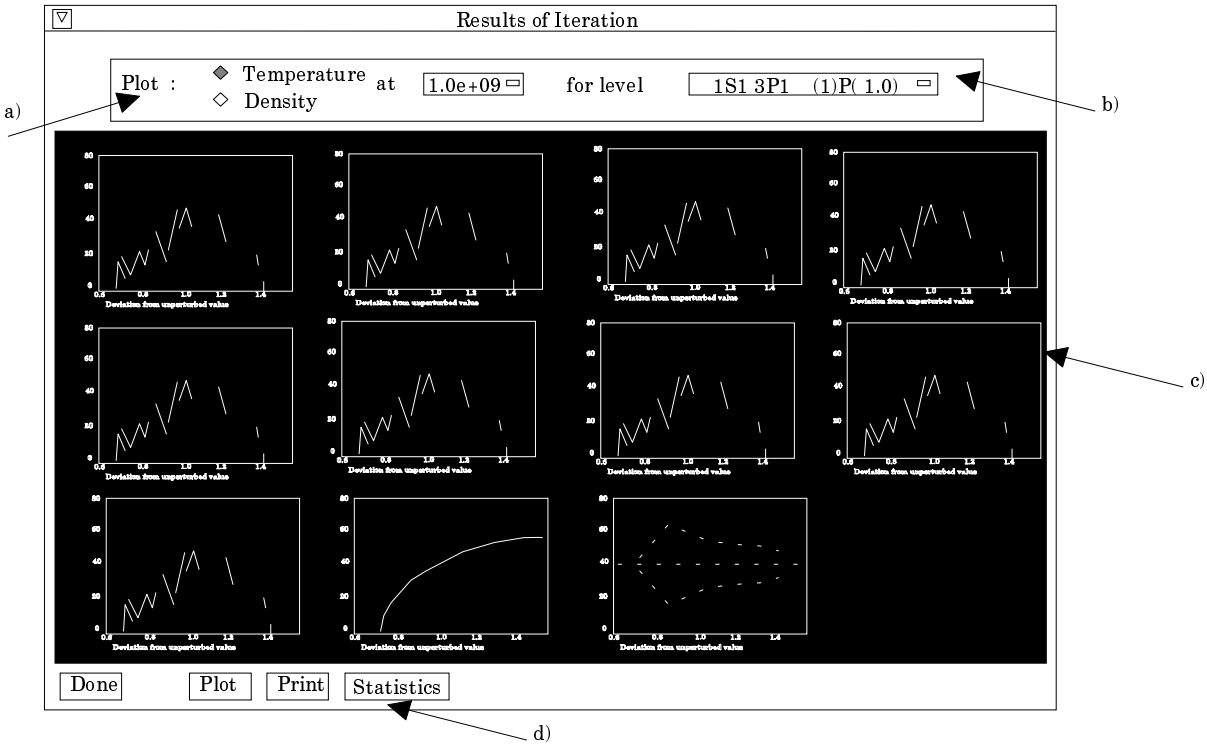
20. Click the *Inspect Results* button at e)to review the complete set of results as shown below.

The **Results of Iteration window** is shown below.

21. Choose to show graphs at different temperatures for a fixed density or vice versa at a). The fixed value is selected from a drop-down menu. Choose the level population for display at b).

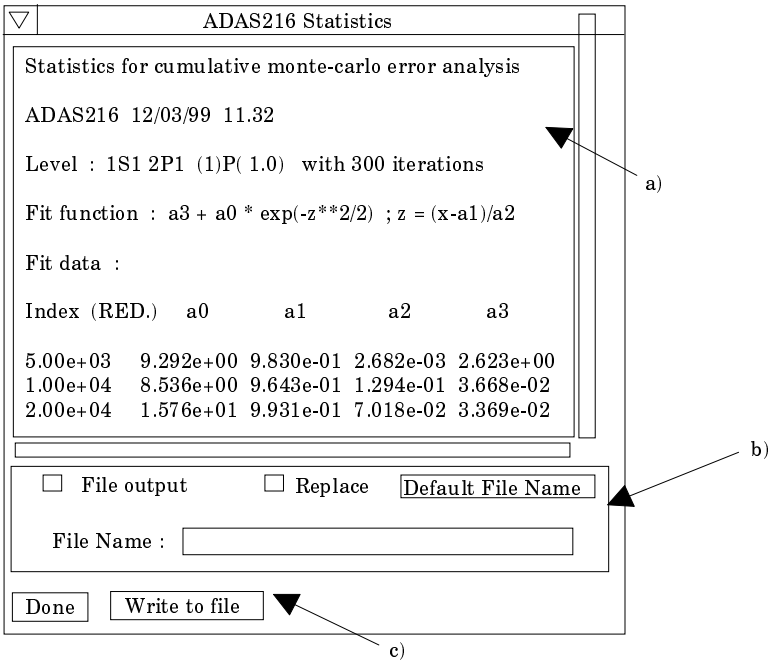
22. Note the two extra graphs at c) which show the relative population and then the mean and half-widths of the Gaussian fits. These last two graphs are plots Vs temperature or density according to the choice at a).

23. *Plot*, *Print* or view the *Statistics* of the analysis by button click at d



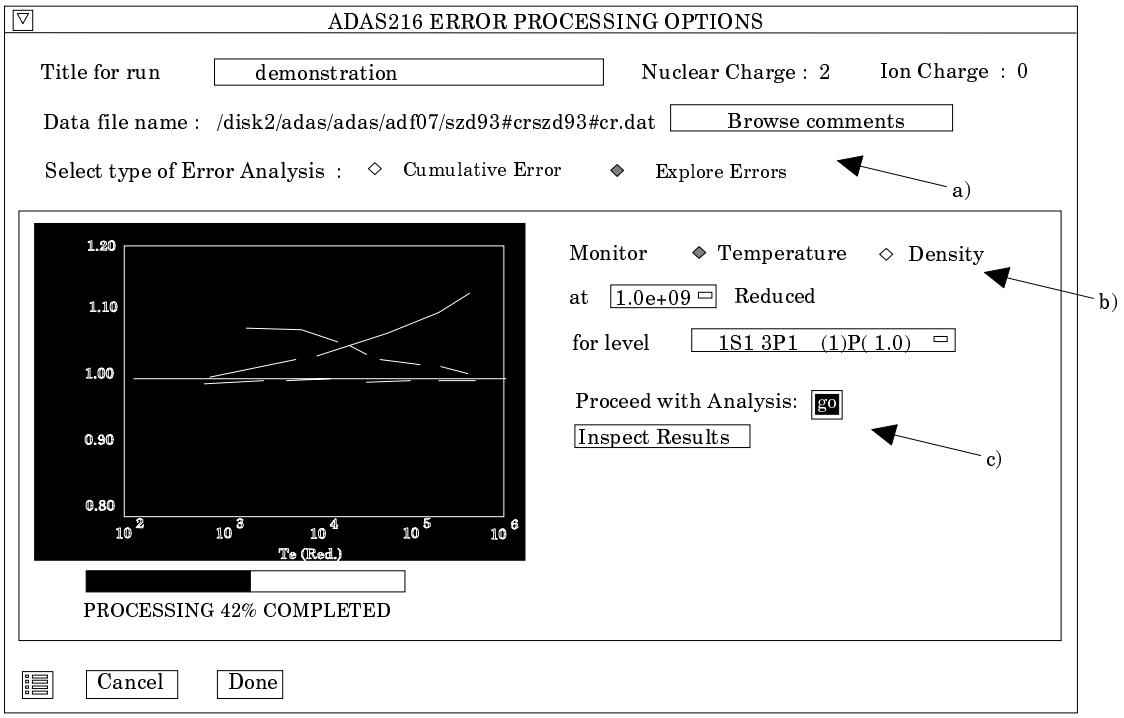
The **Statistics window** is shown below.

25. The numerical results can be inspected at a). At b) and c) output of the results to file can be set up.



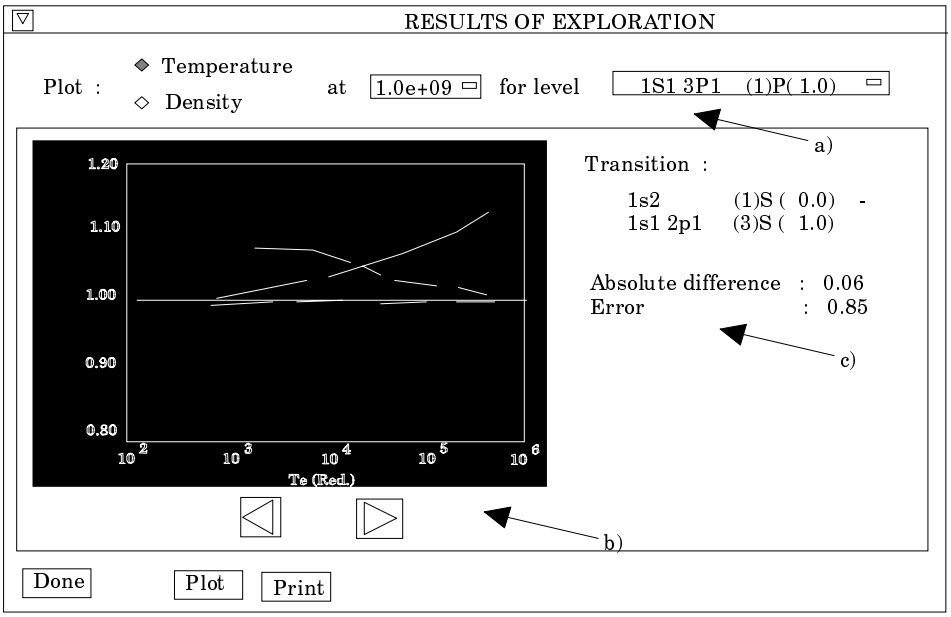
26. The choice of *Explore Errors* on the Error processing options window causes the display of the sub-window at b) as shown below. The graphic display sub-widget is similar to the previous case.

27. Select at b) choice of display Vs temperature or density, then select the specific value of the other fixed parameter. Select also the level whose population is to be monitored. Click Go to initiate the analysis.



28. In the graphic window, the influence of each collisional transition on the population is calculated by shifting the rate coefficient to its positive and negative and error bounds and mapping the population fractional error shift. Separate pairs of curves are given for each transition. Positive shift in the rate is given in white while negative shift is given in yellow. These are not easily distinguished in the evolving graph so a separate more detailed display is provided. Click *Display Results* for this examination in the inspection window.

29. The inspection window, shown below, allows exploration of the largest twenty contributions, distinguished by absolute difference from unity

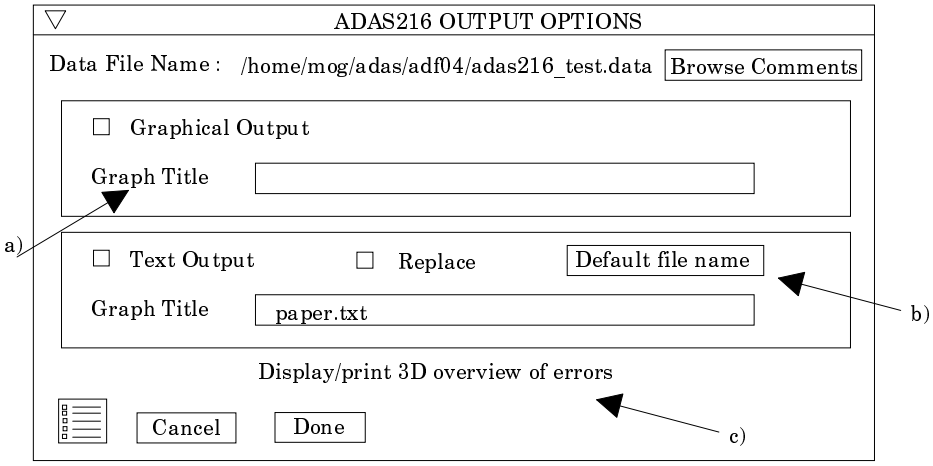


30. The usual choice may be made at a) of the level, temperature and density scans for the display. The forward and reverse buttons beneath the graph display window allows cycling through the individual contributing transitions which are highlighted in yellow. Also the highlighted transition itself is given at c) together with an average difference (over the scan parameter) as a fraction and the individual error from the error block for the transition.

31. Click *Done* to move to the output options window.

The **Output Options** window is shown below:

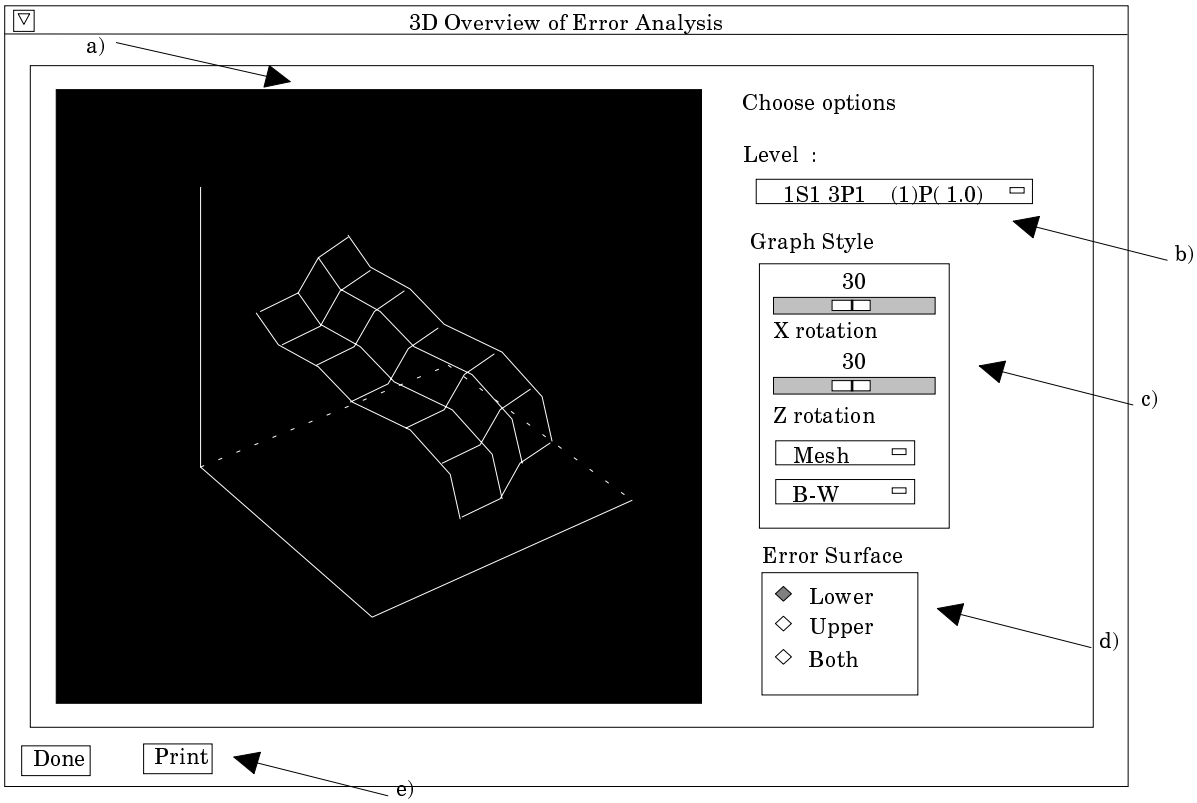
32. The window is simpler than the usual case. If *Graphical Output* is selected a special 3D overview of error analysis widget is displayed as shown below. Hardcopy files are generated as in the inspect error widgets earlier by clicking the *Print* button. The causes a new ADAS File Entry widget to appear which gives complete control.



33. It is to be noted that the ADAS File Entry widget pop-up appears if the *Print* button is clicked on any of the graphic display widgets.

34. The 3D Overview of Error Analysis is controlled by a drop down menu for level selection at b) and controls for rotation, mesh and colour at c).

35. Upper and lower error surfaces can be shown and selected at d).



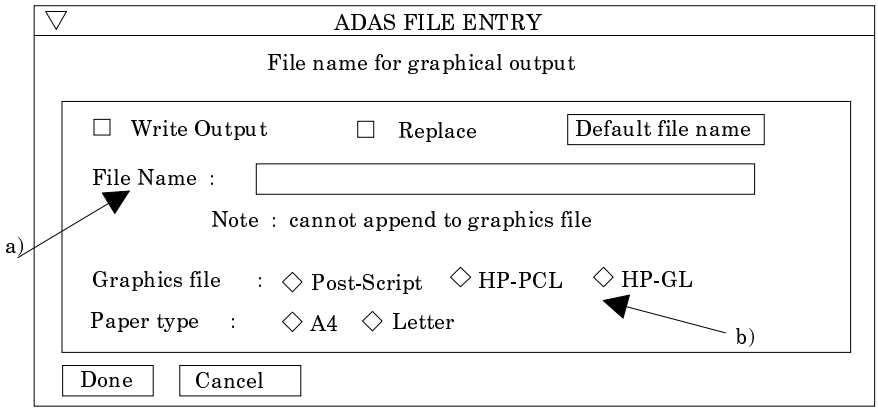


Illustration:

There is no separate illustration.

Notes: