

ADAS207: Metastable and excited population - process line emissivities

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.

Background theory:

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. This is provided by ADAS205 which must be executed before ADAS207. 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 is a set of lines conveniently or necessarily measured together. ADAS207 deals with two line groups which are built up by the user in the data entry section of the code.

From equation 2.5.4, the solution for the ordinary populations is

$$N_j = \sum_{\sigma=1}^M F_{j\sigma}^{(exc)} N_e N_\sigma + F_j^{(rec)} N_e N_1^+ + F_j^{(CX)} N_H N_1^+ \quad 2.7.1$$

where the $F_{j\sigma}^{(exc)}$, $F_j^{(rec)}$ and $F_j^{(CX)}$ 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.

Consider a set of individual lines, or line group, G with upper levels I_G and lower levels J_G . Let $A_{i \rightarrow j}$ be the spontaneous emission coefficient for the line $i \rightarrow j$.

Then the composite emissivity for the line group is

$$\begin{aligned} \mathcal{E}_G &= \sum_{j \in J_G, i \in I_G} \mathcal{E}_{j \rightarrow i} = \sum_{j \in J_G, i \in I_G} A_{j \rightarrow i} N_j \\ &= \sum_{j \in J_G, i \in I_G} A_{j \rightarrow i} \left(\sum_{\sigma=1}^M F_{j\sigma}^{(exc)} N_e N_\sigma + F_j^{(rec)} N_e N_1^+ + F_j^{(CX)} N_H N_1^+ \right) \\ &= N_e N_1 \sum_{j \in J_G, i \in I_G} A_{j \rightarrow i} \left(\sum_{\sigma=1}^M F_{j\sigma}^{(exc)} \frac{N_\sigma}{N_1} + F_j^{(rec)} \frac{N_1^+}{N_1} + F_j^{(CX)} \frac{N_H}{N_e} \frac{N_1^+}{N_1} \right) \end{aligned}$$

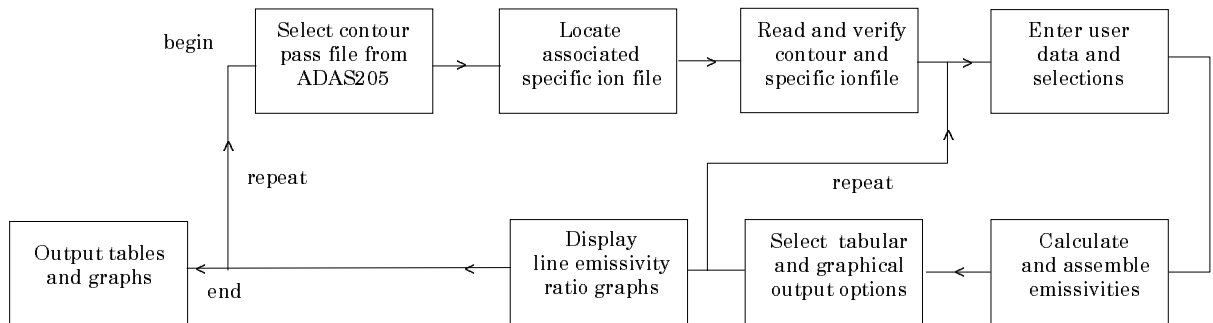
2.7.2

expressed in terms of the ratios N_σ / N_1 , N_1^+ / N_1 and N_H / N_e . The photon emissivity coefficient for the line group is $\mathcal{E}_G / N_e N_1$. The coefficient depends on electron density and temperature in general. Ratios of line group emissivities cancel the leading $N_e N_1$ dependence. The code prepares and operates primarily with a ratio $\mathcal{E}_{G_1} / \mathcal{E}_{G_2}$.

Program steps:

These are summarised in the figure 2.7.

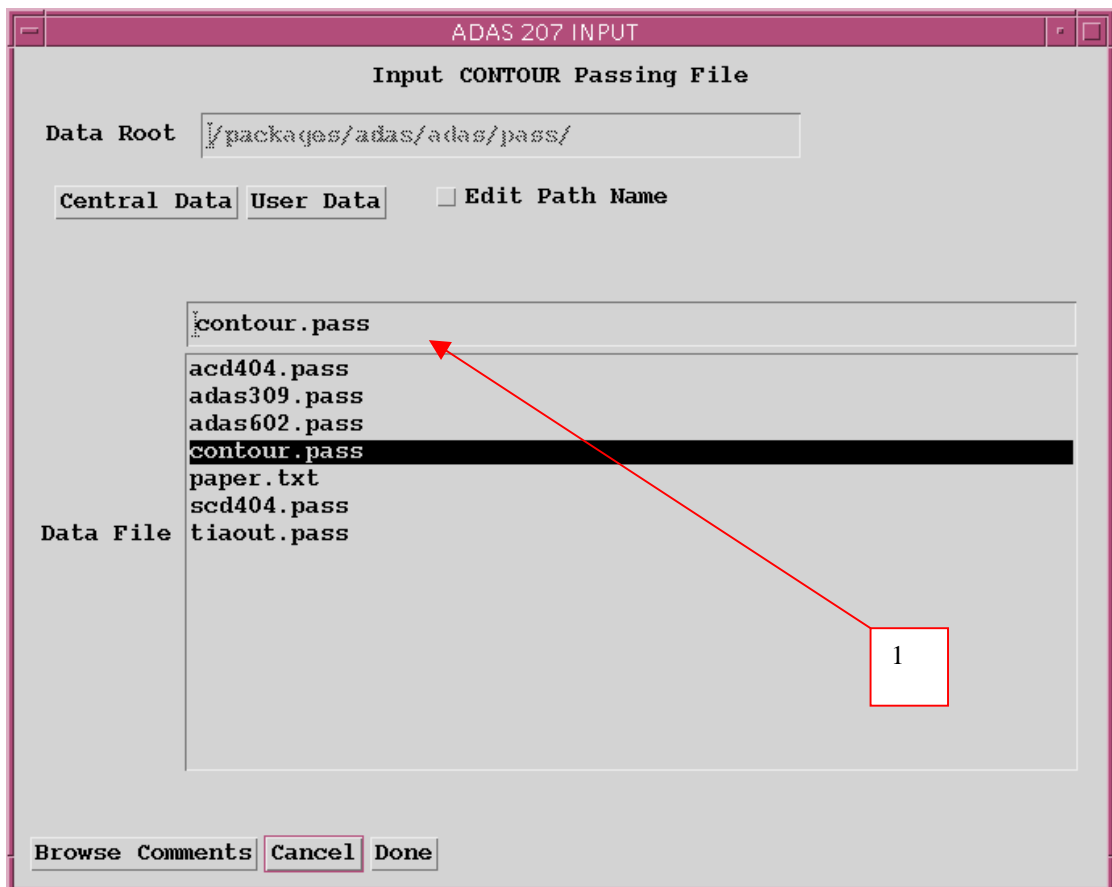
Figure 2.7



Interactive parameter comments:

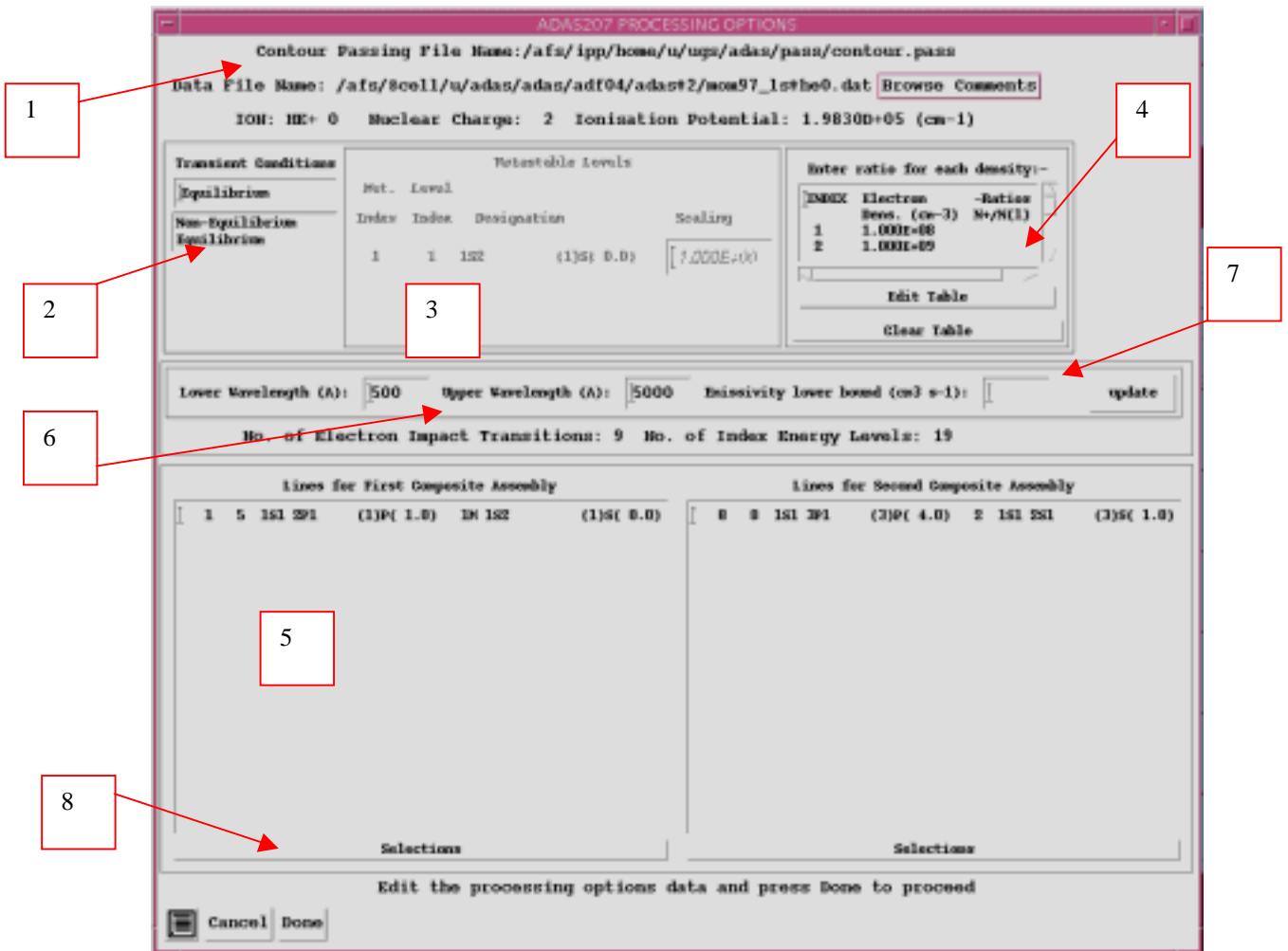
The **file selection window** has the appearance shown below

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.

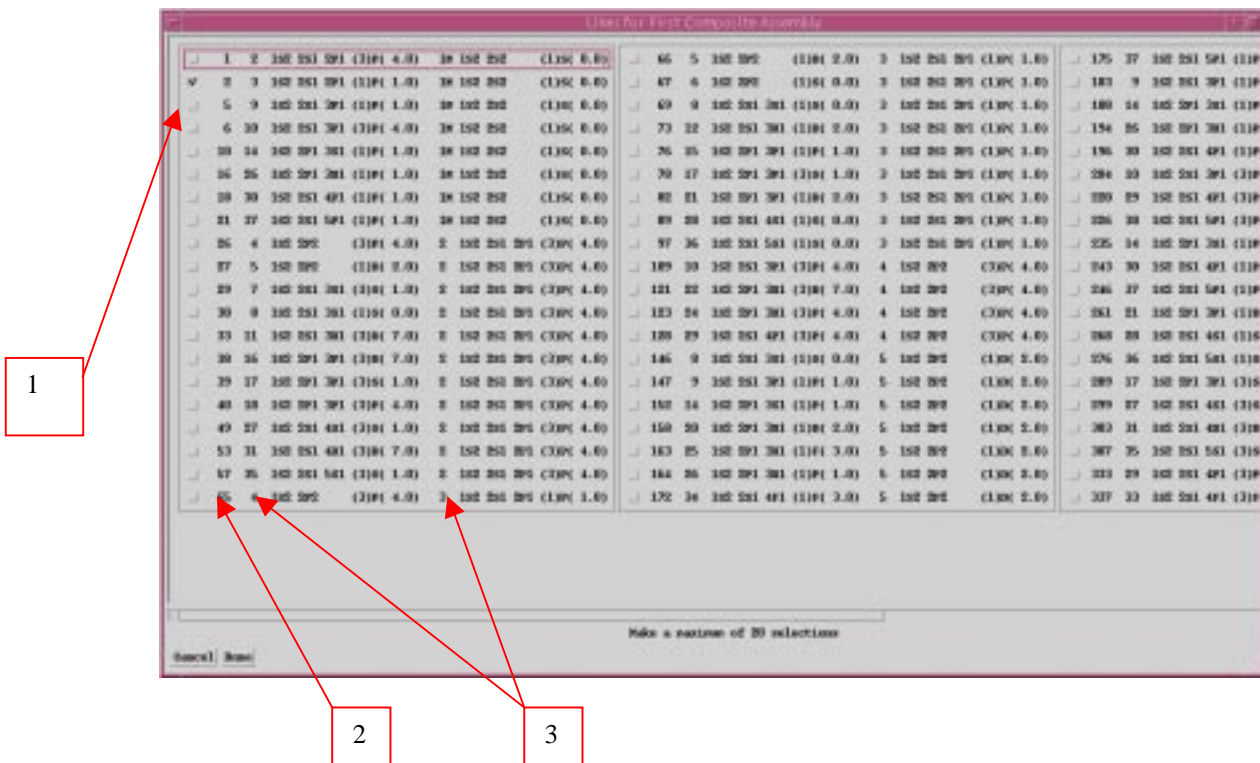


2. Select *Non-equilibrium* or *Equilibrium* conditions by clicking the appropriate case in the list. The selection made is shown in the selection window above. Note that a non-equilibrium choice is only meaningful if there is more than one metastable.
3. The metastables selected in the ADAS205 run are 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 first 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.

- 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.

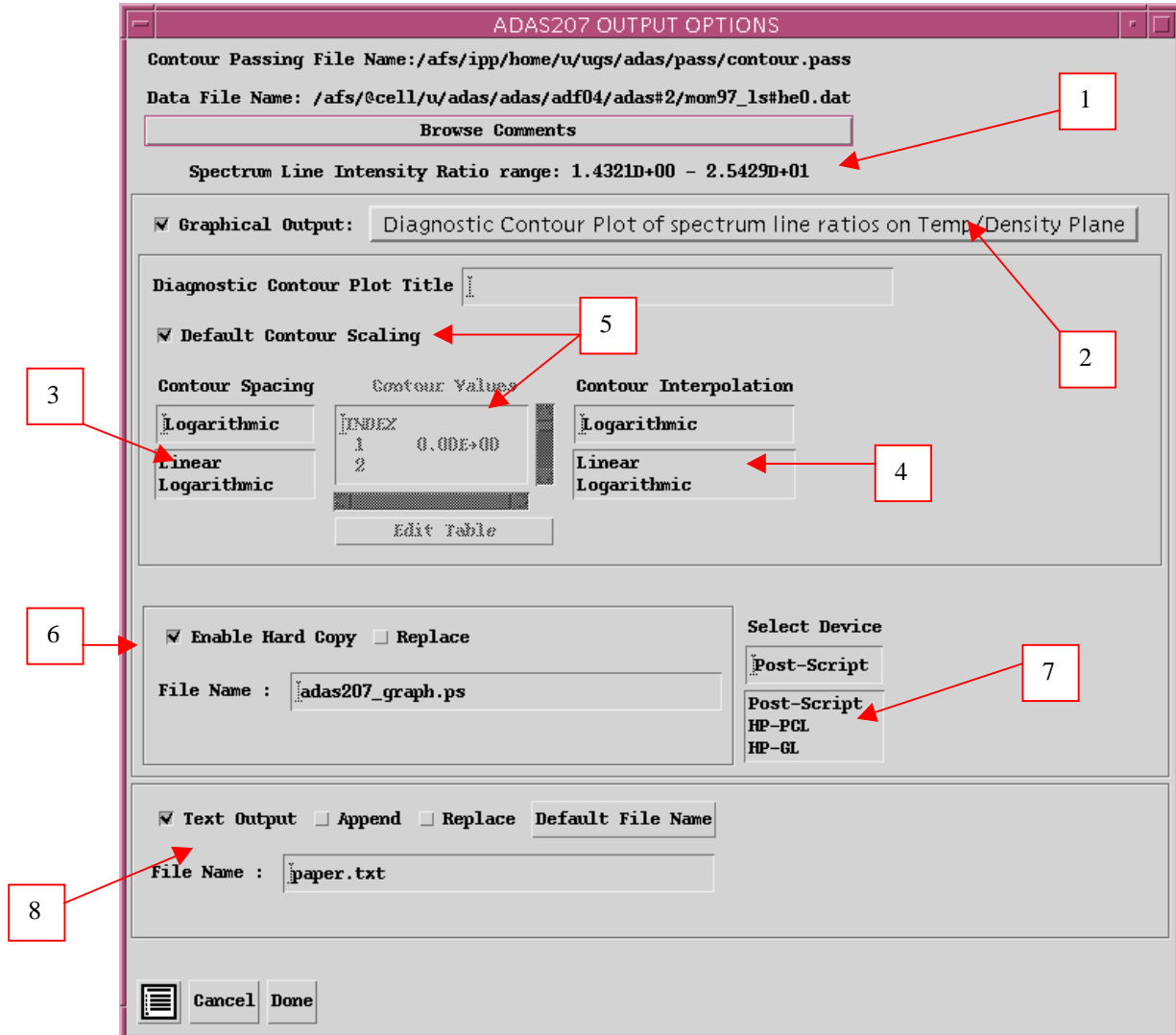
- Clicking on the button alongside a transition allows it to be selected or de-selected.
- The first number is the transition index in the ADF04 file.
- The pair of numbers are the upper and lower level indices form the ADF04 file



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

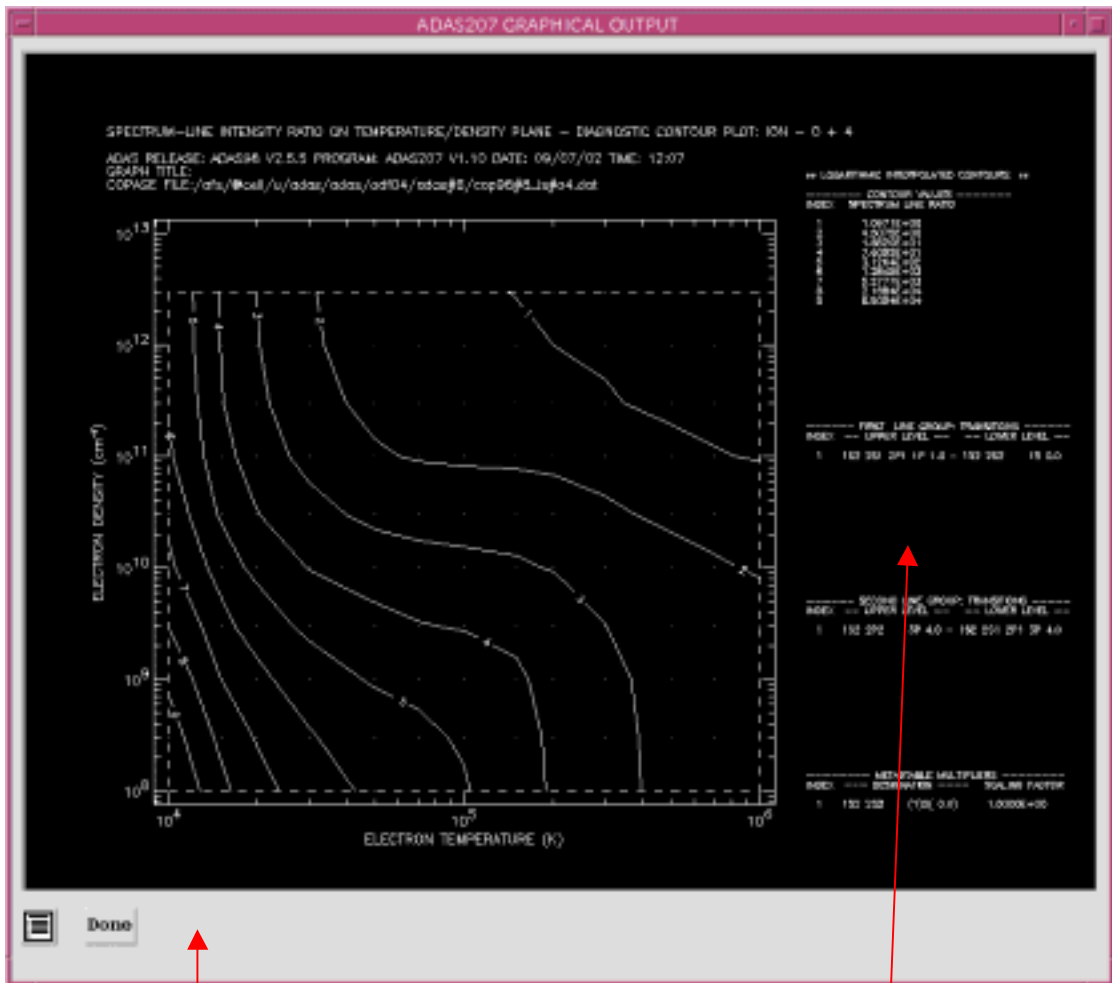
- The limits of the calculated line group ratio are shown on the output window a). It is important to check this range. Subsequent plots may be selected as logarithmic and it is easy to obtain vanishing line ratios by choice of abnormally low temperatures in the ADAS205 run. In these circumstances meaningless contour plots may be produced.
- 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.
- 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.
- Also the interpolation may be chosen.
- If *Default contour scaling* is switched off, the table for specifying contour values is activated.
- Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exists 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.

- 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

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



1

2

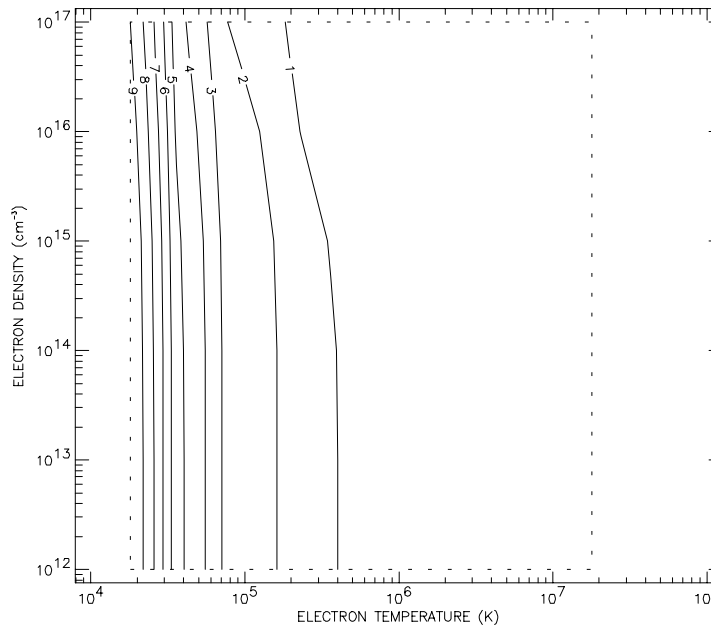
Illustration:

The output from the program is illustrated for the ion O⁺⁵. Figure 2.7a shows a contour plot on the temperature/density plane of the emissivity ratio $\epsilon_{2s_{1/2}-2p_{1/2}}(T_e, N_e) / \epsilon_{2p_{1/2}-3d_{3/2}}(T_e, N_e)$.

Figure 2.7a

SPECTRUM-LINE INTENSITY RATIO ON TEMPERATURE/DENSITY PLANE - DIAGNOSTIC CONTOUR PLOT: ION - O + 5

ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS207 V1.8 DATE: 11/03/99 TIME: 11:16
 GRAPH TITLE: LINE RATIO CONTOUR GRAPH
 COPASE FILE: /packages/adas/adas/adf04/copsm#li/copsm#li_sm#o5.dat



** LOGARITHMIC INTERPOLATED CONTOURS **

----- CONTOUR VALUES -----
 INDEX SPECTRUM LINE RATIO

1	1.0255E+07
2	1.3716E+09
3	1.3344E+11
4	2.4535E+13
5	3.2815E+15
6	4.3800E+17
7	5.8701E+19
8	7.8512E+21
9	1.0501E+24

----- FIRST LINE GROUP: TRANSITIONS -----

INDEX -- UPPER LEVEL -- -- LOWER LEVEL --

1	2p1	2P 0.5 - 2s1	2S 0.5
---	-----	--------------	--------

----- SECOND LINE GROUP: TRANSITIONS -----

INDEX -- UPPER LEVEL -- -- LOWER LEVEL --

1	3d1	2D 1.5 - 3p1	2P 0.5
---	-----	--------------	--------

----- METASTABLE MULTIPLIERS -----

INDEX -- DESIGNATION -- -- SCALING FACTOR

1	2s1	(2)S(0.5)	1.0000E+00
---	-----	------------	------------

The tabular output is shown in table 2.7.

Table 2.7

ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS207 V1.8 DATE: 11/03/99 TIME: 11:16
 ***** TABULAR OUTPUT FROM SPECTRUM LINE DIAGNOSTIC PROGRAM: ADAS207 - DATE: 11/03/99

INPUT CONTOUR-PASSING FILE DSN: /home/loch/adas/pass/contour.pass
 ASSOCIATED COPASE FILE DSN: /packages/adas/adas/adf04/copsm#li/copsm#li_sm#o5.dat

ION	NUCLEAR CHARGE (Z0)	RECOMBINING ION CHARGE (Z1)	----- IONIZATION POTENTIAL ----- (wave number <cm-1>)	(rydbergs)
O + 5	8	6	1114008.	10.1516096

----- ENERGY LEVELS -----

INDEX CONFIGURATION (2S+1)L(J) -- ENERGY RELATIVE TO LEVEL 1 -- ENERGY RELATIVE TO IONISATION POTENTIAL

(rydbergs) (wave number <cm-1>) (rydbergs) (wave number <cm-1>)

1	2s1	(2)0(0.5)	0.	0.0000000	1114008.	
10.1516096	2	2p1	(2)1(0.5)	96376.	0.8782492	1017632.
9.2733604	3	2p1	(2)1(1.5)	96909.	0.8831017	1017099.
9.2685079	23	5g1	(2)4(3.5)	956672.	8.7178535	157336.
1.4337560	24	5g1	(2)4(4.5)	956674.	8.7178736	157334.
1.4337360						

METASTABLE INFORMATION:

NUMBER OF ORDINARY LEVELS = 23
 NUMBER OF METASTABLES = 1

----- METASTABLE DETAILS -----

METASTABLE INDEX	ENERGY LEVEL INDEX	----- DESIGNATION -----
1	23	(2)S(0.5)

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1          1          2s1          (2)S( 0.5)

**** NEUTRAL HYDROGEN CHARGE EXCHANGE NOT INCLUDED ****
****---FREE-ELECTRON-RECOMBINATION---NOT---INCLUDED--- ****

INPUT PLASMA PARAMETERS:
-----

NUMBER OF ELECTRON TEMPERATURES = 10
NUMBER OF ELECTRON DENSITIES     = 6
INDEX ----- TE: ELECTRON TEMPERATURES ----- INDEX -- NE: ELECTRON DENSITIES --
-----
      (kelvin)      (eV)      (reduced)      (cm-3)      (reduced)
-----
1      1.800D+04      1.551D+00      5.000D+02      1      1.000D+12      3.572D+06
2      3.600D+04      3.102D+00      1.000D+03      2      1.000D+13      3.572D+07
3      7.200D+04      6.204D+00      2.000D+03      3      1.000D+14      3.572D+08
4      2.320D+05      1.999D+01      6.444D+03      4      1.000D+15      3.572D+09
5      3.600D+05      3.102D+01      1.000D+04      5      1.000D+16      3.572D+10
6      7.200D+05      6.204D+01      2.000D+04      6      1.000D+17      3.572D+11
7      1.800D+06      1.551D+02      5.000D+04
8      3.600D+06      3.102D+02      1.000D+05
9      7.200D+06      6.204D+02      2.000D+05
10     1.800D+07      1.551D+03      5.000D+05
-----

```

TABLE KEY:

```

-----
NE      = ELECTRON DENSITY
TE      = ELECTRON TEMPERATURE
***** SPECTRUM LINE INTENSITIES & RATIOS: CONTROL DATA *****
*****
TRANSIENT CONDITIONS: NON-EQUILIBRIUM

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----- METASTABLE LEVEL SCALING FACTORS -----
INDEX  LEVEL  DESIGNATION  SCALING FACTOR
-----
1      1      2s1          (2)S( 0.5)      1.0000D+00

```

```

----- FIRST COMPOSITE LINE GROUP ASSEMBLY -----
-----
      TRANSTN  -- UPPER LEVEL -- ----- TRANSITION -----
INDEX  INDEX  INDEX  TYPE  ----- UPPER LEVEL ----- ----- LOWER LEVEL ----- A-VALUE
(SEC-1)
-----
1      1      2      ORD  <2p1          (2)P( 0.5)> - <2s1          (2)S( 0.5)>
4.21D+08

```

```

----- SECOND COMPOSITE LINE GROUP ASSEMBLY -----
-----
      TRANSTN  -- UPPER LEVEL -- ----- TRANSITION -----
INDEX  INDEX  INDEX  TYPE  ----- UPPER LEVEL ----- ----- LOWER LEVEL ----- A-VALUE
(SEC-1)
-----
1      26      7      ORD  <3d1          (2)D( 1.5)> - <3p1          (2)P( 0.5)>
1.08D+06

```

***** SPECTRUM LINE INTENSITIES & RATIOS: RESULTS *****

FIRST COMPOSITE LINE GROUP ASSEMBLY - SPECTRUM LINE INTENSITIES

```

-----
NE (CM-3)      1.00D+12  1.00D+13  1.00D+14  1.00D+15  1.00D+16  1.00D+17
TE (KELVIN)-----
-----
1.80D+04 | 2.63D+01  2.62D+02  2.59D+03  2.30D+04  1.10D+05  1.77D+05
3.60D+04 | 8.79D+02  8.78D+03  8.70D+04  8.00D+05  4.42D+06  8.11D+06
7.20D+04 | 4.36D+03  4.36D+04  4.33D+05  4.07D+06  2.54D+07  5.37D+07
2.32D+05 | 9.81D+03  9.81D+04  9.77D+05  9.41D+06  6.88D+07  1.87D+08
3.60D+05 | 1.02D+04  1.02D+05  1.02D+06  9.87D+06  7.52D+07  2.23D+08
7.20D+05 | 9.81D+03  9.81D+04  9.78D+05  9.53D+06  7.61D+07  2.54D+08
1.80D+06 | 8.33D+03  8.33D+04  8.31D+05  8.15D+06  6.82D+07  2.61D+08
3.60D+06 | 7.08D+03  7.08D+04  7.07D+05  6.95D+06  5.99D+07  2.53D+08
7.20D+06 | 5.89D+03  5.89D+04  5.88D+05  5.80D+06  5.13D+07  2.39D+08
1.80D+07 | 4.50D+03  4.50D+04  4.50D+05  4.45D+06  4.05D+07  2.13D+08

```

SECOND COMPOSITE LINE GROUP ASSEMBLY - SPECTRUM LINE INTENSITIES

```

-----
NE (CM-3)      1.00D+12  1.00D+13  1.00D+14  1.00D+15  1.00D+16  1.00D+17

```


1.80D+04	1.87D-25	1.89D-24	2.06D-23	3.60D-22	1.04D-20	1.80D-19
3.60D+04	6.93D-14	6.98D-13	7.44D-12	1.17D-10	3.39D-09	6.22D-08
TE7 (BDDWOM)	3.60D-08	3.62D-07	3.79D-06	5.42D-05	1.52D-03	3.05D-02
2.32D+05	2.36D-04	2.37D-03	2.44D-02	3.10D-01	7.90D+00	1.85D+02
3.60D+05	8.73D-04	8.75D-03	8.97D-02	1.11D+00	2.71D+01	6.71D+02
7.20D+05	2.58D-03	2.59D-02	2.64D-01	3.17D+00	7.33D+01	1.94D+03
1.80D+06	4.23D-03	4.24D-02	4.31D-01	5.03D+00	1.10D+02	3.16D+03
3.60D+06	4.32D-03	4.32D-02	4.39D-01	5.06D+00	1.09D+02	3.31D+03
7.20D+06	3.83D-03	3.84D-02	3.89D-01	4.45D+00	9.36D+01	3.04D+03
1.80D+07	2.81D-03	2.81D-02	2.85D-01	3.22D+00	6.64D+01	2.36D+03

SPECTRUM LINE INTENSITY RATIO

NE (CM-3)	1.00D+12	1.00D+13	1.00D+14	1.00D+15	1.00D+16	1.00D+17
TE (KELVIN)	-----					
1.80D+04	1.40D+26	1.39D+26	1.26D+26	6.40D+25	1.05D+25	9.85D+23
3.60D+04	1.27D+16	1.26D+16	1.17D+16	6.86D+15	1.31D+15	1.30D+14
7.20D+04	1.21D+11	1.20D+11	1.14D+11	7.51D+10	1.67D+10	1.76D+09
2.32D+05	4.16D+07	4.14D+07	4.01D+07	3.03D+07	8.71D+06	1.01D+06
3.60D+05	1.17D+07	1.17D+07	1.14D+07	8.90D+06	2.77D+06	3.32D+05
7.20D+05	3.80D+06	3.79D+06	3.70D+06	3.01D+06	1.04D+06	1.31D+05
1.80D+06	1.97D+06	1.96D+06	1.93D+06	1.62D+06	6.18D+05	8.28D+04
3.60D+06	1.64D+06	1.64D+06	1.61D+06	1.37D+06	5.52D+05	7.67D+04
7.20D+06	1.54D+06	1.53D+06	1.51D+06	1.30D+06	5.48D+05	7.86D+04
1.80D+07	1.60D+06	1.60D+06	1.58D+06	1.38D+06	6.10D+05	9.05D+04

Notes: