# Lecture 2 The interactive system – working with adf04 datasets and population structure

The population equations for the number densities of excited states of an ion in an optically thin thermal plasma are established and solved. Collisions by free Maxwellian electrons drive the excitation. Basic notation for collisional processes is summarised. The ADAS data sources are identified and ADAS code to examine these data outlined. The code to obtain the populations is described and it is shown how the results can be used in line ratio diagnostic prediction. Some preparation is made in additional processes and data format extensions for later parts of the course.

Preliminaries

Basic electron impact excitation reactions and sources in ADAS

The reaction is

$$X_i^{+z}(E_i) + e(\varepsilon_i) \rightarrow X_j^{+z}(E_j) + e(\varepsilon_j)$$
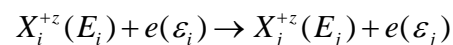
with $\varepsilon_i + E_i = \varepsilon_j + E_j$ where E_i (E_j) is the excitation energy of the state i (j) denoted by X_i^{+z} (X_j^{+z}) from the lowest level of the ion X^{+z} and ε_i (ε_j) is the energy of the incident (scattered) electron. The reaction is described by a *cross-section* for the process denoted by $\sigma_{i \rightarrow j}(\varepsilon_i)$. The reaction requires $\varepsilon_i \geq \Delta E_{ij} = E_j - E_i$. Introduce the threshold parameter $X = \varepsilon_i / \Delta E_{ij}$, with $X \in [1, \infty]$. In preference to the cross-section, use the symmetric, dimensionless, slowly varying *collision strength* Ω_{ij}. The excitation cross-section $\sigma_{i \rightarrow j}(\varepsilon_i)$, the de-excitation cross-section $\sigma_{i \rightarrow j}(\varepsilon_i)$, and the collision strength Ω_{ij}, are connected by

$$\Omega_{ij} = \omega_i(E_i/I_H)(\sigma_{i \rightarrow j}(\varepsilon_i)/\pi a_0^2) = \omega_j(E_j/I_H)(\sigma_{j \rightarrow i}(\varepsilon_j)/\pi a_0^2)$$

Three distinct types of cross-section are recognised, namely, dipole, non-dipole and spin with distinct asymptotic behaviour.

ADAS is principally, but not exclusively, designed for plasmas in which the free electrons are Maxwellian. The collision strength integrated over a Maxwellian distribution of electron energies at an electron temperatures T_e is called the *rate parameter* or *effective collision strength* and written as γ ('gamma') or Y ('Upsilon'). It is defined by

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

Y_{ij} is related to the excitation rate coefficient $q_{i \rightarrow j}(T_e)$ and de-excitation rate coefficient $q_{j \rightarrow i}(T_e)$ as

$$q_{j \rightarrow i}(T_e) = \frac{\omega_i}{\omega_j} \exp(\Delta E_{ij}/kT_e) q_{i \rightarrow j}(T_e) = 2\sqrt{\pi} \alpha c a_0^2 \frac{1}{\omega_j} [I_H/kT_e]^{1/2} Y_{ij}$$

Burgess C-plots: Burgess & Tully (1992) showed that the whole variation of Y and T_e can be mapped onto a finite range by introducing a reduced temperature, x, and reduced Upsilon, y, for four types of transition. Also they introduce a parameter C to balance the spread of x-values across its range ($[0,1]$). Such mapping gives a compact representation of collision data and is used in ADAS for accurate interpolation, checking of the limiting high temperature behaviour of the rate coefficient.

The adf04 data format

The primary repositories of electron impact collision rate coefficient (Upsilon) data are *adf04* files. Such files are for a specific ion and contain energy level lists, level configuration, term and level classification quantum numbers, level energies. Following the level lists, they contain transition lines, which specify the upper and lower levels of each transition, the A-value for the transition and then a set of Upsilons for the transition as a function of electron temperature. The basic layout is as shown below.

Labels: element, ion charge, nuclear charge, Ion charge+1, Ionisation Potential (cm-1), Indexed levels, Configuration, (2S+1)L(J), Energy (cm-1), Transition level pairs, A-values (s-1), Te (K) row vector, Upsilon row vector

```
    H+ 0             1           1            109679.
          1    1S                    (2)0( 0.5)                  0.
          2    2S                    (2)0( 0.5)              82303.
          3    2P                    (2)1( 2.5)              82303.
          .      .        .
         14    5F                    (2)3( 6.5)             105348.
         15    5G                    (2)4( 8.5)             105348.
         -1
      1.00      3       5.80+03 1.16+04 3.48+04 5.80+04 1.16+05 1.74+05 2.32+05 2.90+05
         2     1 0.00+00 2.60-01 2.96-01 3.26-01 3.39-01 3.73-01 4.06-01 4.36-01 4.61-01
         3     1 6.27+08 4.29-01 5.29-01 8.53-01 1.15+00 1.81+00 2.35+00 2.81+00 3.20+00
         4     1 0.00+00 6.51-02 6.96-02 7.76-02 8.13-02 8.70-02 9.21-02 9.66-02 1.01-01
         5     1 1.67+08 1.12-01 1.26-01 1.86-01 2.43-01 3.54-01 4.38-01 5.07-01 5.66-01
         .      .
        12    10 0.00+00 3.48+01 4.05+01 3.97+01 3.70+01 3.32+01 3.11+01 2.98+01 2.89+01
        13    10 5.05+04 7.51+01 1.03+02 1.32+02 1.32+02 1.26+02 1.22+02 1.22+02 1.22+02
        14    10 0.00+00 1.67+02 2.71+02 5.28+02 6.50+02 7.64+02 8.01+02 8.15+02 8.21+02
        15    10 4.26+06 3.87+02 7.33+02 1.76+03 2.46+03 3.64+03 4.48+03 5.14+03 5.69+03
        -1
        -1    -1
```

Note that the configuration of a level is the specification of the orbital occupancies as

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

It is helpful to maintain a consistent pattern for configurations for automatic processing of ADF04 files and for matching of energy levels between different datasets.. In ADAS two conventions are use, namely the *Standard form* and *Eissner form*. *Standard form* represents each shell with three characters with a space separating shells in the whole configuration as ' 1s2 2s2 2p1' representing $1s^2 2s^2 2p^1$. For certain calculations, principal quantum numbers greater than 9 may be required and for complex element ion, shell occupancies greater than 9 also may occur. To maintain the three character shell notation, the integers beyond nine are represented alphabetically, that is $10 \equiv$ 'a', $11 \equiv$ 'b' etc. Thus in *Standard form*, $2p^6 6f^{11} 11s^1$ is represented by ' 2p6 6fb bs1'. In *Eissner form*, each orbital, starting from 1s is indexed. The index is an integer up to 9, but continues through the upper case alphabet and then through the lower case alphabet. Thus $1s \equiv$ '1', $2p \equiv$ '2', $4f \equiv$ 'A'. A portion of the conversion table is

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

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

```
                   ┌─────────────────────┐          ┌─────────────────────┐
                   │  Standard form for  │          │  Eissner form for   │
                   │    configuration    │          │    configuration    │
                   │       = 21512       │          │       = 1s2 4f1      │
                   │   in Eissner form   │          │   in Standard form  │
                   └─────────────────────┘          └─────────────────────┘

  C + 3           6           4          520178.4(1S)
     1 1s2 2s1              (2)0( 0.5)        0.0
     2 1s2 2p1              (2)1( 2.5)    64555.4
     3 1s2 3s1              (2)0( 0.5)   302849.0
     4 1s2 3p1              (2)1( 2.5)   320071.2
     5 1s2 3d1              (2)2( 4.5)   324886.1
     6 1s2 4s1              (2)0( 0.5)   401348.1
     7 1s2 4p1              (2)1( 2.5)   408319.8
     8 1s2 4d1              (2)2( 4.5)   410338.5
     9 2151A                (2)3( 6.5)   410434.2
    10 1s2 5s1              (2)0( 0.5)   445368.5
    11 1s2 5p1              (2)1( 2.5)   448860.5
    12 1s2 5d1              (2)2( 4.5)   449889.2
    13 1s2 5f1              (2)3( 6.5)   449939.8
    14 1s2 5g1              (2)4( 8.5)   449948.4
    -1
```
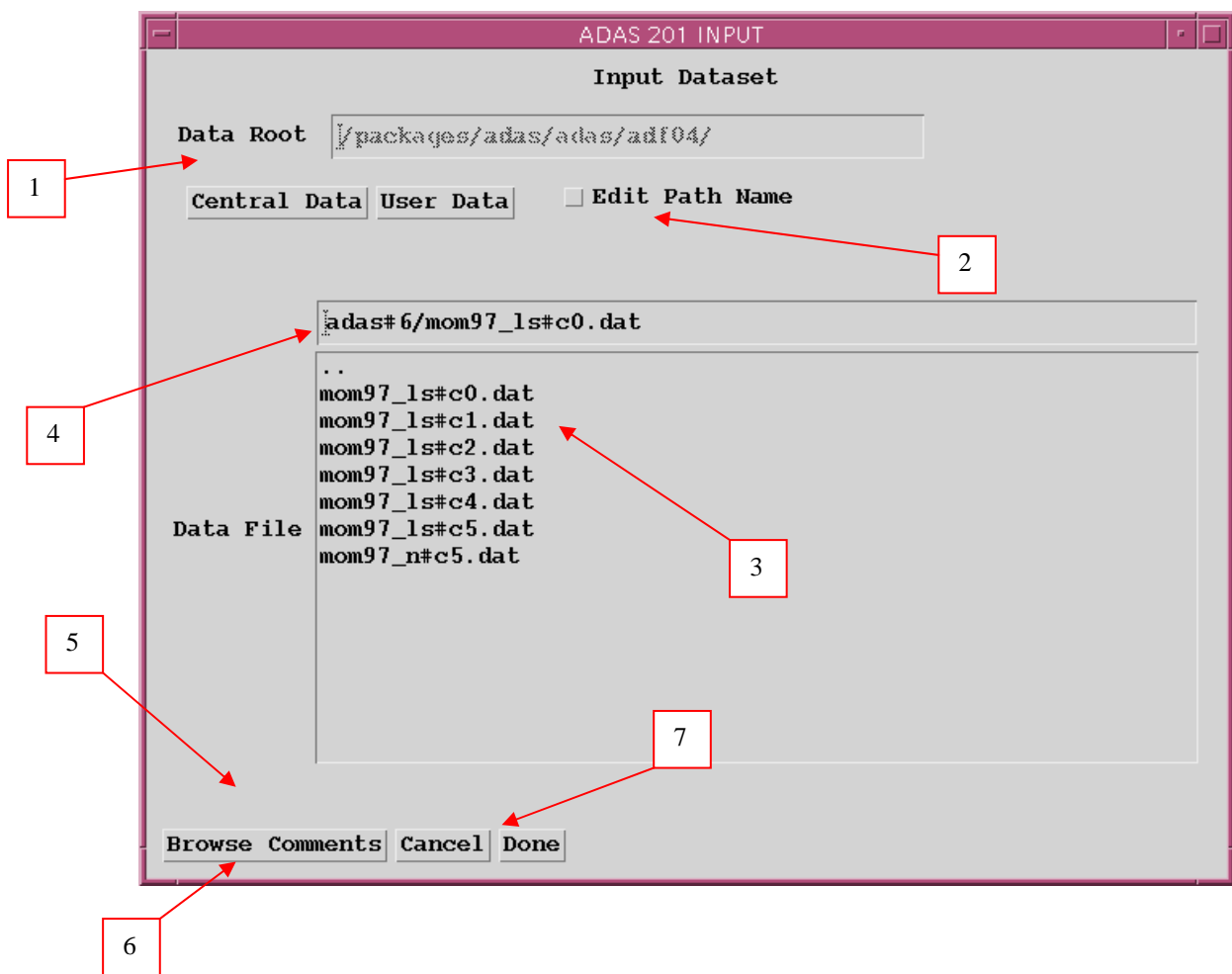
ADAS201

The program interrogates specific ion files of type ADF04. It extracts electron impact rate coefficient data for selected transitions. The data may be interpolated using cubic splines to provide excitation rate coefficients at arbitrarily chosen electron temperatures. A minimax polynomial approximation is also made to the source data. The source and interpolated excitation rate coefficient data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the minimax polynomial approximation.

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 – ADF04 in this case. 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. There are a large number of these, named (a) by iso-electronic sequence (eg. *belike*) (b) by isoelectronic sequence associated with a particular source (eg. *copsm#be*) (c) by iso-nuclear sequence associated with a

particular source (eg. *copmm#16* , where the 16 is the nuclear charge). 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

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. The output data extracted from the datafile, an 'excitation rate coefficient', may be fitted with a polynomial. This is as a function of temperature. Clicking the *Fit Polynomial* button b) 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

3. 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.

4. Your settings of electron temperatures (output) are shown in the temperature display window. The temperature values at which the excitation rate coefficients (in fact 'upsilons') are stored in the datafile (input) are also shown for information. The program recovers the output temperatures you used when last executing the program

5.

5. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures
6. 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.
7. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

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.
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.

4. 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.

5. 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.

6. 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** is shown below

1. Printing of the currently displayed graph is activated by the *Print* button.
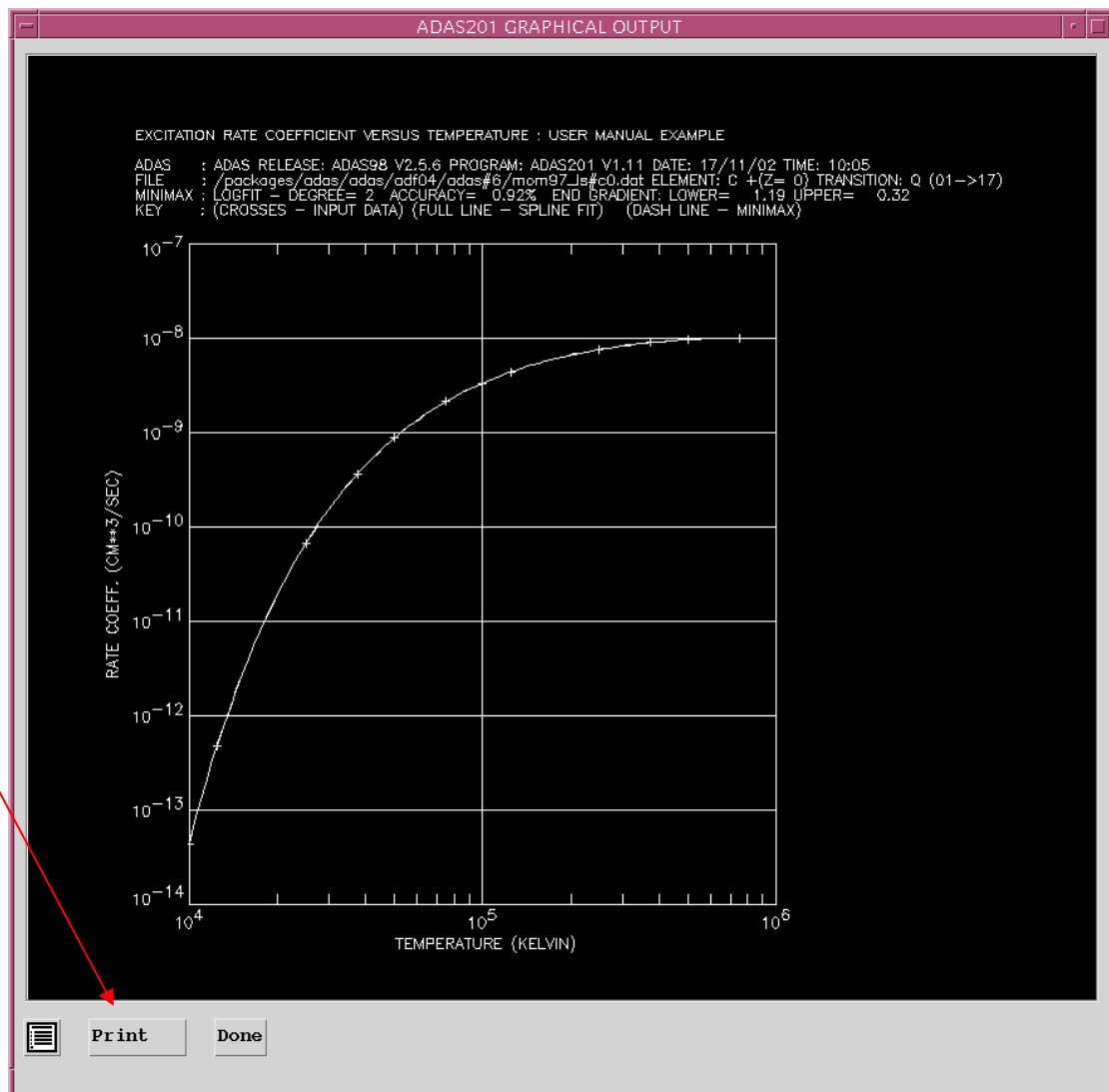
ADAS811

The code is a new and more sophisticated interrogator and comparator of archived ADAS datasets of format *adf04*. It initiates an interactive dialogue with the user in two parts, namely, input file selection and display/comparison of selected data. There is only graphical output.

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

1. Selection of up to three adf04 files is permitted. At least one file, *adf04 file 01*, must be selected.
2. Selection of *adf04 file 01* follows the standard ADAS pattern. 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 *adf04 file 01* is 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 file 01* 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.
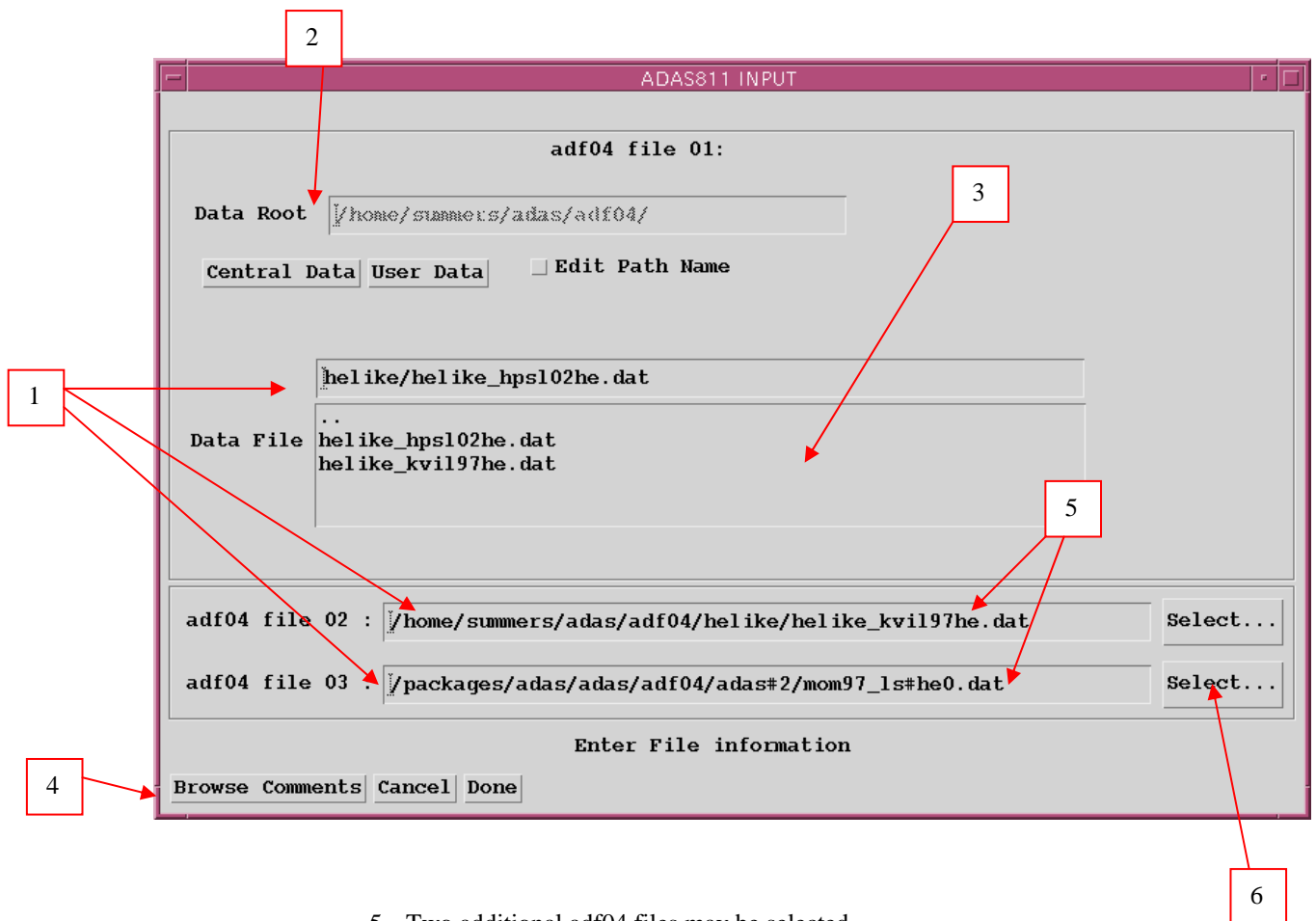

5. Two additional adf04 files may be selected.
6. Click the *Select...* button for *adf04 file 02* or *adf04 file 03*. A pop-up Select-a-File widget is presented as shown below. Note that this is a general non-ADAS specific widget, not targetted specifically on *adf04* files. Only comparison of adf04 files is allowed by ADAS811.
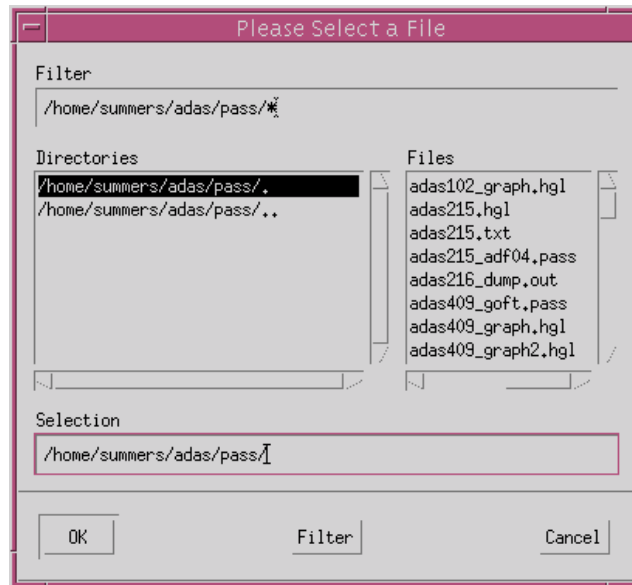
The **processing options window** has the appearance shown below

1. more than one file, click the appropriate button for the primary file you wish to scan through. If there is more than one adf04 file, the program will seek to match transitions between them. The matching does depend on standard configuration labelling and formatting in the adf04 files. The graphical display plots the coefficients from each transition from the primary file but plots the same coefficient from the other files only if it is unambigously matched.
2. Five types of rate coefficient can be displayed, namely electron impact excitation, positive ion excitation, recombination, ionisation and charge exchange. Make the appropriate selection.
3. A number of different forms for display of the selected coefficient may be permitted. The choices are displayed are selected by button click.
4. Coefficients are plotted as a function of temperature. The units, K or eV, may be chosen.
5. The legend of the graph plot line appearances is at the top of the graph and the identification of the particular transition given at the bottom.
6. The selected adf04 files are shown at the top of the screen. If there is
7. Tape recorder type controls are provided to move between transitions.
8. The indices of the transition may be typed in explicitly, then click *Show*.
9. Note that the cursor position in graph axis coordinates is given.
10. The button controls allow printing of the current graph , *Print*, or of all the graphs, *Print All*, of the selected type. Be cautious in using *Print All*. The *Escape to Menu* icon is also available for a quick exit to the main ADAS menu. The *Cancel* button returns the user to the input file selection screen.
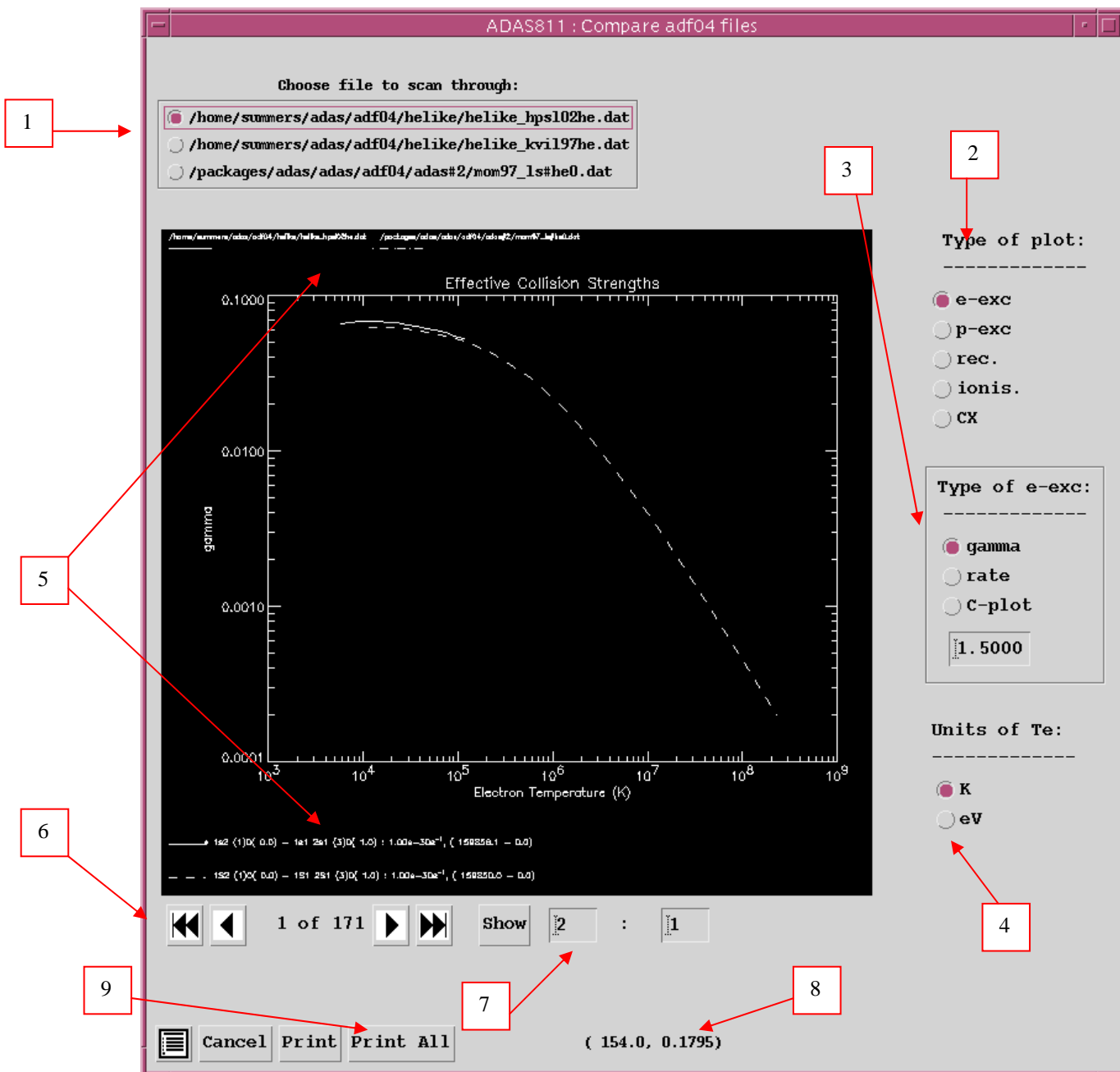
The **graphical file output pop-up** is shown below.
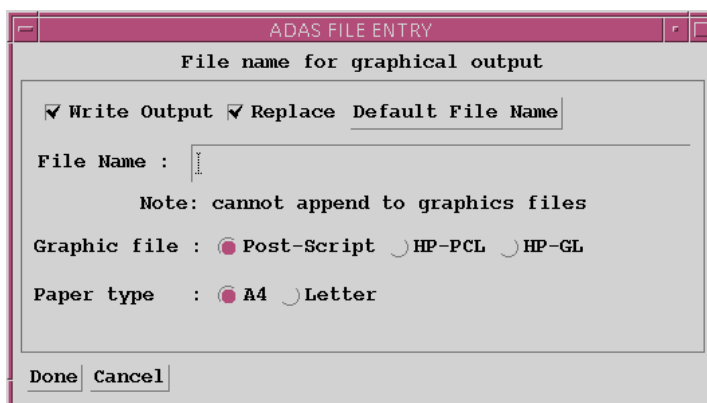
Collisional-radiative modelling of populations

Consider ions X^{+z} of the element X. The adjacent ionisation stages are X^{+z+1} and X^{+z-1}. Let the levels of the ion X^{+z} be separated into the *metastable levels* X_ρ^{+z}, indexed by Greek indices, and *excited levels* X_i^{+z}, indexed by Roman indices. The collective name metastable states as used here includes the ground state. The driving mechanisms considered for populating the excited levels X_i^{+z} are excitation from the metastable levels X_ρ^{+z} and recombination from the ground level of the adjacent ion X_1^{+z+1}. The dominant population densities of the ions in the plasma are those of the levels X_ρ^{+z} and X_1^{+z+1}, denoted by N_ρ and N_1^+ respectively. They, or at least their ratios are assumed known from a dynamical ionisation balance. The other dominant population densities in the plasma are the electron density N_e, the proton density N_p and the neutral hydrogen density N_H. The excited populations, denoted by N_i, are assumed to be in a *quasi-static equilibrium* with respect to the dominant populations. The program evaluates the dependence of the excited populations on the dominant populations with this assumption.

Let M denote the number of metastable levels and O denote the number of excited levels, hereafter called *ordinary* levels. The statistical balance equations take the form

$$\sum_{j=1}^{O} C_{ij} N_j = -\sum_{\sigma=1}^{M} C_{i\sigma} N_\sigma + N_e N_1^+ r_i + N_e N_H q_i^{(CX)} \quad i = 1, 2, ..$$

where the dominant populations (excluding the electron density) have been taken to the right hand side. The C_{ij} and $C_{i\sigma}$ are elements of the collisional-radiative matrix, r_i is the free electron recombination coefficient directly to the level i and $q_i^{(CX)}$ is the charge exchange recombination coefficient from neutral hydrogen to the level i. The element C_{ij} of the collisional-radiative matrix is composed as

$$C_{ij} = -A_{j \rightarrow i} - N_e q_{j \rightarrow i}^{(e)} - N_p q_{j \rightarrow i}^{(p)} \qquad i \neq j$$

where $A_{j \rightarrow i}$, $q_{j \rightarrow i}^{(e)}$ and $q_{j \rightarrow i}^{(p)}$ are the rate coefficients for spontaneous transition, electron induced collisional transition and proton induced collisional transition respectively.

$$C_{ii} = \sum_{j<i} A_{i \rightarrow j} + N_e \sum_{j \neq i} q_{i \rightarrow j}^{(e)} + N_p \sum_{j \neq i} q_{i \rightarrow j}^{(p)} + N_e q_i^{(I)}$$

is the total loss rate from level i, with $q_i^{(I)}$ the electron impact ionisation rate coefficient.
The solution for the ordinary populations is

$$N_j = -\sum_{i=1}^{O} C_{ji}^{-1} \sum_{\sigma=1}^{M} C_{i\sigma} N_\sigma + \sum_{i=1}^{O} C_{ji}^{-1} r_i N_e N_1^+$$

$$+ \sum_{i=1}^{O} C_{ji}^{-1} q_i^{(CX)} N_H N_1^+$$

$$\equiv \sum_{\sigma=1}^{M} \mathsf{F}_{j\sigma}^{(exc)} N_e N_\sigma + \mathsf{F}_{j1}^{(rec)} N_e N_1^+ + \mathsf{F}_{j1}^{(CX)} N_H N_1^+$$

where the $\mathsf{F}_{j\sigma}^{(exc)}$, $\mathsf{F}_{j1}^{(rec)}$ and $\mathsf{F}_{j1}^{(CX)}$ are the effective contributions to the excited populations from excitation from the metastables, from free electron capture and from charge exchange recombination from neutral hydrogen respectively. All these coefficients depend on density as well as temperature. The actual population density of an ordinary level may be obtained from them when the dominant population densities are known.

The emissivity coefficients of specific lines are obtained by multiplying the F s above by the appropriate A-values. They come in the three flavours, (exc), (rec) and (CX) and should be kept distinct in this way for general application. Generalising slightly, there are two kinds of derived

coefficients associated with individual spectrum line emission in common use in fusion plasma diagnosis. These are *photon emissivity coefficients* (PEC) and S/XB ratios (SXB). The reciprocals of the latter are also known as *photon efficiencies*. The emissivity in the spectrum line $j \rightarrow k$, allowing for metastables also in the recombining ion is

$$\varepsilon_{j \rightarrow k} = A_{j \rightarrow k} (\sum_{\sigma=1}^{M} \mathsf{F}_{j\sigma}^{(exc)} N_e N_\sigma + \sum_{\upsilon'=1}^{M_{z+1}} \mathsf{F}_{j\upsilon'}^{(rec)} N_e N_{\upsilon'}^+ +$$

$$\sum_{\upsilon'=1}^{M_{z+1}} \mathsf{F}_{j\upsilon'}^{(CX)} N_H N_{\upsilon'}^+ + \sum_{\mu'=1}^{M_{z-1}} \mathsf{F}_{j\mu'}^{(ion)} N_e N_{\mu'}^-)$$

This allows specification of the *excitation* photon emissivity coefficient

$$\mathsf{PEC}_{\sigma, j \rightarrow k}^{(exc)} = A_{j \rightarrow k} \mathsf{F}_{j\sigma}^{(exc)}$$

the *recombination* photon emissivity coefficient

$$\mathsf{PEC}_{\upsilon', j \rightarrow k}^{(rec)} = A_{j \rightarrow k} \mathsf{F}_{j\upsilon'}^{(rec)}$$

the *charge exchange* photon emissivity coefficient

$$\mathsf{PEC}_{\upsilon', j \rightarrow k}^{(CX)} = A_{j \rightarrow k} \mathsf{F}_{j\upsilon'}^{(CX)}$$

The S/XB are only meaningful for the excitation part of the emissivity and are

$$\mathsf{SXB}_{\sigma, j \rightarrow k} = \sum_{\upsilon=1}^{M_{z+1}} \mathsf{S}_{CD, \sigma \rightarrow \upsilon} / (A_{j \rightarrow k} \mathsf{F}_{j\sigma}^{(exc)})$$

Each of these coefficients is associated with a particular metastable σ, υ' or μ' of the X^{+z}, X^{+z+1} or X^{+z-1} ions respectively. Data format *adf13* encountered in the lecture 2 is the S/XB respository and is interrogated by ADAS501. *adf15* is the repository for the PEC data and is interrogated by ADAS503 in identical manner to ADAS501.

ADAS205

This is the basic code in ADAS for calculating excited state and metastable state populations of a selected ion in a plasma of specified temperatures and densities by drawing on fundamental energy level and rate coefficient data from a specific ion file of type ADF04. It is used principally for displaying the (exc) part of the populations and as a first step in examining diagnostic line ratios.

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. 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

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. There are three 'pop-up' windows for setting temperatures, densities and for designating metastable levels. For the temperature window, click on the *Edit Table* button to open up the table editor. The editing operations are as described in the Chap1-00. 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.

3. The densities table is handled in like manner. 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 and $N(z_1)/N(z)$ **are only used if** neutral hydrogen charge exchange data and free electron recombination data are present in input ADF04 file. These ratio vectors are specified at each electron density so the ratio 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.

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

5. Various processes, supplementary to the primary electron excitation collisions and bound-bound radiative transitions, are activated as desired by clicking on the appropriate buttons. Note again these only have an effect if such data is present in the ADF04 file except for *Ionisation rates*. This activates ionisation out of excited states and is obtained by an internal calculation of these rates in the ECIP approximation. **Warning**-ionisation should **not** be switched on if you have included auto-ionising levels in your ADF04 dataset but have omitted the details of alternative thresholds etc present in advanced ADF04 files.

6. Proton collisions may be present in the ADF04 file. If so, these rate coefficients may be scaled to represent a mixture of other charged projectiles with a mean Z-effective

.
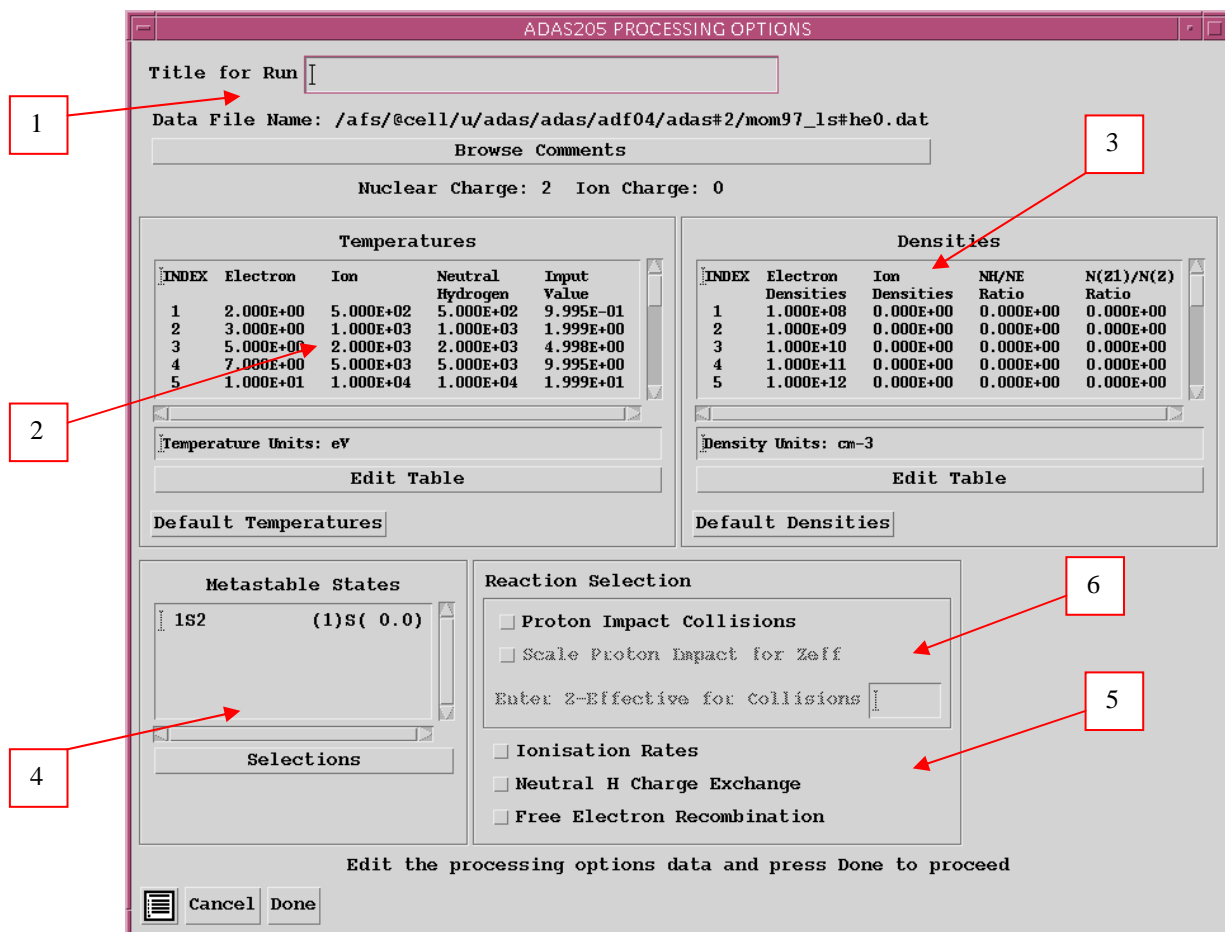
The **output graphic options window** has the appearance shown below

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.
2. Click on the *Graphics* or *Text* buttons to toggle between sub-windows for setting up the graphics output or the text file output.
3. 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.
4. 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.
5. 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.
6. Graphical output is at one selected temperature. Make this choice from the list.
7. 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.
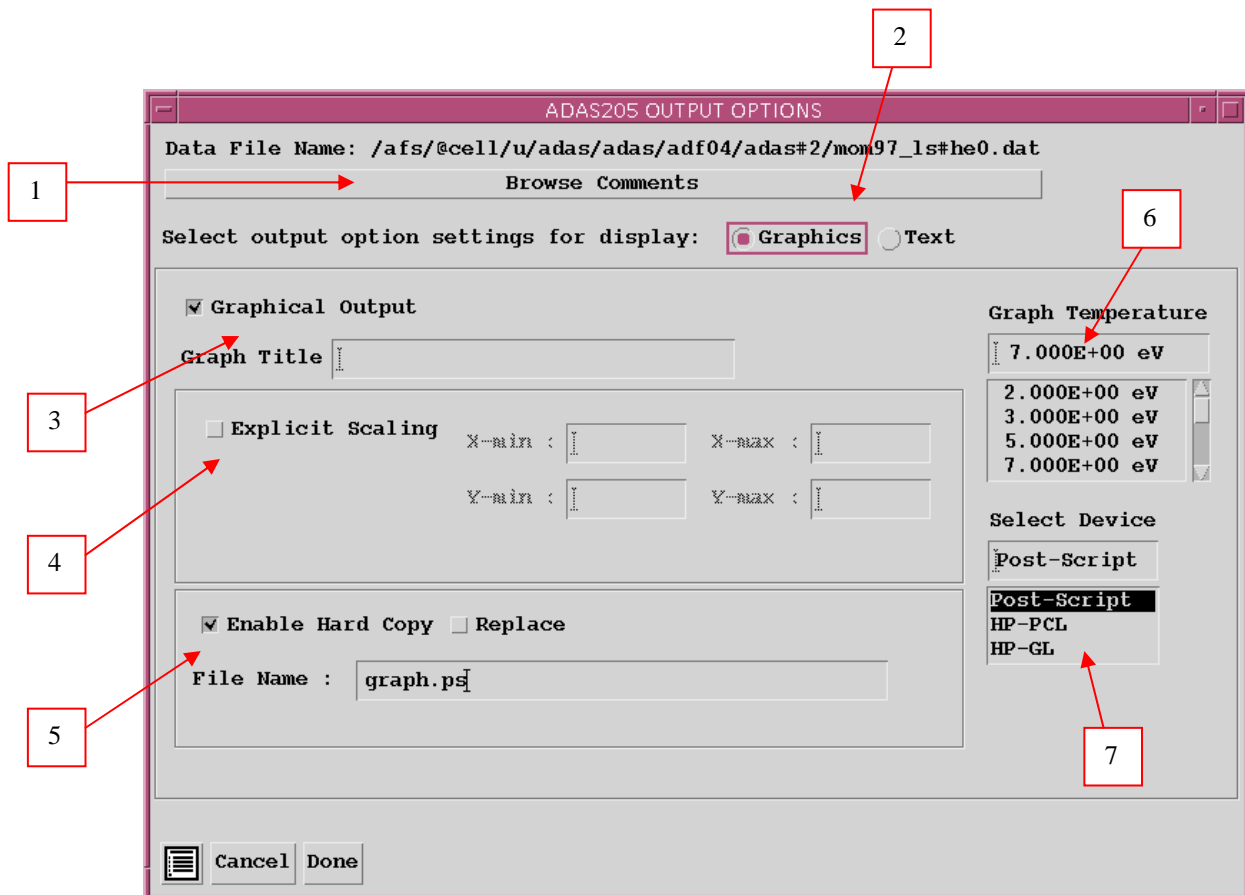
The **output text options sub-window** has the appearance shown below

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 *Contour File* button should be activated to write the passing file for use by the diagnostic line ratio program ADAS207. There is no arrangement for permanent storage of such files which reside only in a user's file space and are generally prepared for temporary immediate use. Usually in ADAS such temporary 'passed files' reside in the *pass/* directory. By default ADAS205 sends the contour file to   */...../<uid>/adas/pass/contour.pass*

3. The *METPOP File* button should be activated to write a passing file of metastable population fractions. It is of data format ADF11 and can be used in ionisation/recombination applications of ADAS4 series programs. It goes by default into

/...../<uid>/adas/pass/metpop.pass
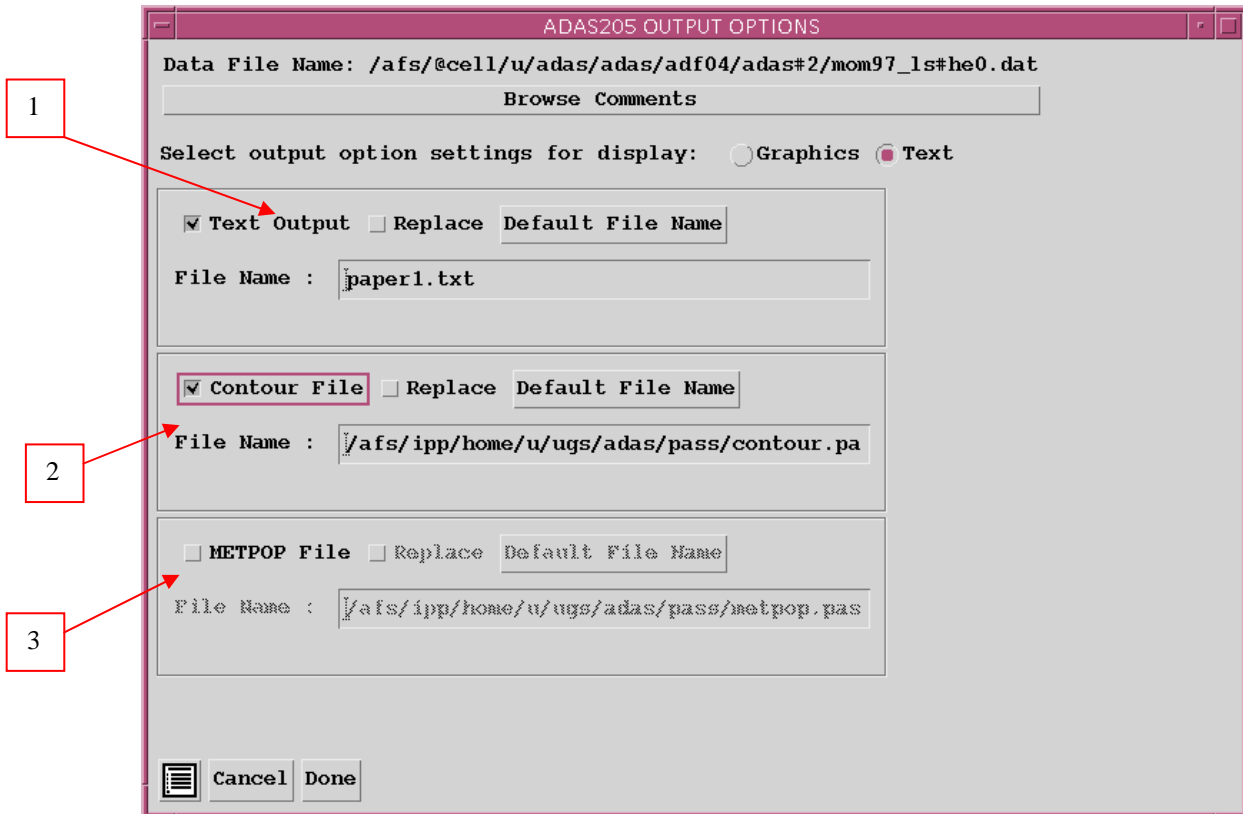
The **Graphical output window** is shown below

2. The graph has at its foot a *Done* button, and possibly *Next* and *Previous* buttons if there is a sequence of graphs to be displayed. A *Print* and *Print all* button is also present if the *Enable Hard Copy* button on the previous window was activated.

3. Press the *Next* button to show the next graph in a sequence and the *Previous* button to show the previous graph.

4. Press the *Print* button to make a hard copy of the currently displayed picture. Print all makes a hard copy of all the pictures.

5. Pressing the *Done* button restores the previous Output Options window.

The graph shows:
POPULATION DEPENDENCE ON METASTABLES: HE 0   ELECTRON TEMP. =   1.00e+01 (eV)

ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS205 V1.10 DATE: 17/11/02 TIME: 16:15
GRAPH TITLE: User manual example
INPUT FILE : /packages/adas/adas/adf04/adas#2/mom97_ls#he0.dat

---- Level Assignments ----
INDEX	DESIGNATION	
1	1S2	(1)S(0.0)
2	1S1 2S1	(3)S(1.0)
3	1S1 2S1	(1)S(0.0)
4	1S1 2P1	(3)P(4.0)
5	1S1 2P1	(1)P(1.0)
6	1S1 3S1	(3)S(1.0)
7	1S1 3S1	(1)S(0.0)
8	1S1 3P1	(3)P(4.0)
9	1S1 3D1	(3)D(7.0)
10	1S1 3D1	(1)D(2.0)
11	1S1 3P1	(1)P(1.0)
12	1S1 4S1	(3)S(1.0)
13	1S1 4S1	(1)S(0.0)
14	1S1 4P1	(3)P(4.0)
15	1S1 4D1	(3)D(7.0)
16	1S1 4D1	(1)D(2.0)
17	1S1 4F1	(3)F(10.0)
18	1S1 4F1	(1)F(3.0)
19	1S1 4P1	(1)P(1.0)

N(I)/(NExN(1)) (cm⁶) versus ELECTRON DENSITY (cm⁻³)

Diagnostic line ratios

Consider emissivities of spectrum lines arising from a single ionisation stage. Ratios of such lines are frequently used as temperature, density or transient state diagnostics in plasmas.   The primary advantage of seeking such ratios of lines from a single ionisation stage is that they are independent of the stage to stage ionisation balance (often uncertain). In general it is matter of some investigation to identify the most diagnostically useful ratios.   The present program is designed to aid such investigation. A necessary preliminary to evaluating line emissivities is a calculation of populations of excited states of the ion as a function of plasma parameters.   In practice, problems of line blending and the spectral resolution of spectrometers mean that it is useful to work with line groups rather than just individual lines. A line group, called a composite assembly in ADAS, is a set of lines conveniently or necessarily measured together. For 'line ratio' diagnostics, we deal with two line groups which are built up by the user in the data entry section of the code.

Reall that the solution for the ordinary populations is

$$N_j = \sum_{\sigma=1}^{M} \mathsf{F}_{j\sigma}^{(exc)} N_e N_\sigma + \mathsf{F}_{j1}^{(rec)} N_e N_1^+ + \mathsf{F}_{j1}^{(CX)} N_H N_1^+$$

where the $\mathsf{F}_{j\sigma}^{(exc)}$, $\mathsf{F}_{j1}^{(rec)}$ and $\mathsf{F}_{j1}^{(CX)}$ are the effective contributions to the excited populations from excitation from the metastables, from free electron capture and from charge exchange recombination from neutral hydrogen respectively. Consider now a set of individual lines, or line group, G with

upper levels I_G and lower levels J_G. Let $A_{i \to j}$ be the spontaneous emission coefficient for the line $i \to j$. Then the composite emissivity for the line group is

$$\varepsilon_G = \sum_{j \in J_G, i \in I_G} \varepsilon_{j \to i} = \sum_{j \in J_G, i \in I_G} A_{j \to i} N_j$$

$$= \sum_{j \in J_G, i \in I_G} A_{j \to i} (\sum_{\sigma=1}^{M} \mathsf{F}_{j\sigma}^{(exc)} N_e N_\sigma + \mathsf{F}_{j1}^{(rec)} N_e N_1^+ + \mathsf{F}_{j1}^{(CX)} N_H N_1^+)$$

$$= N_e N_1 \sum_{j \in J_G, i \in I_G} A_{j \to i} (\sum_{\sigma=1}^{M} \mathsf{F}_{j\sigma}^{(exc)} \frac{N_\sigma}{N_1} + \mathsf{F}_{j1}^{(rec)} \frac{N_1^+}{N_1} + \mathsf{F}_{j1}^{(CX)} \frac{N_H}{N_e} \frac{N_1^+}{N_1})$$

expressed in terms of the ratios N_σ / N_1, N_1^+ / N_1 and N_H / N_1. The photon emissivity coefficient for the line group is $\varepsilon_G / N_e N_1$. The coefficient depends on electron density and temperature in general. Ratios of line group emissivities cancel the leading $N_e N_1$ dependence. Modelling diagnostic line ratios involves preparation and operation primarily with a ratio $\varepsilon_{G_1} / \varepsilon_{G_2}$.

ADAS207

The program evaluates and displays line emissivities and their ratios for an ion. It uses a passing file of excited population data from the code ADAS205.

The **file selection window** has the appearance shown below
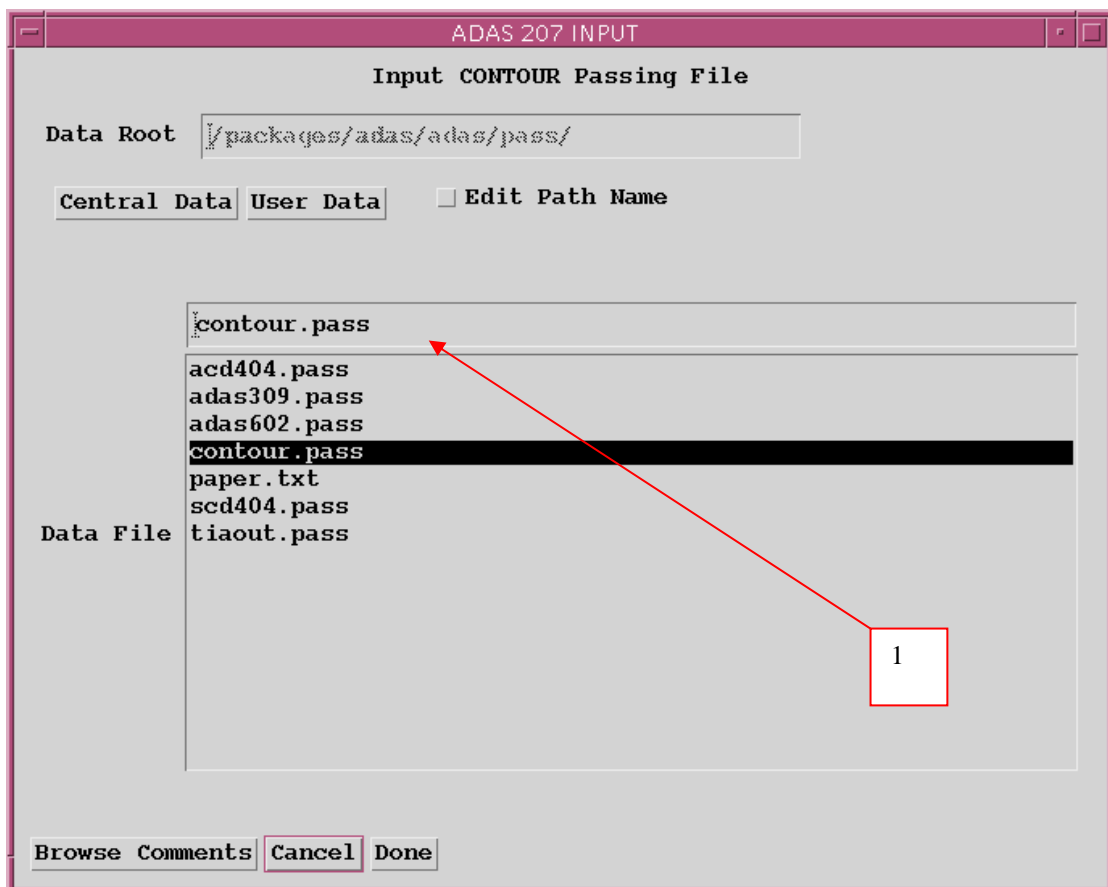
1. The program requires selection of the 'contour' data file prepared as output from ADAS205 (see description of ADAS205). There is no arrangement

for central ADAS storage of such files which reside only in a user's file space and are generally prepared for immediate use

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

1. It displays information from the *contour file* together with information from the ADF04 file used in the prior ADAS205 program run.
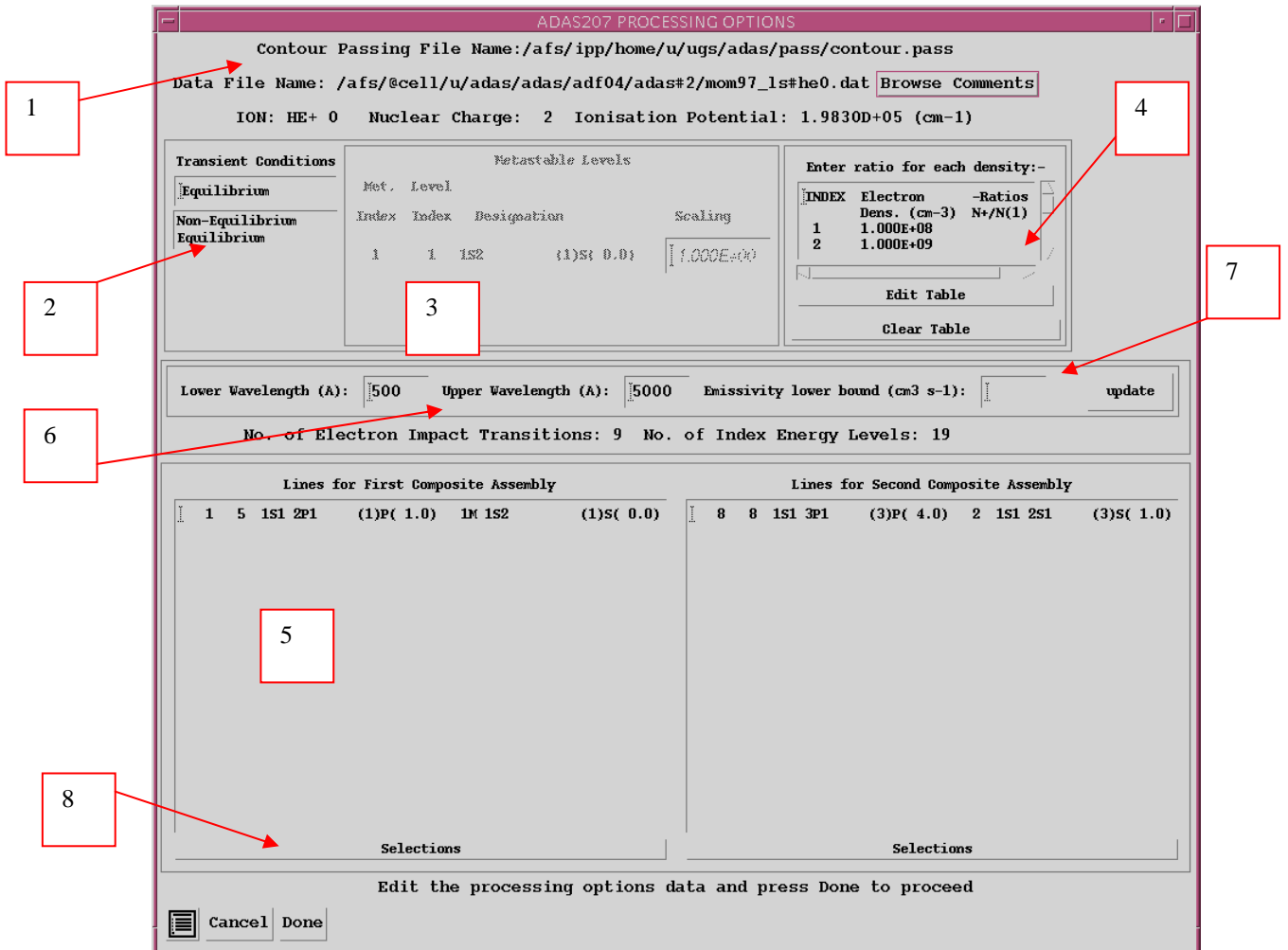
2. Select *Non-equilibrium* or *Equilibrium* conditions by clicking the appropriate case in the list. The selection made is shown in the selection window above. Note that a non-equilibrium choice is only meaningful if there is more than one metastable.

3. The metastables selected in the ADAS205 run are shown in the adjacent window. This window becomes active when non-equilibrium conditions are selected. The values to be entered for each metastable is a multiplier on the equilibrium metastable population. Thus 1.00 for each metastable gives the equilibrium case.

4. If recombination contributions to the line emissivities may be present. Thus the ratio of the number densities of the ground state of the un-ionised ion to the ground state of the ionised ion has to be given.

5. A 'line ratio' in the present context is a ratio of a set of lines for the numerator and a set of lines for the denominator, called first and second composite assemblies respectively. The fist composite assembly is shown in the list window. The columns of each row show the transition index and then for the upper and lower levels of the transition, the level index, configuration designation and the outer quantum numbers. These data are taken from the associated ADF04 file.

6. In practice there may be very many available transitions to make up the composite assemblies. This may be restricted to lines only within a selected wavelength range.
7. A minimum value may also be set for the emissivities of lines to be made available.
8. Each line group is assembled by clicking on the appropriate *Selection* button. A new window is presented with all available transitions listed.

The **composite assembly selection window** has the appearance shown below.

1. Clicking on the button alongside a transition allows it to be selected or de-selected.
2. The first number is the transition index in the ADF04 file.
3. The pair of numbers are the upper and lower level indices form the ADF04 file
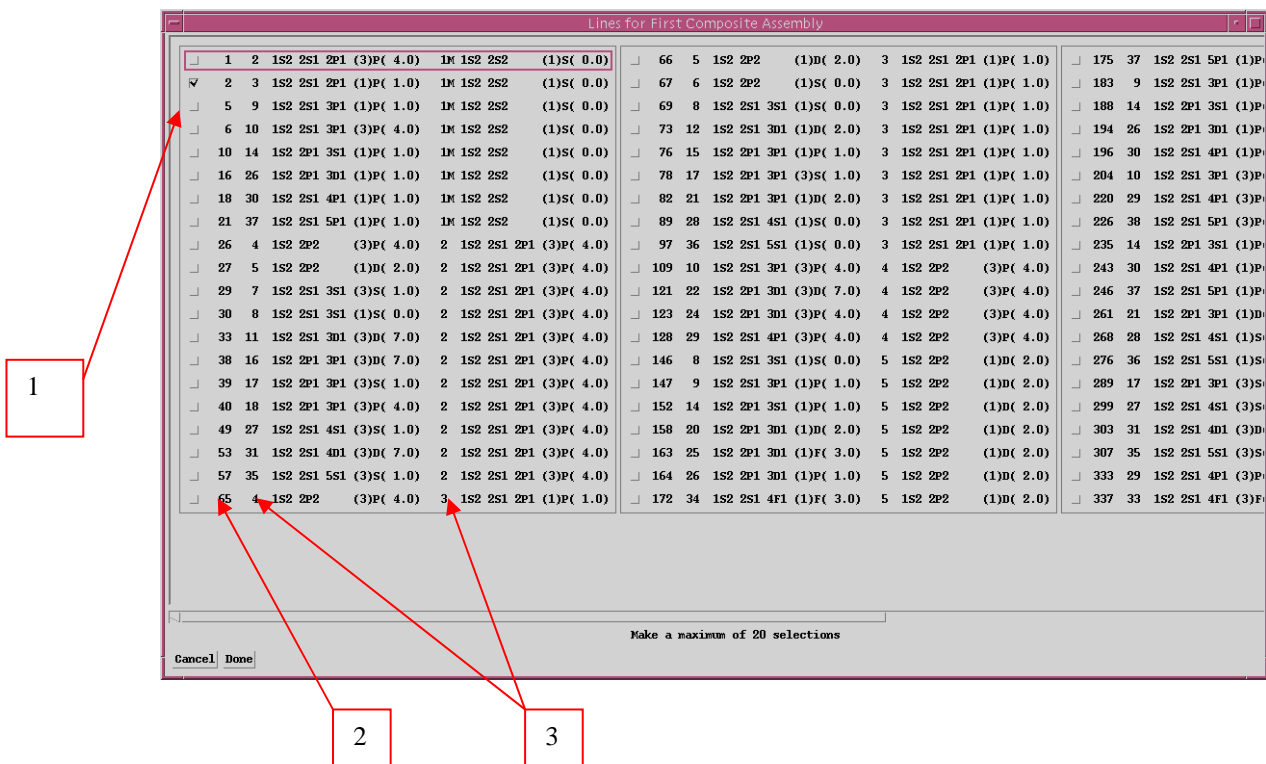
The **output options window** appearance is shown below.

1. The limits of the calculated line group ratio are shown on the output window a). It is important to check this range. Subsequent plots may be selected as logarithmic and it is easy to obtain vanishing line ratios by choice of abnormally low temperatures in the ADAS205 run. In these circumstances meaningless contour plots may be produced.
2. There are three distinct types of plot of the line ratio allowed, namely contours, plots as a function of temperature and plots as a function of density. Click on the appropriate button. The further options selection window changes according to this choice.
3. For the contour plot case, logarithmic or linear choices of contour are permitted. Click on the required type in the lower list window. The chosen type appears in the selection window above.
4. Also the interpolation may be chosen.
5. If *Default contour scaling* is switched off, the table for specifing contour values is activated.

6. 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.
7. 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.
8. 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.
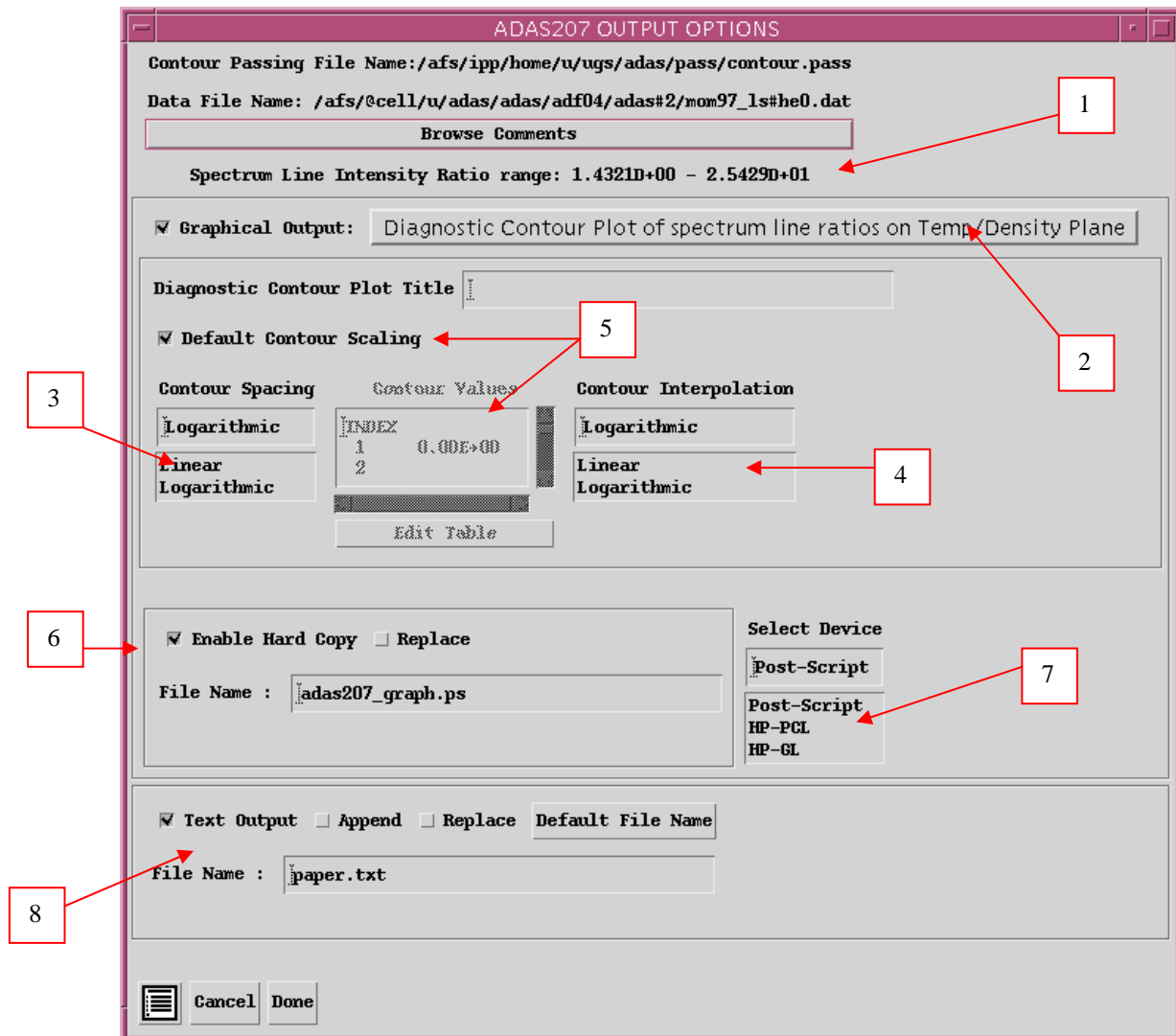
The **Graphical output window** is shown below

1. Printing of the currently displayed graph is activated by the *Print* button.
2. The displayed graph has the usual overall layout, but with supplementary information on the right side listing the line group assemblies and metastable fraction multipliers.
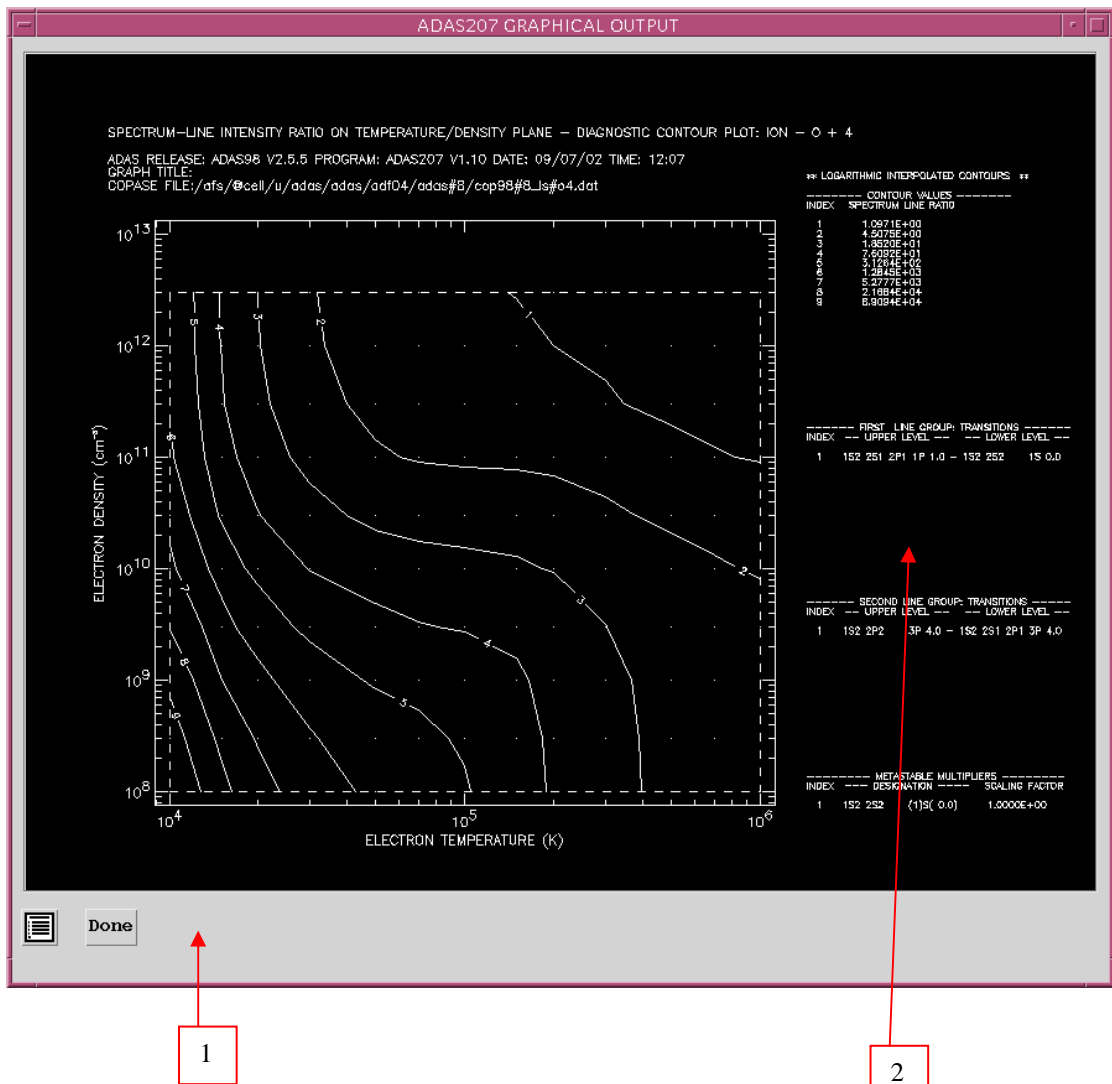
The additional processes and the extended adf04 file

At this stage only the basic adf04 file has been introduced. Full generalised collisional radiative (GCR) modelling requires careful attention to other reactions, especially state selective radiative, dielectronic recombination and electron impact ionisation. Also, by some added care and precision in the specifications of the level list in the *adf04* file, a much higher degree of automatic processing is possible and indeed necessary for complex heavy species. Advanced GCR modelling is addressed later in the course, but some preliminaries are mentioned here

Additional processes and their sources in ADAS

Radiative recombination: State selective radiative recombination coefficients, that is which distinguish the initial recombining ion state (ground or possible metastable) and the final recombined ion state, are archived in data format *adf08*. The code ADAS411 interrogates and displays these data in a similar manner to ADAS201 for electron impact excitation data.

Dielectronic recombination: State selective dielectronic recombination coefficients, that is which again distinguish the initial recombining ion state (ground or possible metastable) and the final recombined ion state, are archived in data format *adf09*. The code ADAS410 interrogates and displays these data. The data are very extensive. Dielectronic recombination is required to very highly excited

states and so the adf09 tabulations include term and level distinguished data for low levels and bundled nl-shell up to n~12 and bundled n-shell data up to n~1000. The precise organisation depends on whether we are working in 'term' resolution or 'level' resolution.

Collisional ionisation: State selective electron impact ionisation coefficients, that is which distinguishes the initial ionising ion state (ground, metastable or excited) and the final ionised ion state (ground or metastable), are archived in data formats *adf07* and *adf23*. *adf23* is the principal data class of this type. *adf07* is restricted to ground and metastables only and was created before the more complete data became available. Code ADAS502 interrogates and displays data of format *adf07*. ADAS413 interrogates and displays data of format *adf23*.

Extending the adf04 file

Transition lines denoting other processes: The first character position of a transition line in an *adf04* file is an alphanumeric code (CCODE –see ADAS User manual appxa-04)

CCODE   transition data type code as follows:

' ' => unspecified electron impact excitation data

'1' => dipole electron impact excitation data

'2' => non-dipole, non-spin change electron impact excitation data

'3' => spin change electron impact excitation data

'p' or 'P' => positive ion impact excitation data

'r' or 'R' => free electron recombination/capture data

'h' or 'H' => charge exchange recombination data from neutral hydrogen

'i' or 'I' => electron impact ionisation data from stage below

's' or 'S' => electron impact ionisation data to stage above

'l' or 'L' => unresolved dielectronic satellite line emission data

```
C + 3        6        4        520178.4(1S)   2931440.0(3S)
    1 1s2 2s1          (2)0( 0.5)        0.0   {1}1.000 {2}1.500
    2 1s2 2p1          (2)1( 2.5)     64555.4  {1}1.000
    3 1s2 3s1          (2)0( 0.5)    302849.0  {1}1.000
  .     .      .
   10 1s2 5s1          (2)0( 0.5)    445368.5  {1}1.000
   11 1s2 5p1          (2)1( 2.5)    448860.5  {1}1.000
   12 1s2 5d1          (2)2( 4.5)    449889.2  {1}1.000
   13 1s2 5f1          (2)3( 6.5)    449939.8  {1}1.000
   14 1s2 5g1          (2)4( 8.5)    449948.4  {1}1.000
   -1
    4.0    3        8.00+03 1.60+04 3.20+04 8.00+04 1.60+05 3.20+05 8.00+05 1.60+06 3.20+06 8.00+06 1.60+07
    3    1 1.00-30 5.68-01 5.49-01 5.16-01 4.46-01 3.96-01 3.84-01 3.87-01 3.83-01 3.83-01 3.85-01 3.86-01
    5    1 4.57+05 4.90-01 4.97-01 5.11-01 5.43-01 5.79-01 6.24-01 7.90-01 9.58-01 1.08+00 1.18+00 1.21+00
        .     .      .
   13   12 1.65+02 3.32+03 3.64+03 3.96+03 4.38+03 4.70+03 5.02+03 5.45+03 5.77+03 6.09+03 6.51+03 6.83+03
   14    9 1.09+09 1.59+02 1.64+02 1.74+02 2.06+02 2.53+02 3.22+02 4.48+02 5.63+02 6.89+02 8.69+02 1.01+03
    9    1 1.00-30 9.51-02 9.39-02 9.15-02 8.57-02 7.94-02 7.31-02 6.89-02 6.82-02 6.81-02 6.80-02 6.80-02
R   1   +1         4.33-13 3.08-13 2.19-13 1.41-13 1.01-13 7.39-14 9.62-14 1.34-13 1.09-13 4.80-14 2.13-14
R   2   +1         1.41-12 9.87-13 6.84-13 4.09-13 2.67-13 1.66-13 1.34-13 1.66-13 1.33-13 5.71-14 2.43-14
        .     .
R  13   +2         4.57-10 1.86-10 7.46-11 2.03-11 7.36-12 2.63-12 6.72-13 2.38-13 8.43-14 2.13-14 7.54-15
R  14   +2         9.73-12 3.92-12 1.56-12 4.24-13 1.53-13 5.49-14 1.40-14 4.96-15 1.76-15 4.44-16 1.57-16
S   1   +1         6.19-10 6.73-10 9.77-10 1.44-09 1.87-09 2.31-09 2.80-09 3.00-09 3.03-09 2.79-09 2.46-09
S   1   +2         4.07-11 4.01-11 3.98-11 5.45-11 8.12-11 1.12-10 1.69-10 2.23-10 2.80-10 3.39-10 3.58-10
   -1
   -1   -1
```

Recombination line

Ionisation line