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

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

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 $A_{i\to j}$ be the spontaneous emission coefficient for the line $i \to j$. Then the composite emissivity for the line group is

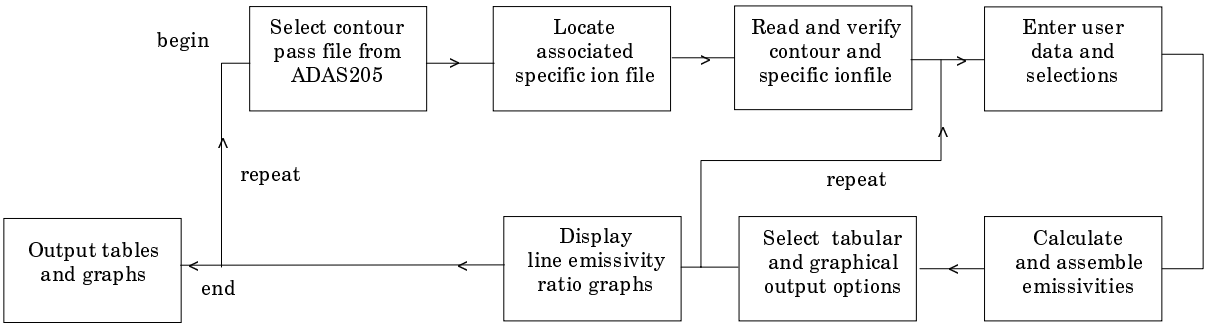
$$\begin{aligned}
\varepsilon_G &= \sum_{j\in J_G, i\in I_G} \varepsilon_{j\to i} = \sum_{j\in J_G, i\in I_G} A_{j\to i} N_j \\
&= \sum_{j\in J_G, i\in I_G} A_{j\to i} \Big(\sum_{\sigma=1}^{M} F_{j\sigma}^{(exc)} N_e N_\sigma + F_j^{(rec)} N_e N_1^+ + F_j^{(CX)} N_H N_1^+\Big) \\
&= N_e N_1 \sum_{j\in J_G, i\in I_G} A_{j\to i} \Big(\sum_{\sigma=1}^{M} F_{j\sigma}^{(exc)} \frac{N_\sigma}{N_1} + F_j^{(rec)} \frac{N_1^+}{N_1} + F_j^{(CX)} \frac{N_H}{N_e} \frac{N_1^+}{N_1}\Big)
\end{aligned} \qquad 2.7.2$$

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. The code prepares and operates primarily with a ratio $\varepsilon_{G_1} / \varepsilon_{G_2}$.

Program steps:

These are summarised in the figure 2.7.

Figure 2.7



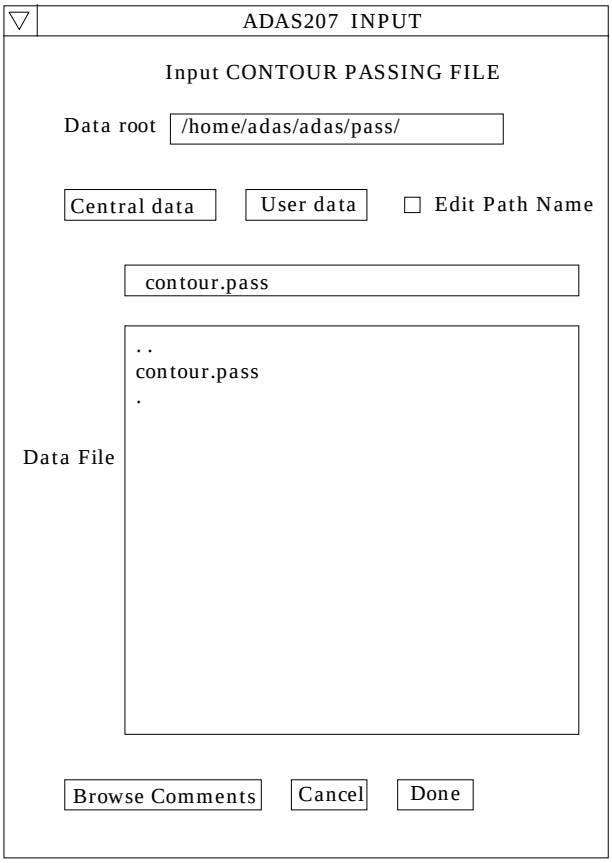
Interactive parameter comments:

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

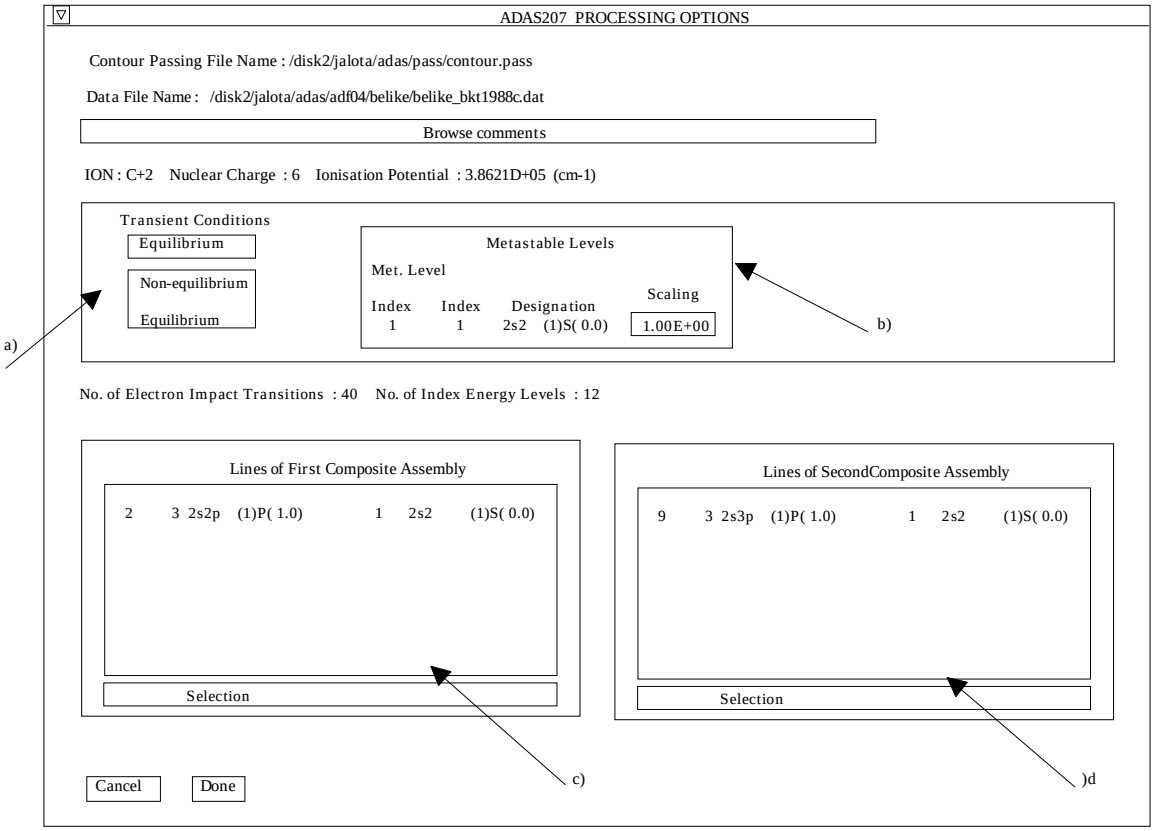
1. The program requires selection of the 'contour' data file prepared as output from ADAS205 (see description of ADAS205). There is no arrangement for central ADAS storage of such files which reside only in a user's file space and are generally prepared for immediate use. Usually in ADAS we store such temporary 'passed files' in a *pass* sub-library. You should create this at the first level within the adas database as

   /...../<uid>/adas/pass

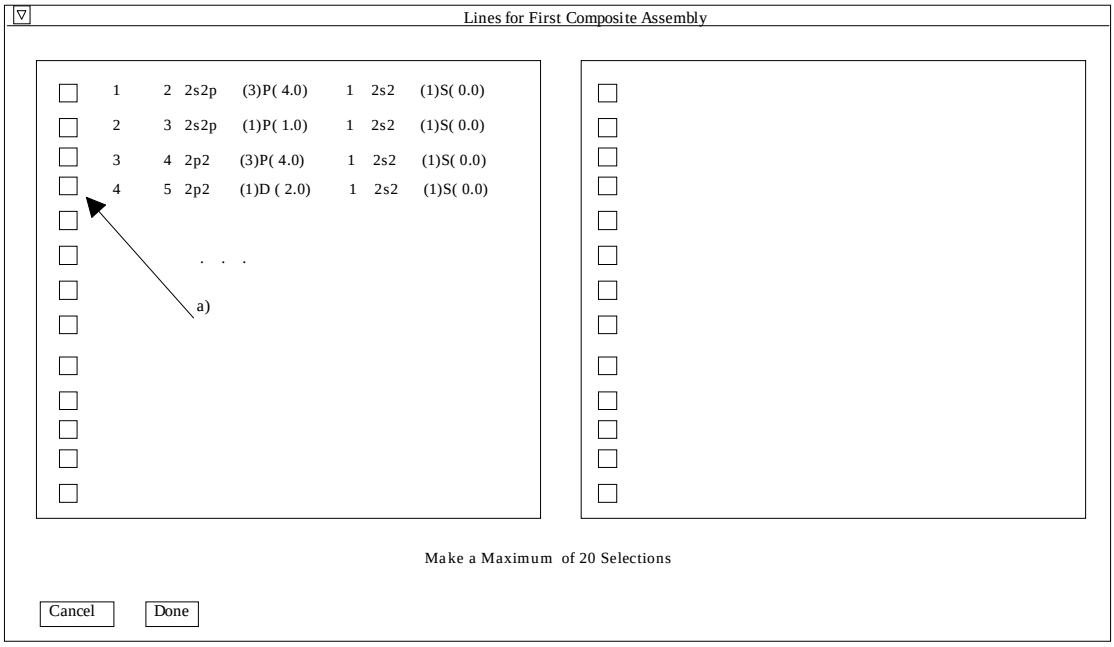
   to which the program looks by default.



The **processing options window** has the appearance shown below. 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 a). 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. The metastables selected in the ADAS205 run are shown in the adjacent window b). 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.



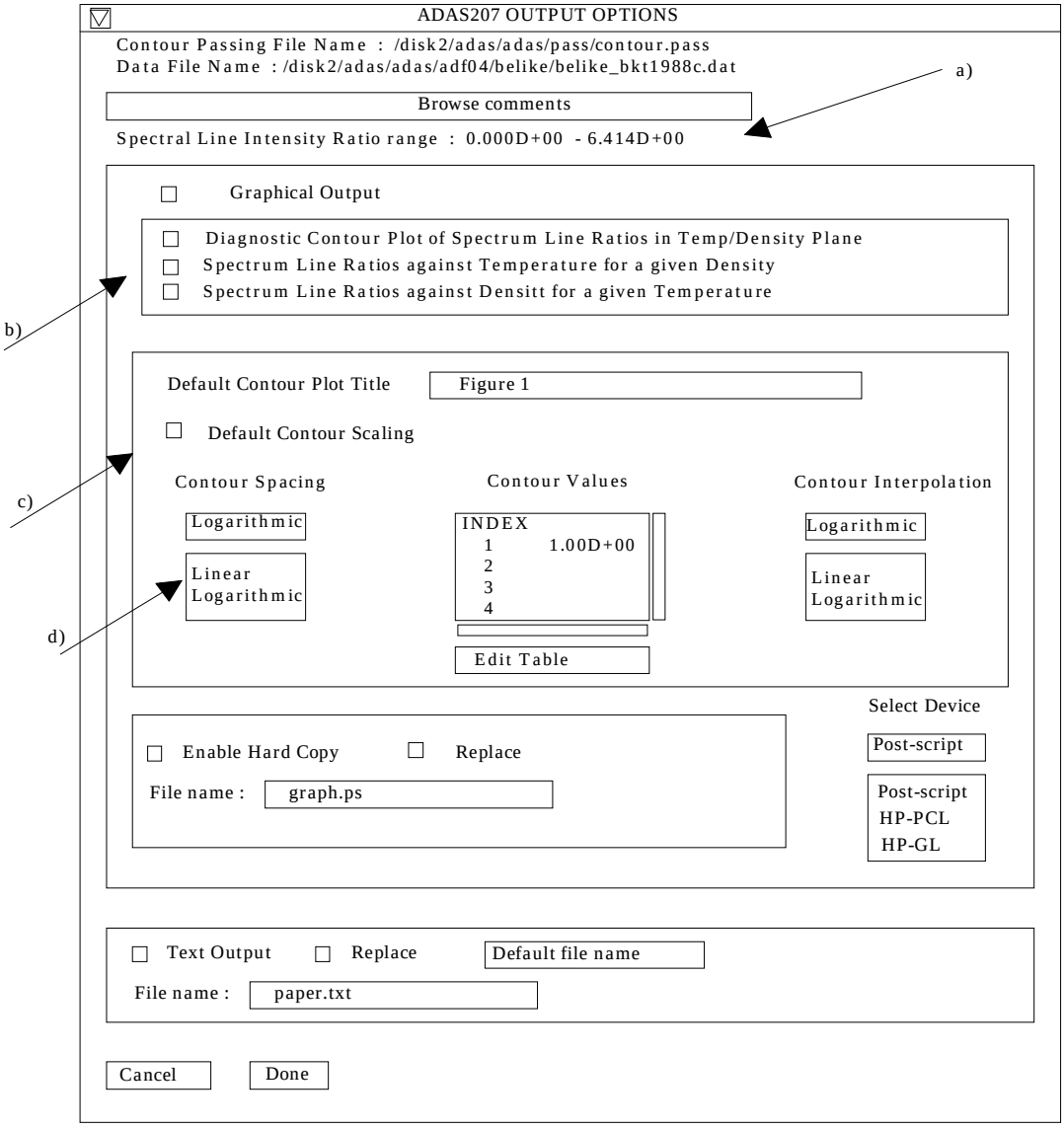
3. A ‘line ratio’ in the present context is a ratio of line groups. The current line groups are shown in the list windows. The columns of the each row show the transition

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.

4. Each line group is assembled by clicking on the appropriate *Selection* button c) or d). A new window is presented with all available transitions listed. This is shown above. Clicking on the button alongside a transition a) allows it to be selected or de-selected.

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

5. 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.



6. There are three distinct types of plot of the line ratio allowed b), 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 c) changes according to this choice.

7. For the contour plot case, logarithmic or linear choices of contour are permitted. Click on the required type in the lower list window d). The chosen type appears in the selection window above.

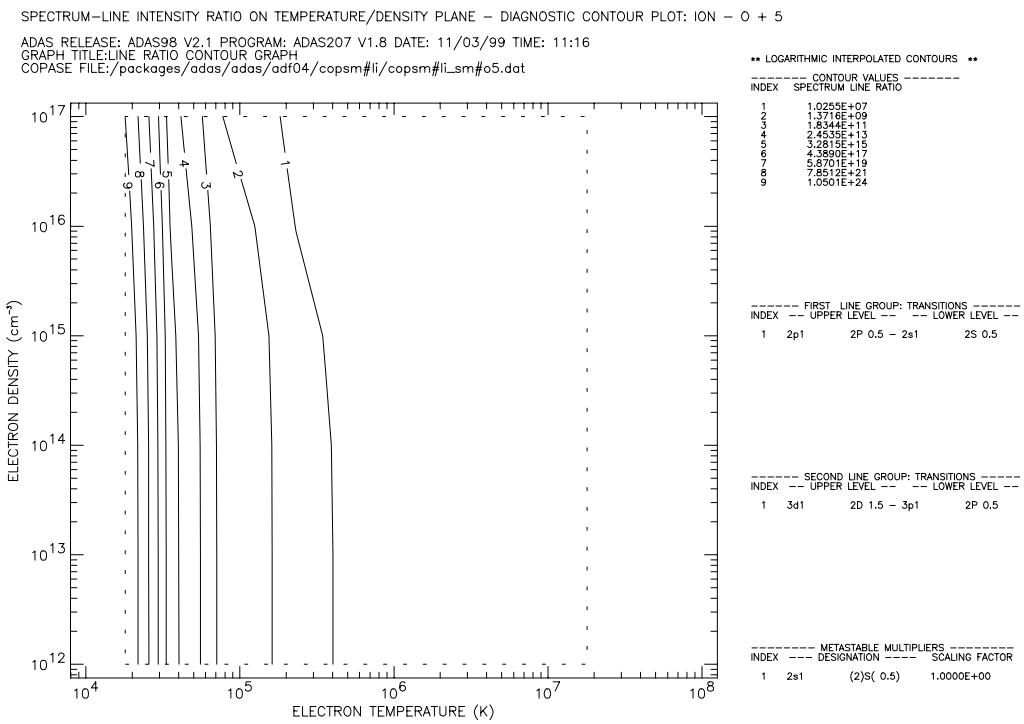
8. The displayed graph has the usual overall layout, but with supplementary information on the right side listing the line group assemblies and metastable fraction multipliers.

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

$$\varepsilon_{2s_{1/2}-2p_{1/2}}(T_e, N_e) / \varepsilon_{2p_{1/2}-3d_{3/2}}(T_e, N_e).$$

Figure 2.7a



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        RECOMBINING      ------- IONIZATION POTENTIAL -------
        CHARGE (Z0)    ION CHARGE (Z1)    (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
                                (wave number <cm-1>) (rydbergs)  (wave number <cm-1>)     (rydbergs)
-----------------------------------------------------------------------------------------------------
 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:
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```
NUMBER OF ORDINARY LEVELS        =  23
```

```
---------------- METASTABLE DETAILS ----------------
METASTABLE    ENERGY LEVEL    ---- DESIGNATION -----
  INDEX          INDEX
NUMBER OF METASTABLES ---------------- = 1 ---------------
    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

---------- 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
TE (KELVIN)-----------------------------------------------------------------------------------------
  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
  7.20D+04 |   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
```

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NE  (CM-3)     1.00D+12  1.00D+13  1.00D+14  1.00D+15  1.00D+16  1.00D+17
TE (KELVIN)------------------------------------------------------------------------------- ------------
SPECTRUM LINE INTENSITY RATIO
  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: