2a. The interactive system - working with adf04 datasets

- Preliminaries
  - » Electron impact cross-sections and rate coefficients
  - » The ADF04 file format
  - » Interrogating adf04 collisional excitation data using ADAS201 and ADAS811

Electron impact cross-sections and rates

The excitation reaction $X_i^{+z}(E_i) + e(\varepsilon_i) \rightarrow X_j^{+z}(E_j) + e(\varepsilon_j)$

is described by an excitation cross-section $\sigma_{i\rightarrow j}(\varepsilon_i)$

More useful for tabulation is the collision strength Ω_{ij} with independent variable

$X = \varepsilon_i / \Delta E_{ij}$ with $X \in [1, \infty]$

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

ADAS principally deals with Maxwell averaged rate coefficients $q_{i\rightarrow j}(T_e)$

Υ_{ij} $\quad \Upsilon_{ij} = \int_0^\infty \Omega_{ij}(\varepsilon_j) \exp(-\varepsilon_j / kT_e)\, d(\varepsilon_j / kT_e)$

Electron impact cross-sections and rates (contd.)

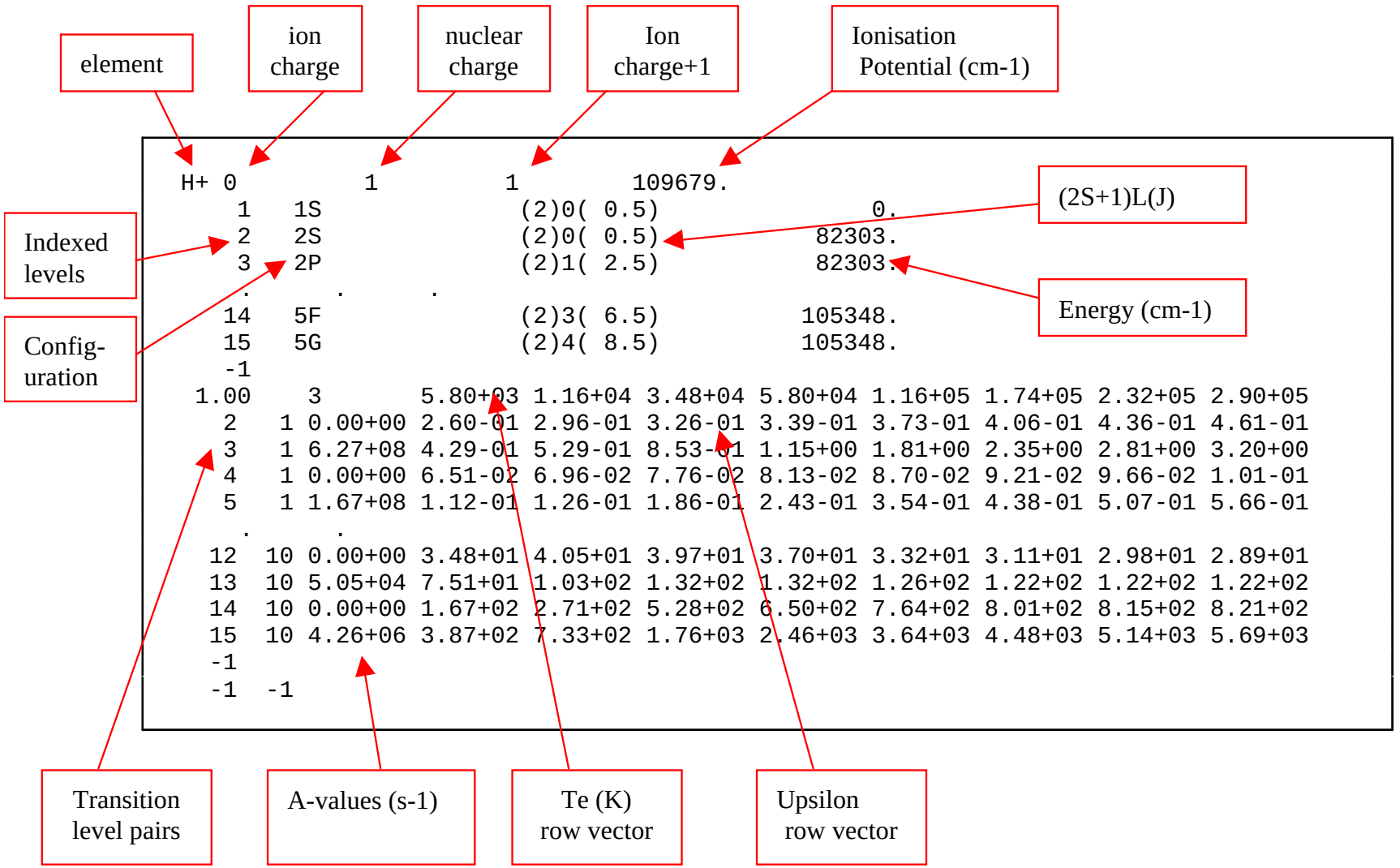
More useful for tabulation is the Maxwell averaged collision strength $\Upsilon_{ij}(T_e)$

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

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

The ADAS adf04 format is used to archive sets of energy level lists, A-values and Maxwell averaged collision strengths for an ion sufficient to allow a population calculation.

The basic adf04 file




```
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
```

Configuration specification

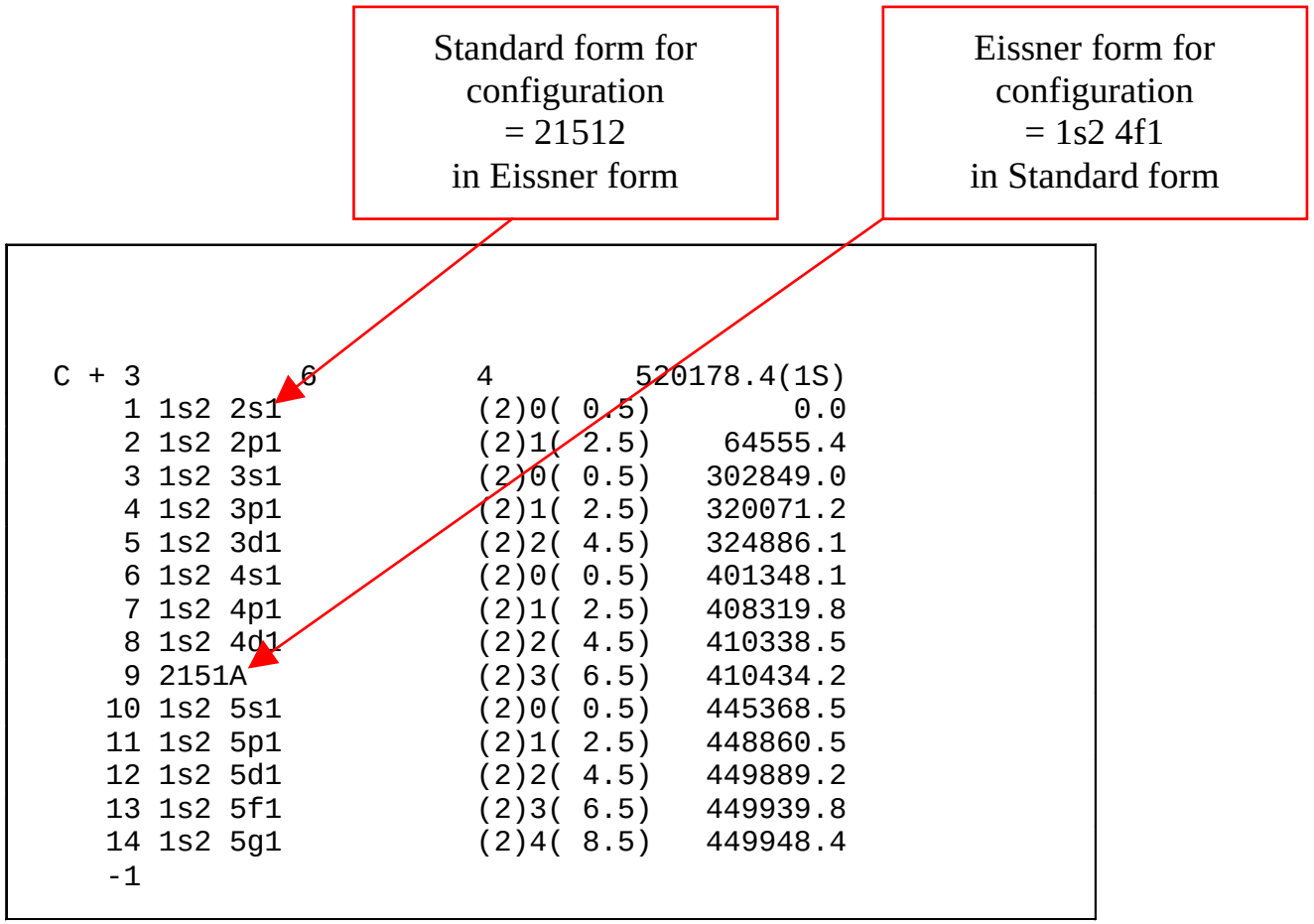
$$\Gamma = n_1 l_1^{q_1} n_2 l_2^{q_2} \ldots\ldots n_m l_m^{q_m}$$

where $q_i > 0$ for $i = 1,\ldots,m$ and $\sum_{i=1}^{m} q_i = N$

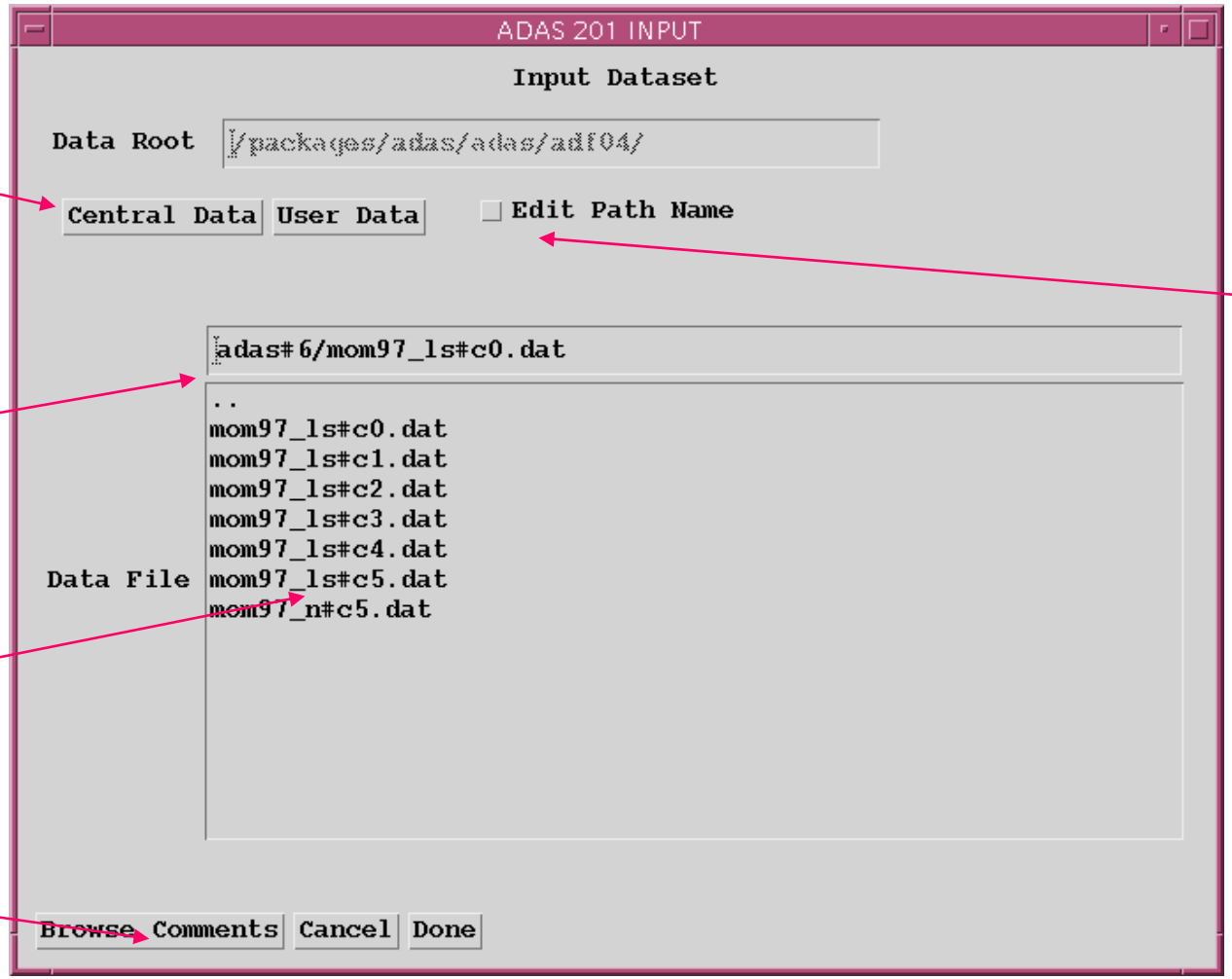
ADAS prefers Standard and Eissner configuration representations in ADF04 files for automatic processing and matching of levels between different data sets.

Configuration	Standard form	Eissner form
$1s^2 2s^2 2p^4$	1s2 2s2 2p4	21522543
$1s^2 2s^2 2p^6 6f^{11}$	1s2 2s2 2p6 6fb	2152254361J

The basic adf04 file



ADAS201 input



click to use central ADAS data

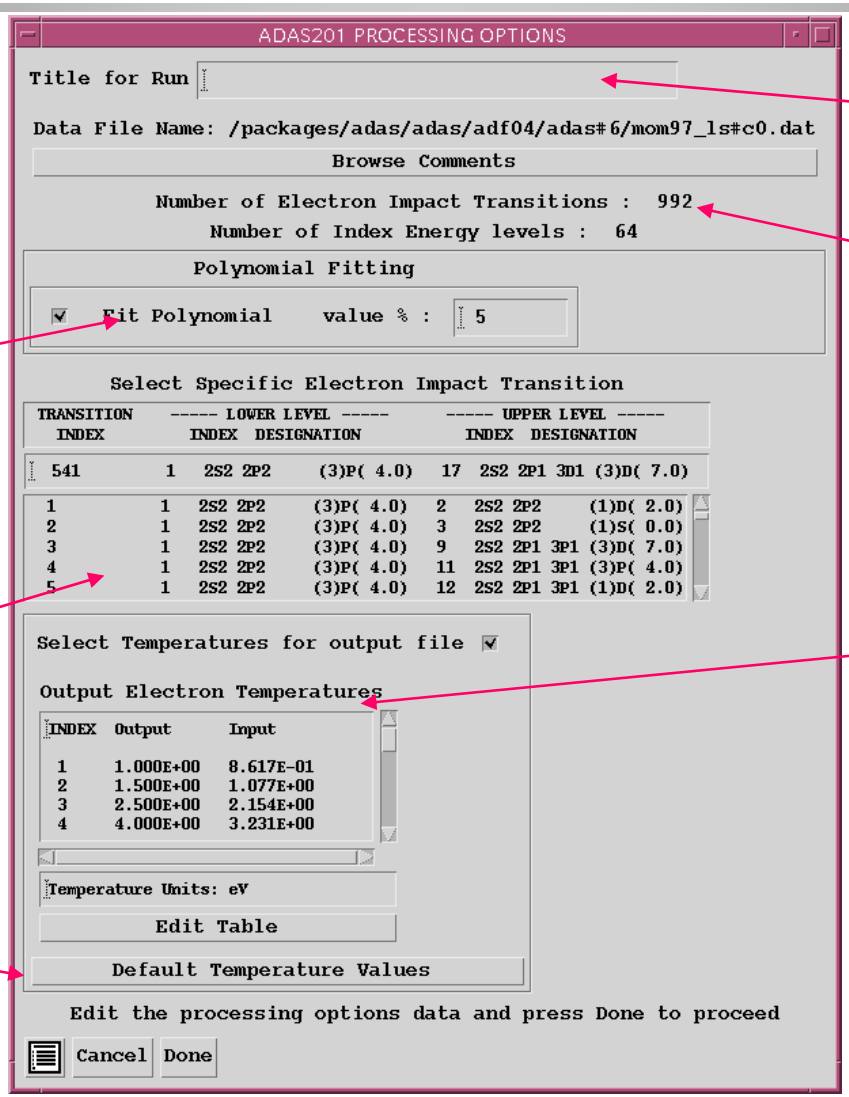
selected file for processing

ADF04 data file list

browse comments from selected data set

click to edit pathway

ADAS201 Processing



your title to appear on graphs & tables

number of transitions and levels

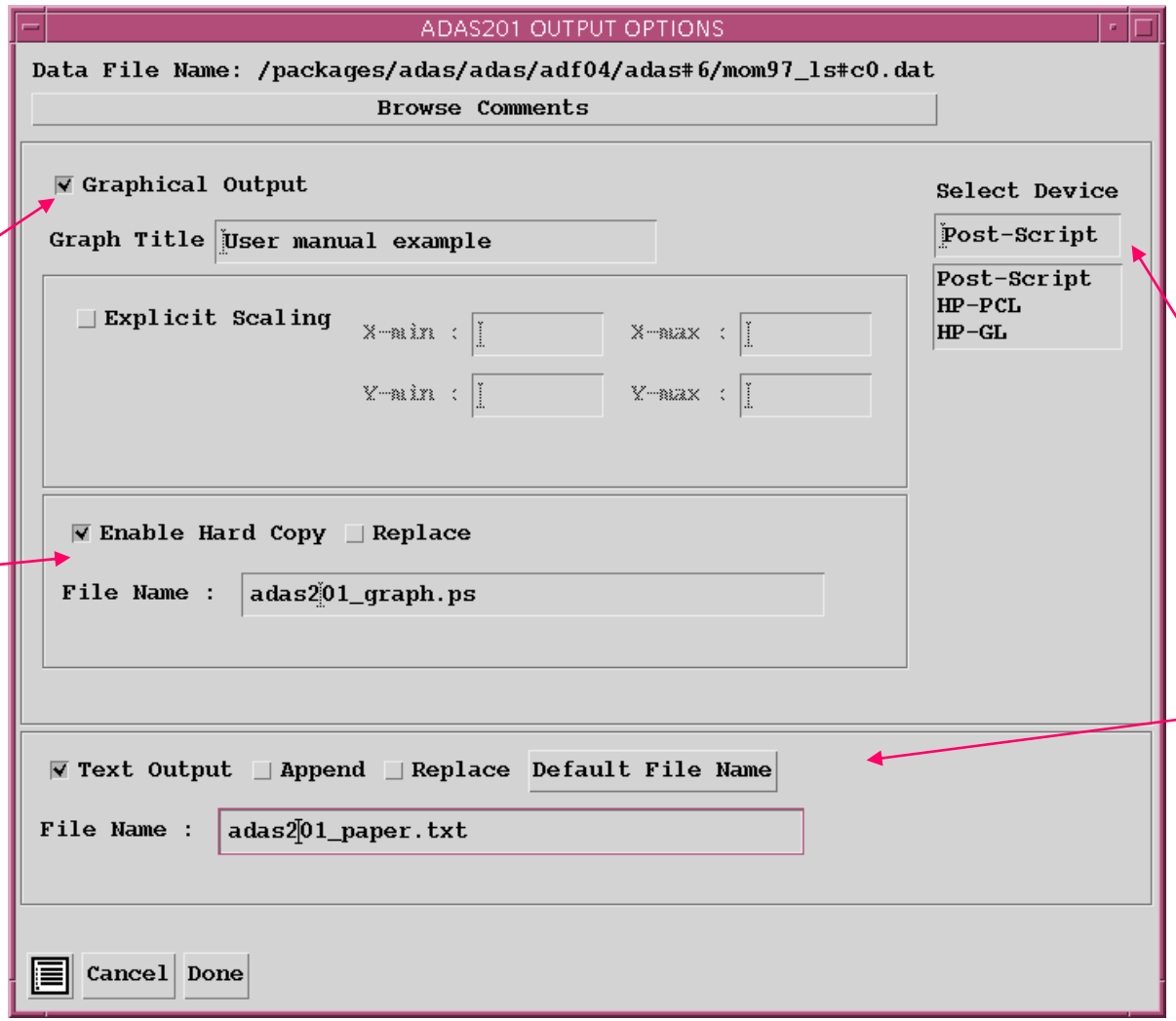
make polynomial fit to data

select transition for analysis

Select & enter Te values for output

set default output values

ADAS201 Output



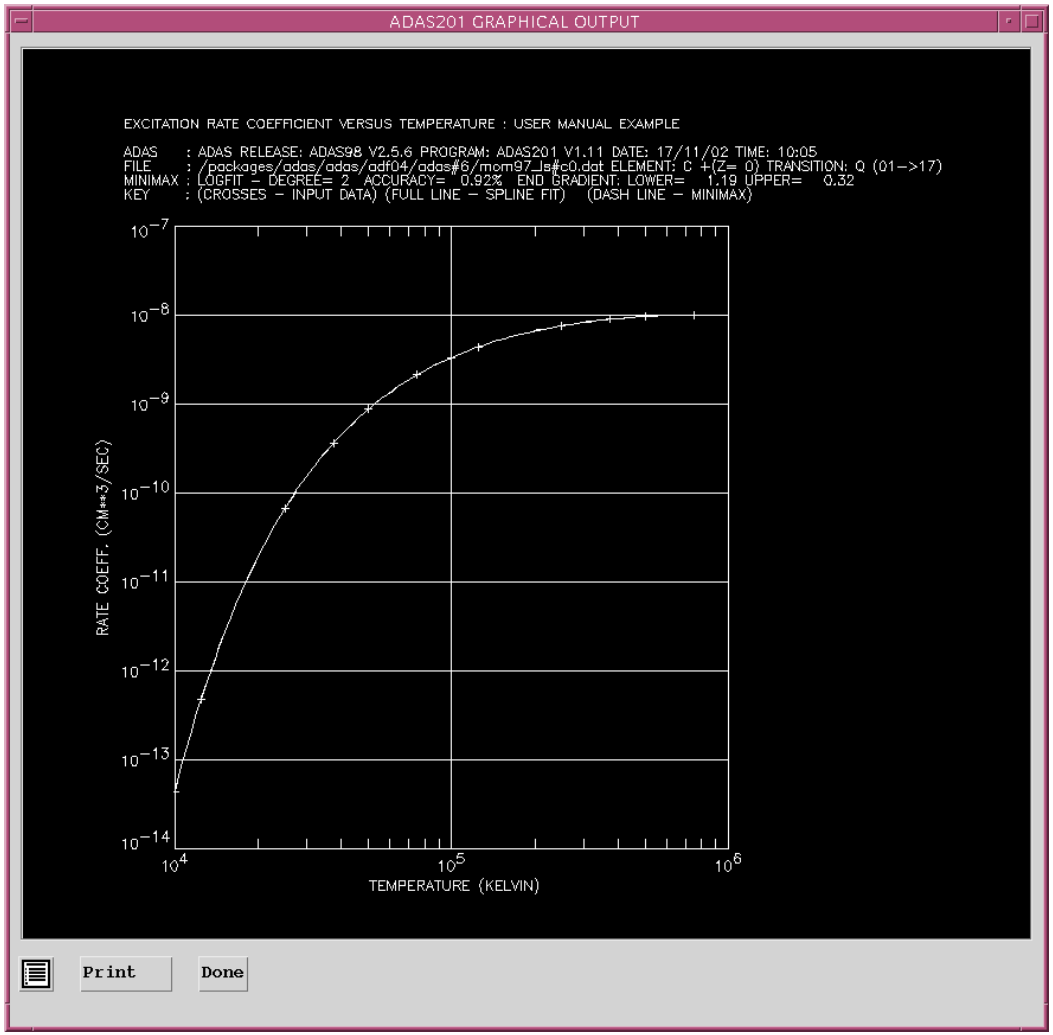
provide graphical output

allow graphical hard copy

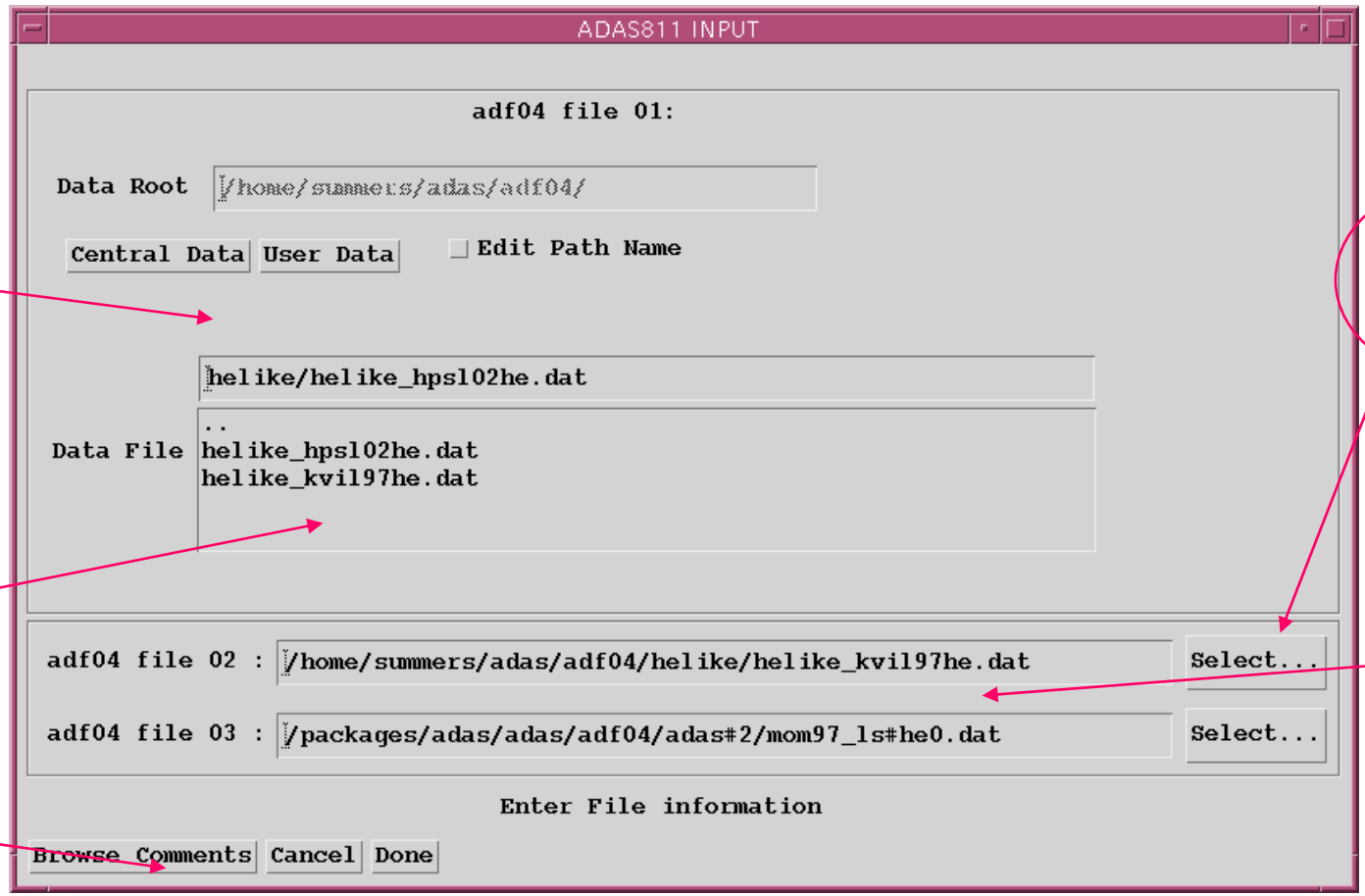
graphical output file coding

tabular output of results

ADAS201 Graph



ADAS811 input



Select first file

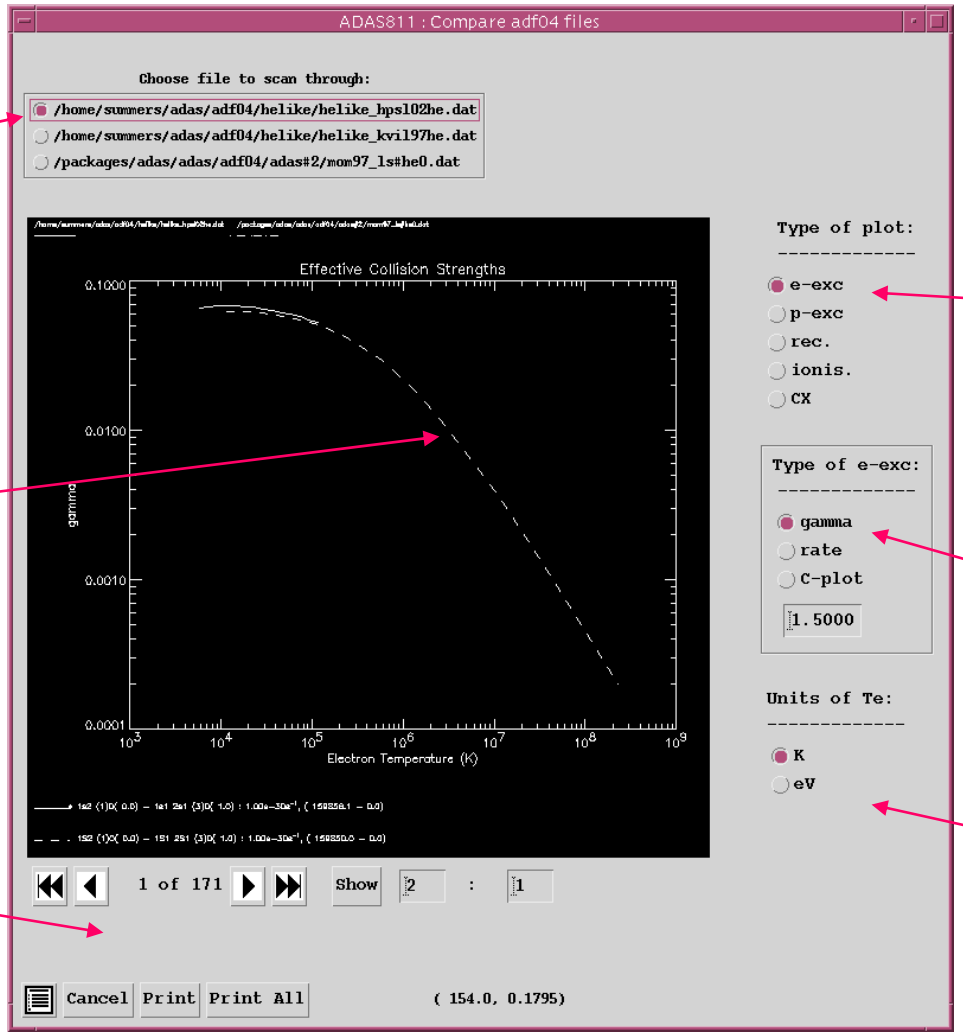
ADF04 data file list

browse comments from first data set

Click to show file chooser pop-up

Second and third files

ADAS811 Processing



select file to cycle through

comparative graph for matched transitions

tape recorder keys

select type e-exc

select type of e-exc display

select Te units

2b. The interactive system – working with excited population structure

- Datasets of class ADF04 contain all the information necessary to evaluate excited populations of an ion. It is called a ‘specific ion file’.
- Code ADAS205 computes the populations at temperatures and densities of your choice.
- The input, data set selection, screen is very similar to that for ADAS201

Populations calculation (contd.)

Distinguish metastable levels X_{ρ}^{+z} indexed by Greek letters

and ordinary levels X_{i}^{+z} indexed by Roman letters

Write the quasi-static equations for the ordinary levels populations in terms of the metastable populations as:

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

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

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

Populations calculation (contd.)

Solution for the ordinary populations is

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

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

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

Populations calculation (contd.)

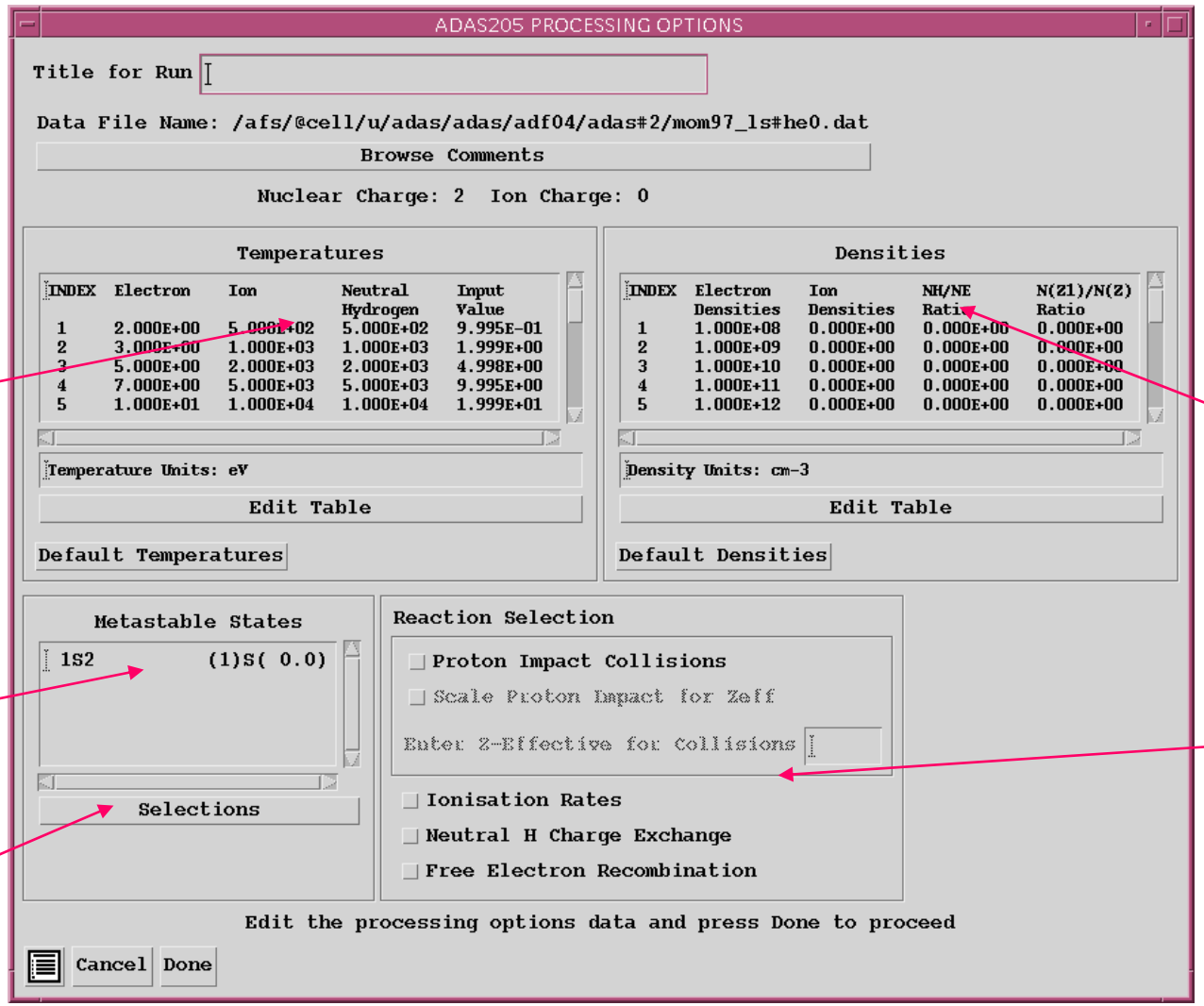
Spectrum line emissivities are

$$\varepsilon_{j\to k} = A_{j\to k}\Big(\sum_{\sigma=1}^{M} \mathrm{F}_{j\sigma}^{(exc)} N_e N_\sigma + \sum_{\upsilon'=1}^{M_{z+1}} \mathrm{F}_{j\upsilon'}^{(rec)} N_e N_{\upsilon'}^{+} + \sum_{\upsilon'=1}^{M_{z+1}} \mathrm{F}_{j\upsilon'}^{(CX)} N_H N_{\upsilon'}^{+} + \sum_{\mu'=1}^{M_{z-1}} \mathrm{F}_{j\mu'}^{(ion)} N_e N_{\mu'}^{-}\Big)$$

Identify excitation and recombination photon emissivity coefficients as

$$\boxed{\mathrm{PEC}_{\sigma,j\to k}^{(exc)} = A_{j\to k}\mathrm{F}_{j\sigma}^{(exc)}} \qquad \mathrm{PEC}_{\upsilon',j\to k}^{(rec)} = A_{j\to k}\mathrm{F}_{j\upsilon'}^{(rec)}$$

ADAS205 processing



Te grid specification

Ne grid specification

Designated metastables

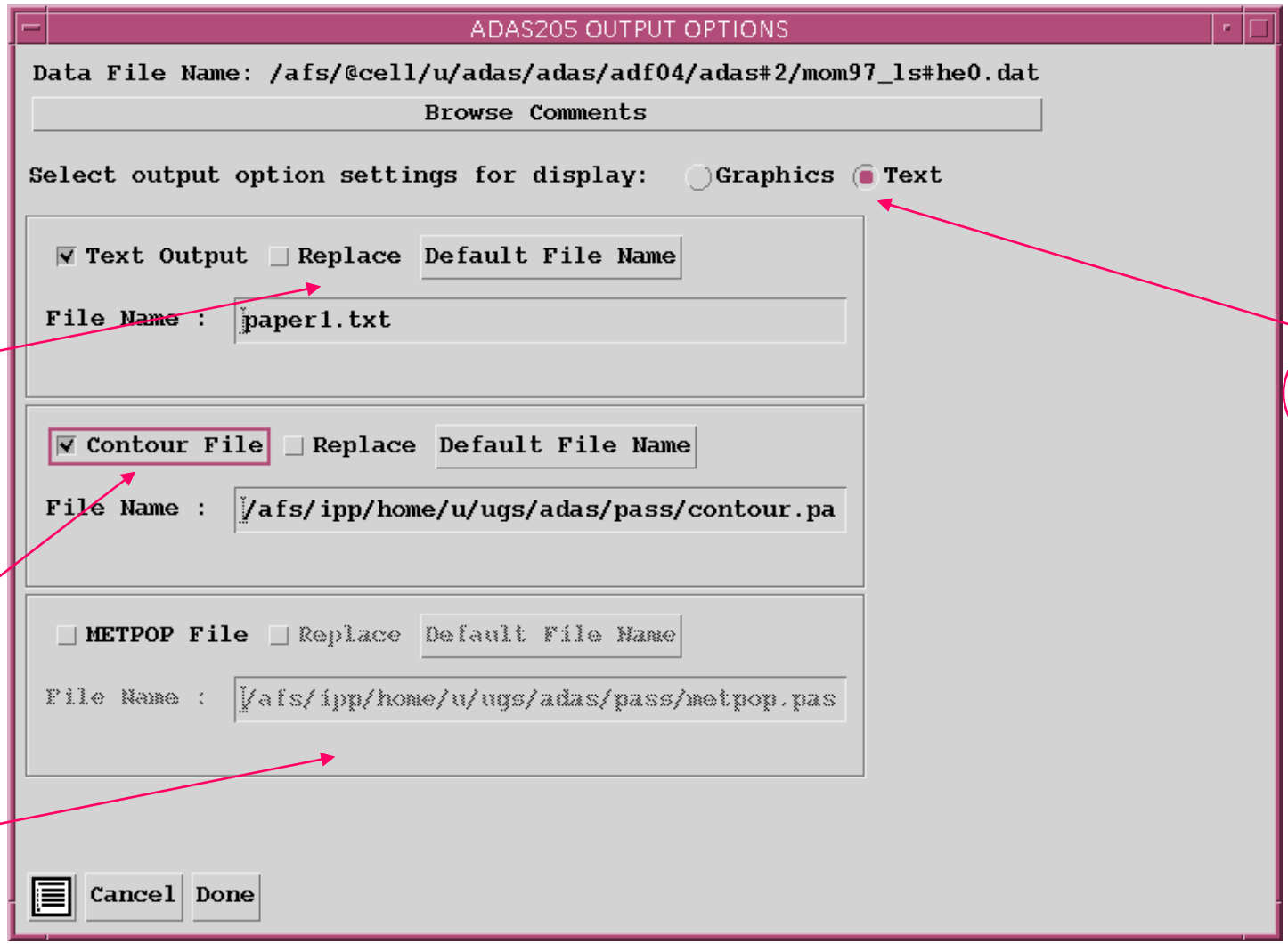
advanced process control

activate to select metastables

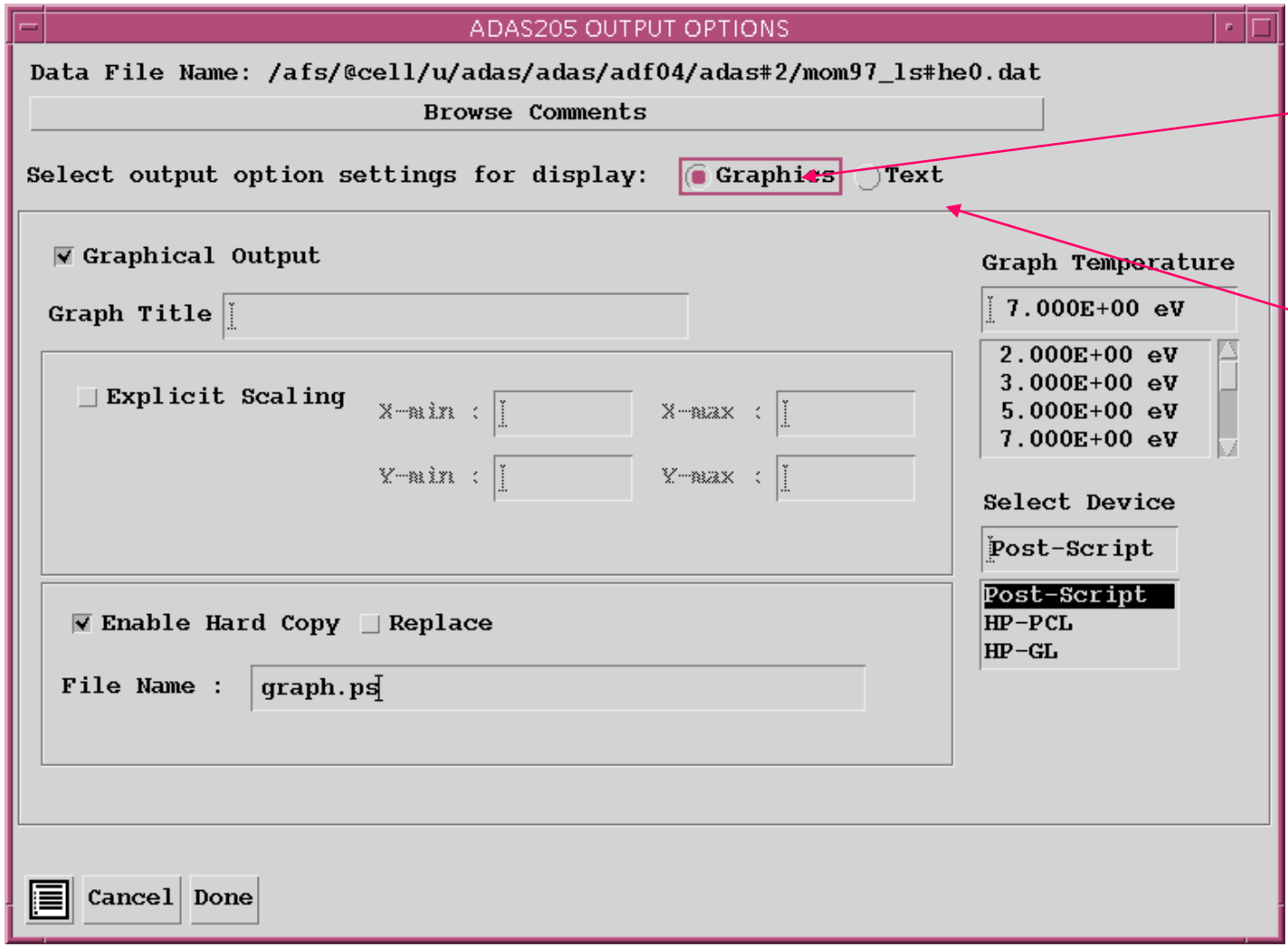
Populations and line ratio studies (contd.)

- Output options
  - » Graphical display of the $F_{j\sigma}^{(exc)}$ as a function of density is allowed.
  - » An output file of the $F_{j\sigma}^{(exc)}$, called the ‘contour’ pass file, can be generated. This file must be created to allow the next step of looking a line ratios.

ADAS205 output - text



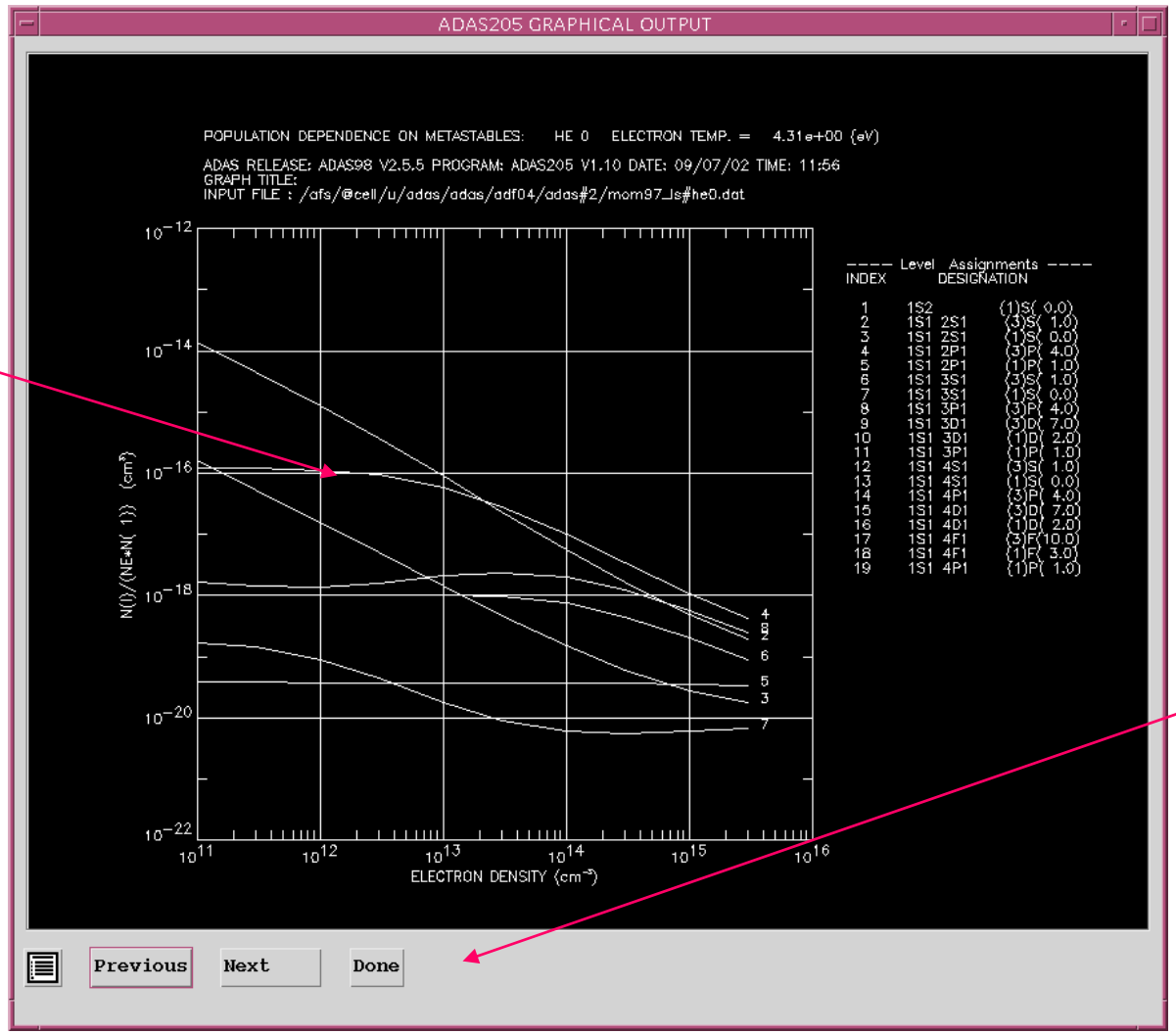
ADAS205 output - graphics



show graphic output choices

graphs may be shown at one Te only

ADAS205 graph



excited population graph

Print button is present if graphic file chosen

Setting up lines

- Code ADAS207 is the diagnostic analysis program which allows study of line ratios.

- It needs the ‘contour’ pass file of populations. It also fetches the specific ion file, of type ADF04, which was used in the population calculation.

Setting up lines (contd.)

The program in deals with two line assemblies which from the numerator and denominator of the line ratio.

The composite emissivity for a line assembly is written as

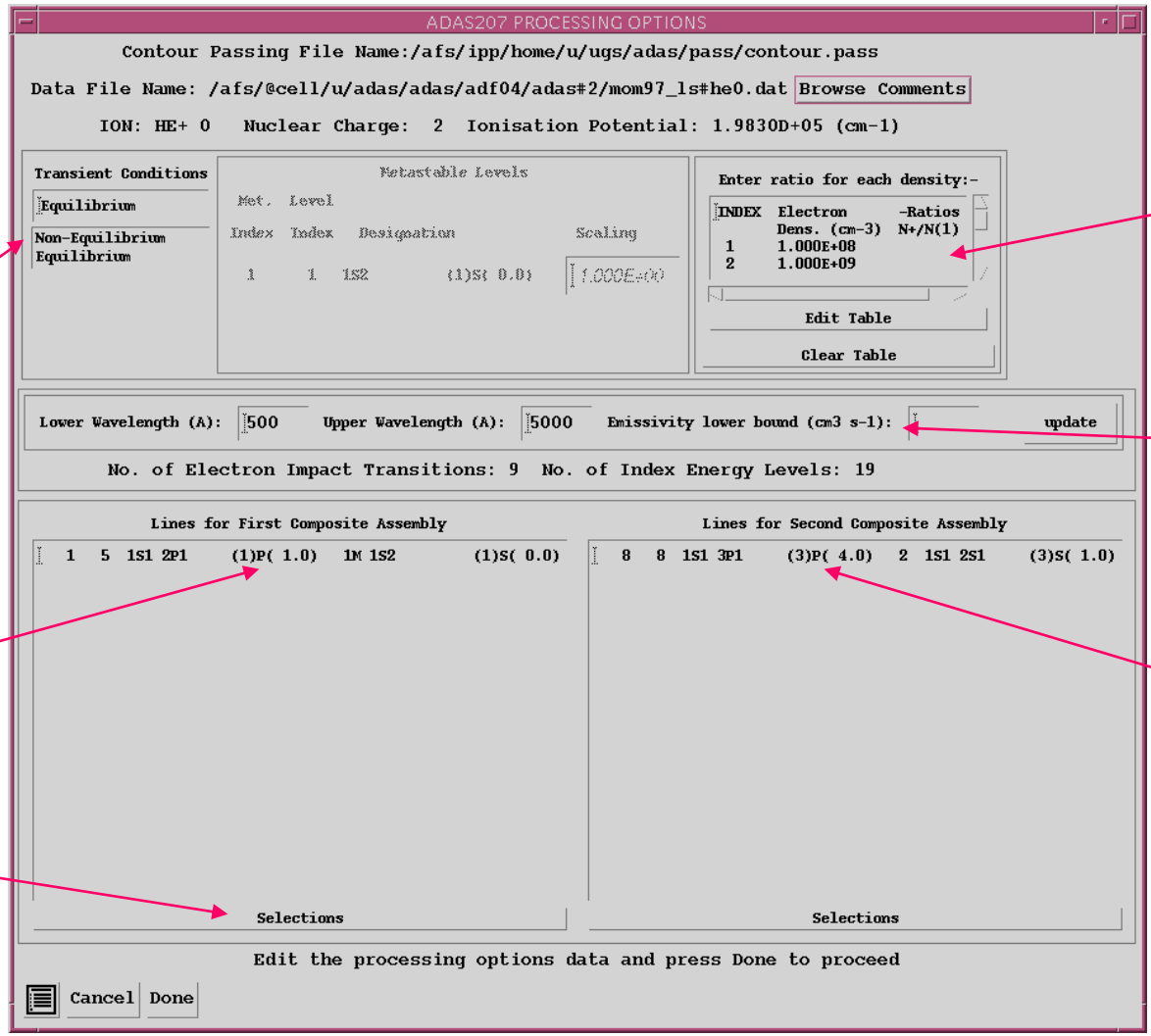
$$\varepsilon_G = \sum_{j\in J_G, i\in I_G} \varepsilon_{j\to i} = \sum_{j\in J_G, i\in I_G} A_{j\to i} N_j$$

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

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

Diagnostic line ratio modelling deals with $\varepsilon_{G_1} / \varepsilon_{G_2}$

ADAS207 processing



advanced use with metastables

lines in numerator of ratio

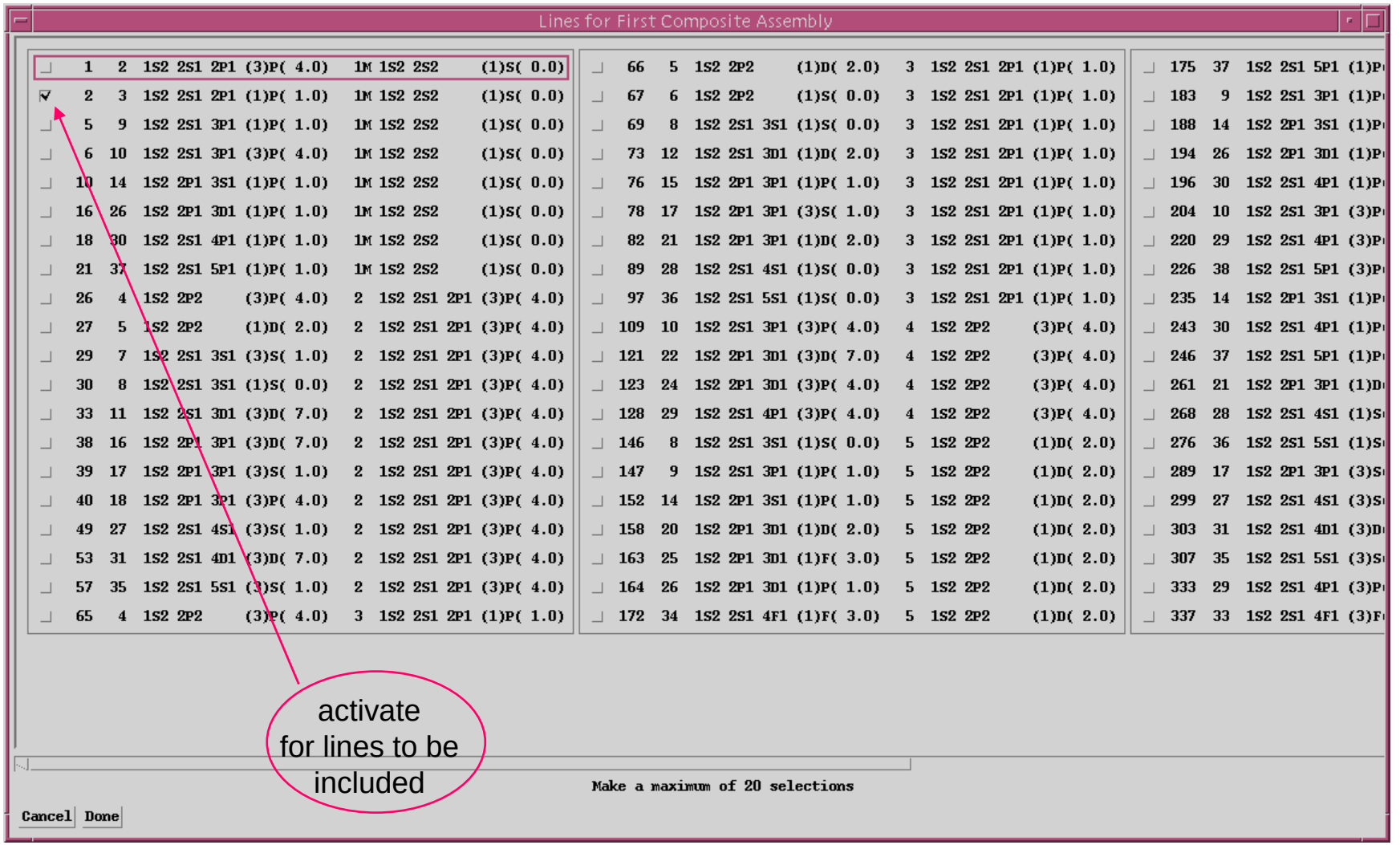
show line selection list

advanced use for recombination

restrict the choice of lines

lines in denominator of ratio

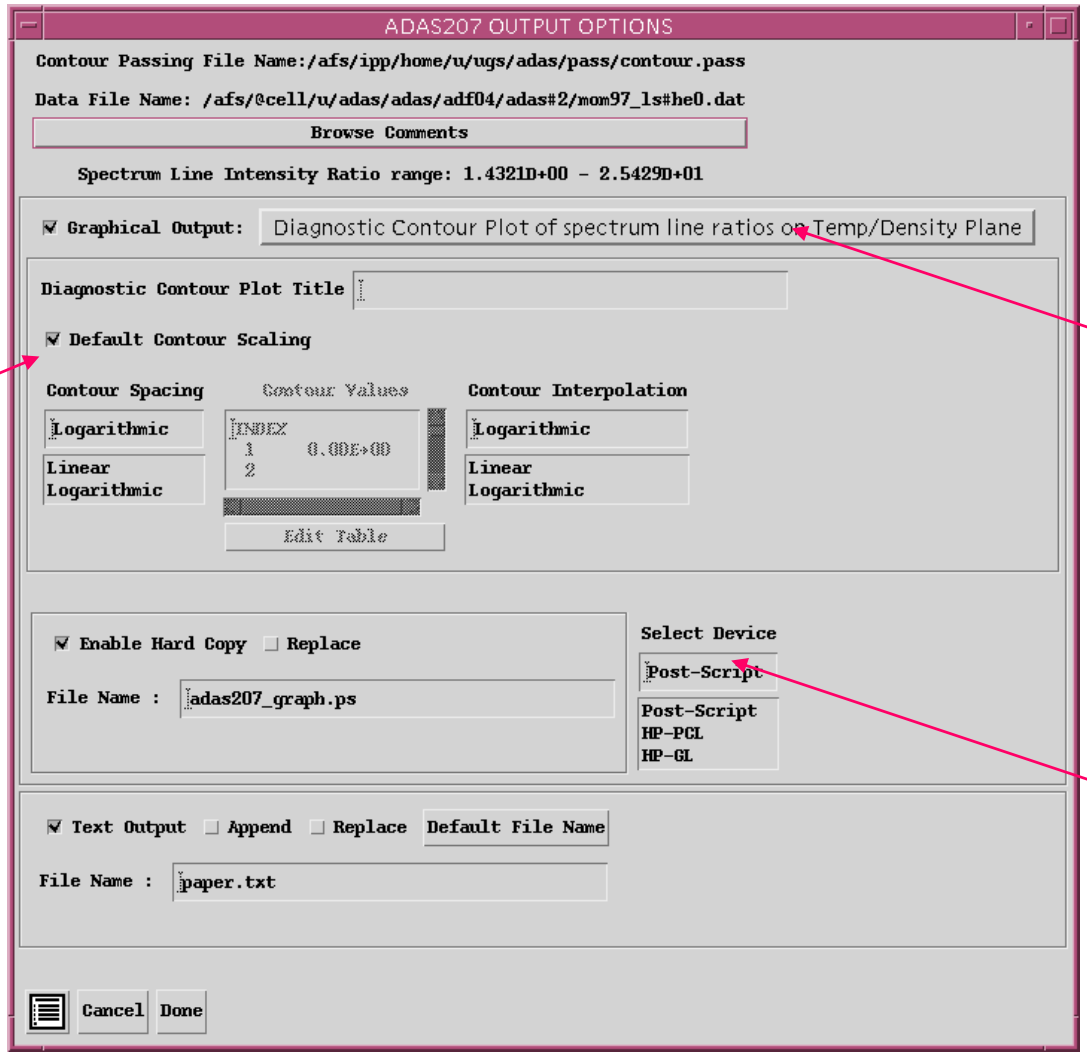
ADAS207 line assembly



Displaying line ratios

- Output options
  - » The type of display of the ratio of line assemblies may be chosen.
  - » The contour form on the Te/Ne plane seems to be the favourite.
  - » Crosses on the graph mark the tabular points at which the populations were explicitly evaluated.
  - » The extensive range of controls on the plot scales and contour lines should be used to refine the diagnostic plot.

ADAS207 output

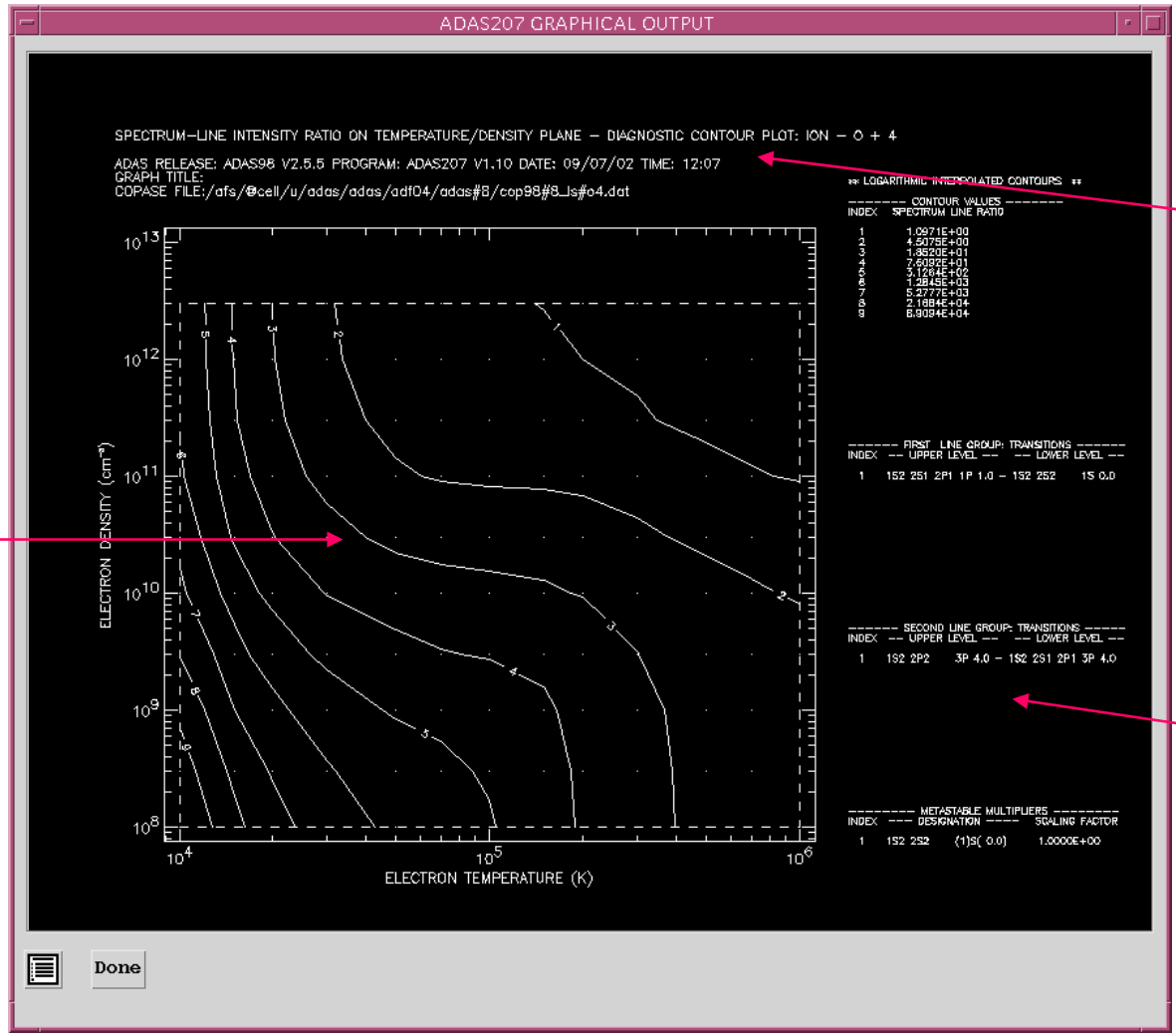


controls on contour plotting

select type of plot

usual graph and text output choices

ADAS207 graph



unique record of case studied

final line ratio contours

details of graph presented