

ADAS707: Metastable and excited populations - process line emissivities

The program evaluates and displays line emissivities and their ratios from a pair of adjacent ions of an element. It uses a passing file of excited population data from the code ADAS705 which includes ionisation data linking the two ion stages. The code is specifically designed to enable study of satellite lines and related resonance lines.

Background theory:

This is a new code in preparation. The following theory and interactive widget designs are developmental only.

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 ADAS706 which must be executed before ADAS707. 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. ADAS707 deals with two line groups which are built up by the user in the data entry section of the code.

From equation 8.6.4, the solution for the ordinary populations of the first stage is

$$N_j = \sum_{\sigma=1}^{M_z} F_{j\sigma}^{(exc)} N_e N_\sigma + \sum_{\tau=1}^{M_{z+1}} F_{j\tau}^{(rec)} N_e N_\tau^+ + \sum_{\tau=1}^{M_{z+1}} F_{j\tau}^{(CX)} N_H N_\tau^+ \quad 8.7.1$$

where the $F_{j\sigma}^{(exc)}$, $F_{j\tau}^{(rec)}$ and $F_{j\tau}^{(CX)}$ 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. Similarly for the second stage ordinary populations.

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

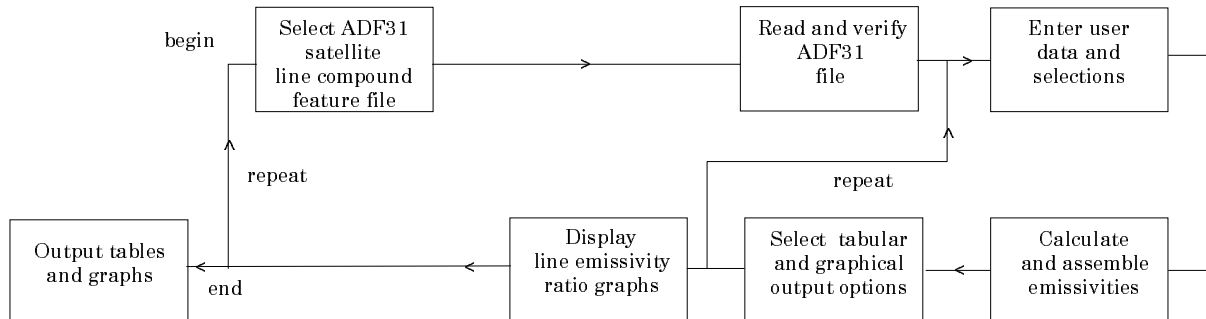
$$\begin{aligned} \mathcal{E}_G &= \sum_{j \in J_G, i \in I_G} \mathcal{E}_{j \rightarrow i} = \sum_{j \in J_G, i \in I_G} A_{j \rightarrow i} N_j \\ &= \sum_{j \in J_G, i \in I_G} A_{j \rightarrow i} \left(\sum_{\sigma=1}^{M_z} F_{j\sigma}^{(exc)} N_e N_\sigma + \sum_{\tau=1}^{M_{z+1}} F_{j\tau}^{(rec)} N_e N_\tau^+ + \sum_{\tau=1}^{M_{z+1}} F_{j\tau}^{(CX)} N_H N_\tau^+ \right) \\ &= N_e N_1 \sum_{j \in J_G, i \in I_G} A_{j \rightarrow i} \left(\sum_{\sigma=1}^M F_{j\sigma}^{(exc)} \frac{N_\sigma}{N_1} + \sum_{\tau=1}^{M_{z+1}} F_{j\tau}^{(rec)} \frac{N_\tau^+}{N_1} + \sum_{\tau=1}^{M_{z+1}} F_{j\tau}^{(CX)} \frac{N_H}{N_e} \frac{N_\tau^+}{N_1} \right) \end{aligned} \quad 8.7.2$$

expressed in terms of the ratios N_σ / N_1 , N_τ^+ / N_1 and N_H / N_1 . 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 8.7.

Figure 8.7



Interactive parameter comments:

The program requires selection of the ADF31 compound feature file of satellite line type prepared as output from ADAS706 (see description of ADAS205). ADAS707 initiates an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition and display of output.

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. 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.

The screenshot shows a window titled 'ADAS706 INPUT'. Inside, there is a section for 'Input satellite line compound feature file'. The 'Data root' is set to '/packages/adas/adas/adf31/'. Below this are two buttons: 'Central data' and 'User data', along with an unchecked checkbox for 'Edit Path Name'. A text field contains the file name 'sat_li_he/ic#n4.dat'. A 'Data File' list box shows a list of files: '..', 'ic#be1.dat', 'ic#b2.dat', 'ic#c3.dat', 'ic#n4.dat', and '.'. At the bottom of the window are three buttons: 'Browse Comments', 'Cancel', and 'Done'.

2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing. 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.

- 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*.
- Once a data file is selected, the set of buttons at the bottom of the main window become active.
- 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.

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

▽
ADAS706 PROCESSING OPTIONS

Compound feature file : /packages/adas/adas/adf31/sat_li_he/ic#n4.dat

Nuclear Charge : 7

1st. stage charge : 4
 No. of index energy levels : 10
 No. of metastables : 1
 No. of radiative transitions: 40
 No. of s-lines : 5

1st. stage charge : 5
 No. of index energy levels : 5
 No. of metastables : 1
 No. of radiative transitions: 20
 No. of s-lines : 5

Browse comments

Transient Conditions

Equilibrium

Non-equilibrium
Equilibrium

1st. stage Metastable Levels

Met. Level

Index	Designation	Scaling
1	2s1 (2)S(0.5)	1.00E+00

2nd.. stage Metastable Levels

Met. Level

Index	Designation	Scaling
1	1s2 (1)S(0.0)	1.00E+00

3rd.. stage Metastable Levels

Met. Level

Index	Designation	Scaling
1	1s1 (2)S(0.5)	1.00E+00

Lines of First Composite Assembly

Index	lvl.	desig.	-	lvl.	desig.	stge/code
2	3	1s2p (1)P(1.0)	1	1s2	(1)S(0.0)	5
10						4/s
11						4/s

Selection

Lines of Second Composite Assembly

Index	lvl.	desig.	-	lvl.	desig.	stge/code
8	5	2s2p (1)P(1.0)	1	1s2s	(1)S(0.0)	4

Selection

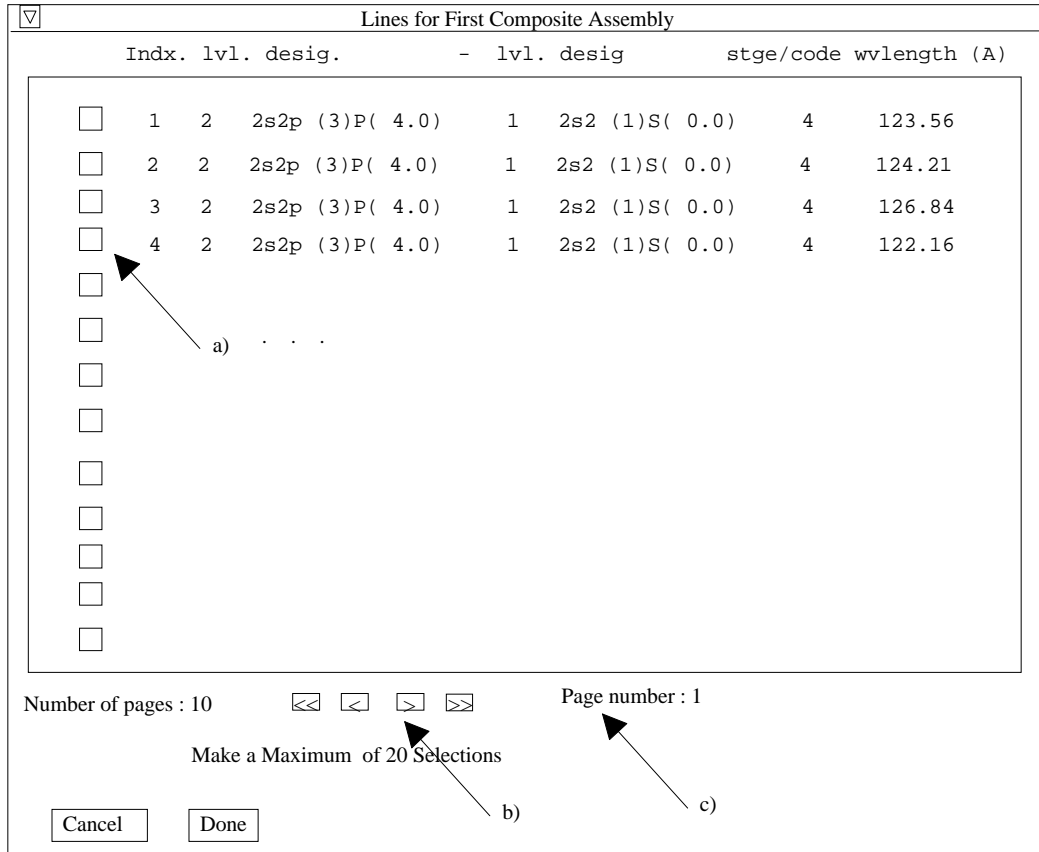
1

Cancel

Done

- 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. The metastables selected in the ADAS705 run are shown in the windows at b). These windows become 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.
- 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, then for the upper and lower levels of the transition, the level index, configuration designation and the outer quantum numbers and finally the ionisation stage to which the transition belongs. The code identifies if it is an s-line. These data are taken from the ADF31 file.
- 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 below.
- There may be very many transitions, so they are grouped into pages. The current page number is shown at c).
- The page controls at b) are like tape recorder controls going forward and back and fast forward or fast back. The latter jump three pages at a time.

11. Clicking on the button alongside a transition a) allows it to be selected or de-selected.



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

12. 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 ADAS706 run. In these circumstances meaningless contour plots may be produced.
13. 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.
14. 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.
15. 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.

ADAS706 OUTPUT OPTIONS

Compound feature file : /packages/adas/adas/adf31/sat_li_he/ic#n4.dat

Browse comments a)

Spectral Line Intensity Ratio range : 0.000D+00 - 6.414D+00

Graphical Output

Diagnostic Contour Plot of Spectrum Line Ratios in Temp/Density Plane

Spectrum Line Ratios against Temperature for a given Density

Spectrum Line Ratios against Densitt for a given Temperature

b)

Default Contour Plot Title

Default Contour Scaling

Contour Spacing	Contour Values	Contour Interpolation
<input type="button" value="Logarithmic"/>	INDEX 1 1.00D+00 2 3 4	<input type="button" value="Logarithmic"/>
<input type="button" value="Linear"/> <input type="button" value="Logarithmic"/>	<input type="text"/> <input type="button" value="Edit Table"/>	<input type="button" value="Linear"/> <input type="button" value="Logarithmic"/>

c)

d)

Enable Hard Copy Replace

File name :

Select Device

Text Output Replace

File name :

Illustration:

Figure 8.7a

Table 8.7

Notes: