

ADAS412: Equilibrium ionisation - prepare G(Te) function tables

The program interrogates *GFT* files of type ADF20. The $G(T_e)$ function is extracted for a selected radiative transition of an ion. The data may be interpolated using cubic splines at selected electron temperatures. A minimax polynomial approximation is made to the interpolated data. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the polynomial approximation.

Background theory:

This new code allows the full calculation of solar astrophysical G(Te) functions. It does this by carrying out an excited population calculation from an *adf04* dataset in the manner of ADAS205, generating an ionisation balance from *adf11* datasets and finally assembling the G(Te) function. The code is the interactive implementation of the program used to create the main *adf20* datasets. The new code can create output data sets fully formatted to the *adf20* specification. Probable special uses of the code will be to check the sensitivity of G(Te) functions to small alterations in underlying collisional rates from *adf04* datasets or to focus on a restricted number of G(Te) functions. Thus we have allowed restriction of the number of G(Te) functions created by wavelength interval or by initial and final level. The theory of the G(Te) functions is given in the 'cde_manual' (*./.../adas/docs/cde-manual/...*). One of the most widely used methods available for the interpretation of astronomical spectral intensities is the emission measure technique. This method is less familiar in spectroscopic studies of fusion plasma. However it and variants designed to determine impurity concentration, impurity variation in time and impurity influx are applicable in fusion.

The intensity of a spectral line from a column of optically thin plasma of cross-sectional area \mathbf{A} and due to a transition from upper level j to lower level k may be written as

$$I_{j \rightarrow k} = \frac{1}{4\pi\mathbf{A}} \iiint A_{j \rightarrow k} N_j dz dy dx \quad 5.12.1$$

where N_j denotes the population density of ions in the upper state j , $A_{j \rightarrow k}$ is the radiative transition probability for the transition and the integral is taken over the volume of the plasma viewed.

The excited population may be expressed in terms of the ground and metastable populations of the ionisation stage to which it belongs and to those of the adjacent higher ionisation stage by a quasi-equilibrium collisional radiative calculation as

$$N_j = \sum_{\sigma=1}^{M_z} F_{j\sigma}^{(exc)} N_e N_\sigma + \sum_{\nu=1}^{M_{z+1}} F_{j\nu}^{(rec)} N_e N_\nu^+ \quad 5.12.2$$

Usually contributions to the population of the excited state by excitation from the metastables of its own ionisation stage only need to be considered so that

$$N_j = \sum_{\sigma=1}^{M_z} F_{j\sigma}^{(exc)} N_e N_\sigma \quad 5.12.3$$

In differential emission measure analysis, the assumption of ionisation balance is normally made. Although a time dependent ionisation could be used, the method would be specific to a particular model for the dynamic behaviour of the plasma and the universality of the emission measure technique would be lost. Thus it is convenient to write.

$$N_\sigma \equiv N_\sigma^{(z)} = \frac{N_\sigma^{(z)}}{N_{tot}} \frac{N_{tot}}{N_H} \frac{N_H}{N_e} N_e \quad 5.12.4$$

where the ratio $N_\sigma^{(z)} / N_{tot}$ is evaluated in equilibrium at the local temperature and density. For the solar plasma, the generally accepted assumption is that the abundance of the element N_{tot} / N_H does not vary through the depth of the atmosphere. Then gathering terms

$$A_{j \rightarrow k} N_j = \frac{N_{tot}}{N_H} N_e^2 G(T_e, N_e) \quad 5.12.5$$

where

$$G_{j \rightarrow k}(T_e, N_e) = A_{j \rightarrow k} \frac{N_H}{N_e} \sum_{\sigma=1}^{M_z} F_{j\sigma}^{(exc)} \frac{N_{\sigma}^{(z)}}{N_{tot}} \quad 5.12.6$$

Then the spectral intensity may be written as

$$I_{j \rightarrow k} = \frac{1}{4\pi\mathbf{A}} \frac{N_{tot}}{N_H} \iiint G_{j \rightarrow k}(T_e, N_e) N_e^2 dz dy dx \quad 5.12.7$$

It is convenient to change the variable of the integral to electron temperature. However the atomic coefficient depends on both electron temperature and electron density so it is necessary to make some assumption about the relation between them. A common assumption is that the plasma pressure is constant over the relatively small range of temperature where the $G(T_e, N_e)$ function has significant values. In any event a model assumption is made even though the $G(T_e)$ function is usually written as function of temperature alone. Also introduce the concept of surfaces of constant temperature of which there may be more than one in the viewed volume. The intensity then may be rewritten as

$$I_{j \rightarrow k} = \frac{1}{4\pi\mathbf{A}} \frac{N_{tot}}{N_H} \int_{T_1}^{T_2} G_{j \rightarrow k}(T_e, N_e) \sum_l \int_{S_l(T_e)} |\nabla T_e|^{-1} N_e^2 dS_l dT_e \quad 5.12.8$$

The limits of the integral T_1 and T_2 are the minimum and maximum electron temperatures in the part of the atmosphere contributing to the spectrum. Introduce the differential emission measure, $\phi(T_e)$, defined by

$$\phi(T_e) = \frac{1}{\mathbf{A}} \sum_l \int_{S_l(T_e)} |\nabla T_e|^{-1} N_e^2 dS_l \quad 5.12.9$$

where the sum is taken over all l of the isothermal surfaces $S_l(T_e)$ and $|\nabla T_e|$ is the modulus of the temperature gradient perpendicular to the surface. By this definition $\phi(T_e)$ is the average value for the differential emission measure over the area viewed by the spectrometer. It is noted that $\phi(T_e)$ is the part of the integral it is sought to extract since it is the part which gives information about the structure of the atmosphere. The above analysis leads to the following expression for the spectral intensity

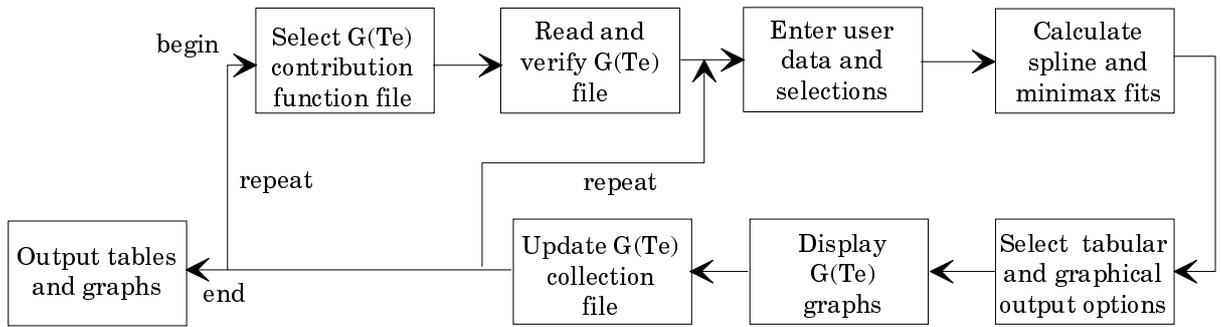
$$I_{j \rightarrow k} = \frac{1}{4\pi} \frac{N_{tot}}{N_H} \int_{T_1}^{T_2} G_{j \rightarrow k}(T_e, N_e) \phi(T_e) dT_e \quad 5.12.10$$

The program interrogates $G(T_e)$ data sets prepared according to the prescription of equation 6.6.6. Details of the model relating temperature, density, pressure and hydrogen to electron number densities are stored in the $G(T_e)$ datasets and this information is accessed simultaneously with the $G(T_e)$ in the interrogation. Interpolation of the $G(T_e)$ to arbitrary temperatures is done by cubic splines. This implies an implicit interpolation in the other model parameters. For completeness these model parameters are also explicitly interpolated as a function of temperature.

Program steps:

These are summarised in figure 5.12.

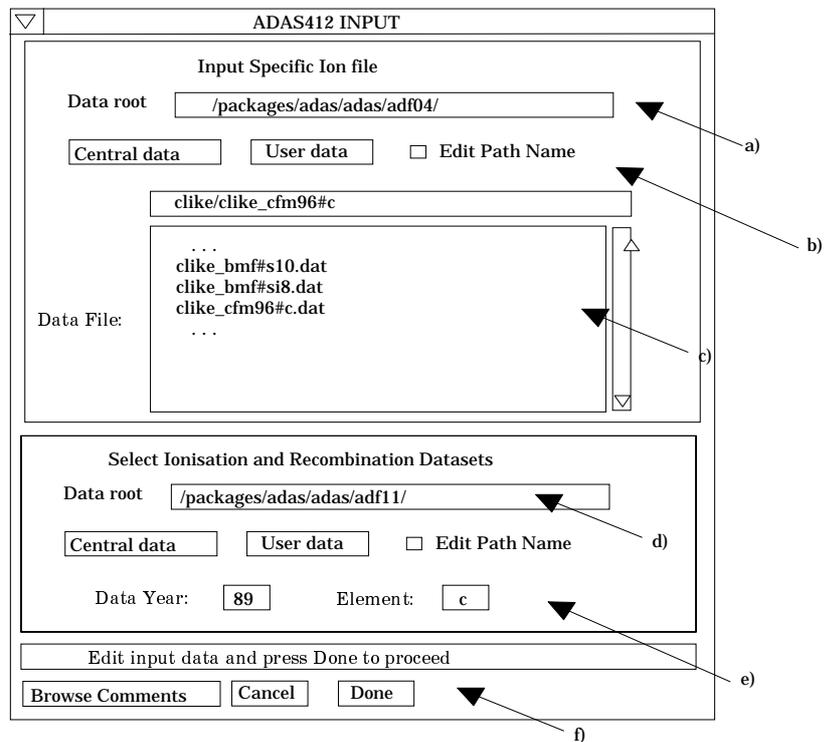
Figure 5.12



Interactive parameter comments:

The **file selection window** has the appearance shown below. It is composed of two sub-windows. The upper sub-window is a conventional file selection window used to select the specific ion file for the excited population part of the calculation, while the lower one allows an ionisation balance to be selected.

1. Data root a) shows the full pathway to the appropriate data subdirectories of type *adf04*. 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.
2. The Data root can be edited directly. Click the *Edit Path Name* button at b) first to permit editing.
3. Available sub-directories are shown in the large file display window c). 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.
5. The ionisation balance is selected at d) and e). The appropriate data class is *adf11*.
6. Data root at d) shows the full pathway to the appropriate data subdirectories of type *adf11*. 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.
7. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
8. The particular ionisation and recombination data is selected by *Data Year* and then by *Element* at e). Enter the two digit year number. Note that the G(Te) code uses ionisation and recombination data unresolved by metastable. Thus it looks for sub-directories *acd<year>* and *scd<year>*, not *acd<year>r* and *scd<year>r*. Most of such data are in years '74', '85' and '89'.
9. Enter the element symbol at *Element*. The code will check that the same element is being used for the ionisation balance as for the excited population calculation.



10. Once a data file is selected, the set of buttons at the bottom of the main window become active.
11. Clicking on the *Browse Comments* button displays any information stored in the *adf04* file.
12. 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

13. An arbitrary title may be given for the case being processed. For information the full pathway to the *adf04* dataset being used is also shown at a). The button *Browse comments* again allows display of the information field section at the foot of the selected *adf04* dataset, if it exists. Information on the ionisation and recombination data in use is given below.
14. At b) and c) the model data for the calculation are entered. The code will allow calculation of the $G(\text{Te})$ functions at either a fixed electron pressure or a fixed electron density.
15. Click the *Default Data* button to begin. A pop-up widget appears as shown at g). Select either *Density* or *Pressure*, enter a value in the editable box and press Return. Default model values of the selected type appear at b). The default temperature values come from the selected ionisation and recombination data sets. Note that the ratio of hydrogen to electron number densities is also inserted. This is required from the definition of the astrophysical type of $G(\text{Te})$ function. Standard solar atmosphere model data is used.
16. The model data is editable. Click on the *Edit Table* button to activate Table Editor. Note that the whole table becomes editable. It is the user's responsibility to modify the last column of $N_{\text{H}}/N_{\text{e}}$ values according to changes in temperature. It is not recomputed from the standard built in atmosphere model.
17. The production of $G(\text{Te})$ functions is controlled and restricted by the selections at d). Activate the appropriate button at d) to enable selection by *Indices* or *Wavelengths*. The relevant part of the widget becomes activated.

ADAS412 PROCESSING OPTIONS

Title for Run

Data File Name : /packages/adas/adas/adf04/clike/clike_cf96#e.dat

adf11 year : 89 Element : c

Model Data

Electron Temp. (log(K))	Electron Density (cm-3)	NH/NE Ratio	
-------------------------	-------------------------	-------------	--

INDEX	Electron Temp. (log(K))	Electron Density (cm-3)	NH/NE Ratio
1	4.065E+00	1.000E+11	1.394E+00
2	4.115E+00	1.000E+11	1.303E+00
3			
4			

Select Transitions by : Indices Wavelengths

<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="width: 5%;">INDEX</th> <th style="width: 45%;">Upper level</th> <th style="width: 45%;">Lower level</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>2s(2) 2p(2)</td> <td>(3)P(4.0)</td> </tr> <tr> <td>2</td> <td>2s(2) 2p(2)</td> <td>(1)D(2.0)</td> </tr> <tr> <td>3</td> <td>2s(2) 2p(2)</td> <td>(1)S(0.0)</td> </tr> <tr> <td>4</td> <td>...</td> <td></td> </tr> </tbody> </table>	INDEX	Upper level	Lower level	1	2s(2) 2p(2)	(3)P(4.0)	2	2s(2) 2p(2)	(1)D(2.0)	3	2s(2) 2p(2)	(1)S(0.0)	4	...		<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="width: 5%;">INDEX</th> <th style="width: 35%;">Upper level</th> <th style="width: 35%;">Lower level</th> <th style="width: 25%;">Assign Wavelength</th> </tr> </thead> <tbody> <tr> <td>1</td> <td></td> <td></td> <td></td> </tr> <tr> <td>2</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3</td> <td></td> <td></td> <td></td> </tr> <tr> <td>4</td> <td></td> <td></td> <td></td> </tr> </tbody> </table> <p style="text-align: center;"><input type="button" value="Edit Table"/></p>	INDEX	Upper level	Lower level	Assign Wavelength	1				2				3				4			
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Wavelength Max. : Wavelength Min. : Highest Level Included

Edit the processing options data and press Done to proceed

DEFAULT DENSITY/PRESSURE

Select Transitions by :

Default : Density (cm-3) Pressure (cm-3 K)

18. Selecting by *Indices* is as shown at e). The complete indexed level list from the *adf04* file is shown on the left. In the editable table on the right, enter the upper and lower level indices of transitions you wish. Note that you must click the *Edit Table* button first to start Table Editor. The table allows you to enter the precise, spectroscopic accuracy wavelength of the line if you have it available. The output tables of the G(Te) function will provide the approximate theoretical wavelength from the *adf04* level energies. These are not of spectroscopic quality unless hand prepared. Browse the comments section of the *adf04* file to see if this is so. The precise wavelength you assign will appear in the output G(Te) tables along with the approximate theoretical one.
19. Selecting by *Wavelengths* activates the widgets at f). You can enter a *Minimum* and *Maximum* wavelength (in Angstroms) and further restrict by the *Highest level included*, that is the highest indexed level from the *adf04* file which will be considered in setting up possible lines.

- At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

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

- As in the previous window, the full pathway to the file being analysed is shown for information at a). Also the *Browse comments* button is available.
- Graphical display of the G(Te) functions is activated by the *Graphical Output* button at b). 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.
- Hard copy is activated by the *Enable Hard Copy* button at c). 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 to the right. Clicking on the required device selects it. It appears in the selection window above the Device list window.

ADAS412 OUTPUT OPTIONS

Data File Name : /packages/adas/adas/adf04/clike/clike_cfm96#c.dat

Graphical Output

Graph Title

Explicit scaling

X-min X-max

Y-min Y-max

Enable Hard Copy Replace

File Name :

Text Output Replace Default File Name

File Name :

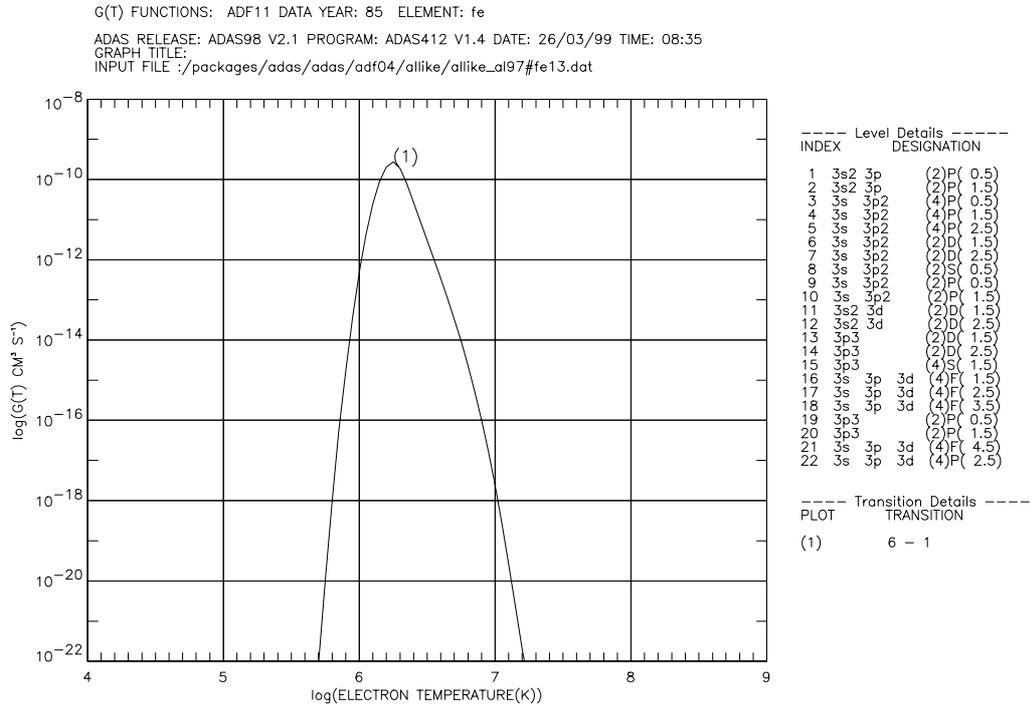
Select Device

- The *Text Output* button at d) 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 is *goft.pass* and it is sent to your *././adas/pass* directory. Note that the
- At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

Illustration:

Figure 5.12a shows the G(Te) function for 6-1 transition FeXIV. The GFT data set was prepared for a constant pressure model at 1×10^{13} K cm⁻³. The model includes the variation of the ratio N_H / N_e in the solar atmosphere with temperature in the G(Te) functions.

Figure 5.12a



The tabulation is given in table 5.12a. For completeness, interpolation with temperature of the model electron density, electron pressure and N_H / N_e is given in the table. Only a single G(Te) function has been calculated in this case. Selection options in the processing screen allow mass generation formatted as illustrated in this example.

Table 5.12a

```

FE+13 /NLEVELS= 40/NKNOTS= 82/NLINES= 1/

SOURCE FILES:
-----
IONISATION BALANCE DATA - /packages/adas/adas/adf11/.<>cd85#FE.dat
SPECIFIC ION FILE DATA - /packages/adas/adas/adf04/alllike/allike_al97#fe13.dat

PROCESSING CODE          DATE          USER IDENTIFIER
-----
ADAS 412                 26/03/99    summers

ENERGY LEVEL INDEXING
-----
INDX   CODE          S L IJ
-----
  1    3s2 3p          2(1) 0.5
  2    3s2 3p          2(1) 1.5
  3    3s  3p2         4(1) 0.5
  4    3s  3p2         4(1) 1.5
  5    3s  3p2         4(1) 2.5
  6    3s  3p2         2(2) 1.5

38    3s  3p  3d      2(2) 2.5
39    3s  3p  3d      2(1) 0.5
40    3s  3p  3d      2(1) 1.5

PLASMA MODEL (FINITE DENSITY IONISATION BALANCE =YES)
-----
TE(K)    NE(CM-3)    P(KCM-3)    NH/NE    TIME(S)    LOG(TE)    LOG(NE)    LOG(P)
-----
8.91D+04  1.12D+08    1.00D+13    8.55D-01  -----    4.95      8.05      13.00
1.00D+05  1.00D+08    1.00D+13    8.49D-01  -----    5.00      8.00      13.00
1.12D+05  8.91D+07    1.00D+13    8.42D-01  -----    5.05      7.95      13.00
1.26D+05  7.94D+07    1.00D+13    8.35D-01  -----    5.10      7.90      13.00

```

6.31D+08	1.58D+04	1.00D+13	8.27D-01	8.80	4.20	13.00
7.08D+08	1.41D+04	1.00D+13	8.27D-01	8.85	4.15	13.00
7.24D+08	7.06D+04	1.00D+13	8.27D-01	8.90	4.20	13.00
8.91D+08	1.12D+04	1.00D+13	8.27D-01	8.95	4.05	13.00
1.00D+09	1.00D+04	1.00D+13	8.27D-01	9.00	4.00	13.00

TABLE OF G(T) VALUES (CM3 S-1) FOR FE XIV

TRANS INDEX	1	2	3	4	5	6	7	
APPROX WLENGTH	334.2	0.0	0.0	0.0	0.0	0.0	0.0	0.
SPECTR WLENGTH	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.
TRANSITION	1- 6	0- 0	0- 0	0- 0	0- 0	0- 0	0- 0	0-
LOG(TE(K))								
4.95	1.000D-99	0.000D+00						
5.00	4.003D-98	0.000D+00						
5.05	6.230D-88	0.000D+00						
5.10	5.875D-79	0.000D+00						
8.85	1.174D-47	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+
8.90	3.436D-48	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+
8.95	1.043D-48	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+
9.00	3.227D-49	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+

C-----

C

C TRANSITION LIST FOR FE XIV

C-----

C IND	TRANSITION	APP. WVL. (A)	EXACT WVL. (A)	LOWER ST.	UPPER ST.
C 1	1 - 6	334.2	0.0	2(1) 0.5	2(2) 1.5
C					
C				summers	26/03/99
C					
C					
C					

C-----

Notes: