ADAS508: GTN - graph and fit G(Te,Ne) functions

The program interrogates *GTN* files of type ADF32. The $G(T_e, N_e)$ function is extracted for a selected radiative transition of an ion. The data may be interpolated using cubic splines at selected electron temperatures and electron densities. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be displayed. Additionally a collection file may be prepared for double differential emission measure analysis.

Code under design and development

Background theory:

One of the most widely used methods available for the interpretation of astronomical spectral intensities is the emission measure technique. This method is less familar 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 **A** and due to a transition from upper level j to lower level k may be written as

$$I_{j \to k} = \frac{1}{4\pi \mathbf{A}} \iiint A_{j \to k} N_j dz dy dx \qquad 6.8.1$$

where N_j denotes the population density of ions in the upper state j, $A_{j \to k}$ 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

$$N_j = \sum_{\sigma=1}^{M_z} \mathscr{F}_{j\sigma}^{(exc)} N_e N_\sigma + \sum_{\upsilon'=1}^{M_{z+1}} \mathscr{F}_{j\upsilon'}^{(rec)} N_e N_{\upsilon'}^+ \qquad 6.8.2$$

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

$$N_j = \sum_{\sigma=1}^{M_z} \mathscr{F}_{j\sigma}^{(exc)} N_e N_\sigma \qquad 6.8.3$$

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.

$$N_\sigma \equiv N_\sigma^{(z)} = \frac{N_\sigma^{(z)}}{N_{tot}} \frac{N_{tot}}{N_H} \frac{N_H}{N_e} N_e \qquad 6.8.4$$

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

$$A_{j \to k} N_j = \frac{N_{tot}}{N_H} N_e^2 G(T_e, N_e) \qquad 6.8.5$$

where

$$G_{j \to k}(T_e, N_e) = A_{j \to k} \frac{N_H}{N_e} \sum_{\sigma=1}^{M_z} \mathscr{F}_{j\sigma}^{(exc)} \frac{N_\sigma^{(z)}}{N_{tot}} \qquad 6.8.6$$
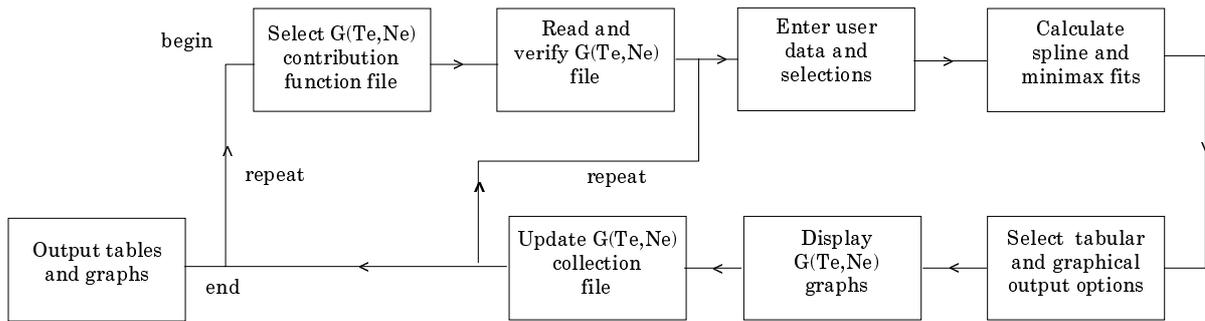
Then the spectral intensity may be written as

This is a place holder for double differential emission measure theory.

The program interrogates $G(T_e, N_e)$ data sets prepared according to the prescription of equation 6.8.6. Interpolation of the $G(T_e, N_e)$ to arbitrary temperatures and densities is done by cubic splines.
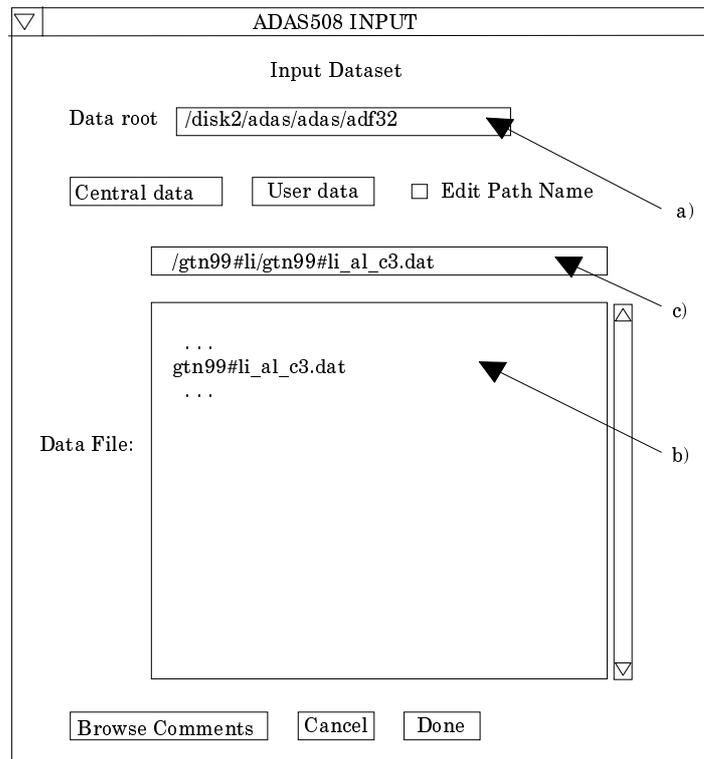
Program steps:

These are summarised in figure 6.8.

Figure 6.8

Interactive parameter comments:

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. The appropriate ADAS data format for input to this program is ADF32 ('G(Te,Ne) files'). 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 first to permit editing.

3. 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. They are named by iso-electronic sequence (eg. *Gtn99#li*). specific file names include a source identifier (eg. *al*) and the specific ion symbol (eg. *c3*).

4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then the individual datafiles are presented for selection. Datafiles all have the termination *.dat* (eg. *Gtn99#li_al#c3.dat*).

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

6. 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 has gone into the dataset and the attribution of the dataset. The possibility of browsing the comments appears in the subsequent main window also.

7. 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.

8. Transitions for which G(Te,Ne) data are available in the data set are displayed in the line list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a line to select it. The selected transition appears in the selection window a) just above the line list display window.

9. Your settings of electron temperatures (output) are shown in the temperature display window d). The temperature values at which the G(Te,Ne) coefficients are stored in the datafile (input) are also shown for information.

10. The program recovers the output temperatures you used when last executing the program. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures

11. The Temperature Values are editable. Click on the *Edit Table* button if you wish to change the values. A 'drop-down' window, the ADAS Table Editor window: It follows the usual pattern of operation.

12. Your settings of electron densities (output) are shown in the density display window e). The density values at which the G(Te,Ne) coefficients are stored in the datafile (input) are also shown for information.

13. The program recovers the output densities you used when last executing the program. Pressing the *Default Density values* button inserts a default set of densities equal to the input densities

14. The Density Values are editable. Click on the *Edit Table* button if you wish to change the values. A 'drop-down' window, the ADAS Table Editor window: It follows the usual pattern of operation.

15. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **output options window** has the appearance shown below.

16. 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.

```
┌─────────────────────────────────────────────────────────────────────┐
│ ☑              ADAS508  OUTPUT OPTIONS                               │
│                                                                     │
│   Data file name  :  /home/lanzafam/adas/adf32/gtn99#li/gtn99#li_al_c3.dat │
│   ┌─────────────────────────────────────────────────────────────┐   │
│   │                    Browse Comments                          │   │
│   └─────────────────────────────────────────────────────────────┘   │
│   ┌─────────────────────────────────────────────────────────────┐   │
│   │  ☐    Graphical Output                      Default Device   │   │
│   │  Graph Title    ┌──────────────────────┐    ┌────────────┐   │   │
│   │                 │   Figure 1           │    │ Post-script│   │   │
│   │    ┌──────────────────────────────────────┐ └────────────┘   │   │
│   │    │  ☐    Explicit Scaling               │  ┌────────────┐  │   │
│   │    │            X-min ┌──────┐  X-max ┌──────┐ │ Post-script│  │   │
│   │    │                                          │ HP-PCL     │  │   │
│   │    │            Y-min ┌──────┐  Y-max ┌──────┐ │ HP-GL      │  │   │
│   │    │                                          └────────────┘  │   │
│   │    │            Z-min ┌──────┐  Z-max ┌──────┐              │   │
│   │    └──────────────────────────────────────┘                 │   │
│   │    ┌──────────────────────────────────────┐                 │   │
│   │    │  ☐ Enable Hard Copy   ☐  Replace     │                 │   │
│   │    │  File name  : ┌────────────────────┐ │                 │   │
│   │    │               │  graph.ps          │ │                 │   │
│   │    └──────────────────────────────────────┘                 │   │
│   └─────────────────────────────────────────────────────────────┘   │
│   ┌─────────────────────────────────────────────────────────────┐   │
│   │  ☐ Text Output   ☐ Replace   ┌──────────────────┐           │   │
│   │                              │ Default file name│           │   │
│   │  File name  : ┌────────────────────┐                        │   │
│   │               │  paper.txt         │                        │   │
│   └─────────────────────────────────────────────────────────────┘   │
│   ┌─────────────────────────────────────────────────────────────┐   │
│   │  ☐  Collection File ☐  Replace                              │   │
│   │  File name  : ┌────────────────────┐                        │   │
│   └─────────────────────────────────────────────────────────────┘   │
│    ┌──┐   ┌────────┐   ┌──────┐                                     │
│    │▤ │   │ Cancel │   │ Done │                                     │
│    └──┘   └────────┘   └──────┘                                     │
└─────────────────────────────────────────────────────────────────────┘

a)   b)   c)   d)
```

17. Graphical display is activated by the *Graphical Output* button a). 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.

18. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button at b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable. In this case, a three-dimensional surface plot is presented with x-axis: beam energy, y-axis: density, z-axis: selected coefficient.

19. 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.

20. A choice of output graph plotting devices is given in the Device list window at c). Clicking on the required device selects it. It appears in the selection window above the Device list window.

21. Writing to the collection file is activated by clicking the *Collection File* button at d). The operation is slightly different from the usual text output. The collection file is composed of blocks of data for each spectrum line. Each block includes a header line which enables the code to construct an indexed list of lines present in the collection file. A line which is already present in the collection is replaced if the *Replace* button is activated, otherwise it is disallowed. Thus the G(Te,Ne) collection file contains any one line only once.

The graph is displayed in a following **graphical output** window.

22. This is a new style of graphical output widget to ADAS. A three-dimensional surface plot is given at a). There is much more control over it than in our usual graph displays.

23. At b), there are the controls for the orientation of the figure. By clicking repeatedly on a button, the figure may be rotated clockwise or anti-clockwise is small steps. You may rotate about a vertical or horizontal axis.

24. At c), there are two buttons to zoom in or out on the figure.

25. At d), the controls on the appearance of the figure are available. Note the nesting of menu buttons in more than one layer. The choices are laid out at e) below the main figure. Thus one may choose a meshed surface or shaded surface, the colour of the shaded surface may be selected and so on. You may feel we have gone to overkill here.

26. Then there are choices on the axes, whether they are linear or logarithmic, whether they are to be displayed or not etc. There is an additional point. At b) when the figure is rotated the position of the axis of rotation matters. For rotations about a vertical axis, the figure Z-axis is used and it may be moved to any corner of the projected area on the X/Z plane.

27. Finally note that when the figure is printed, it is the figure as displayed in the graphic output window which you get.

28. 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 3 menu. Remember that *Done* takes you back to the previous screen. The *Print* button appears if graphical hard-copy is selected on the output options window.

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ADAS508 : GRAPH

a)

b)

Rotate Image about vertical axis	Rotate Image about horizonal axis	Magnify Image	Image Display
Anti-clockwise	Anti-clockwise	Step in	Surface Properties
Clockwise	Clockwise	Step out	Axis Properties

Done   Print

c)

d)

Surface Properties —— Meshed Surface ▷
Shaded Surface ▷ —— Stacked Histogram
Horizontal Lines
Wire Mesh

Colour ▷ —— Blue
Orange
Grey

Axis Properties —— Log Plots ▷
Axis Style ▷
Z-axis ▷

X-axis
Y-axis
Z-axis

Show axis
Extend axis
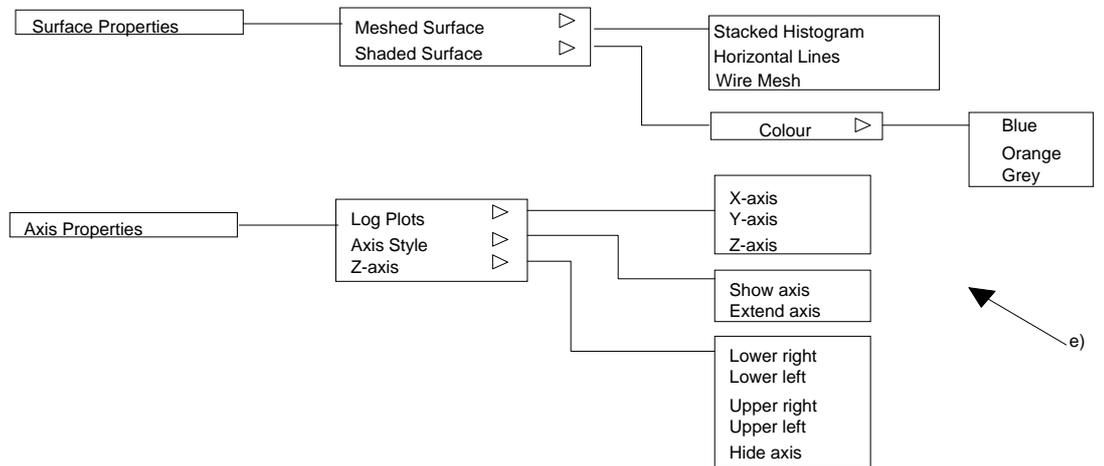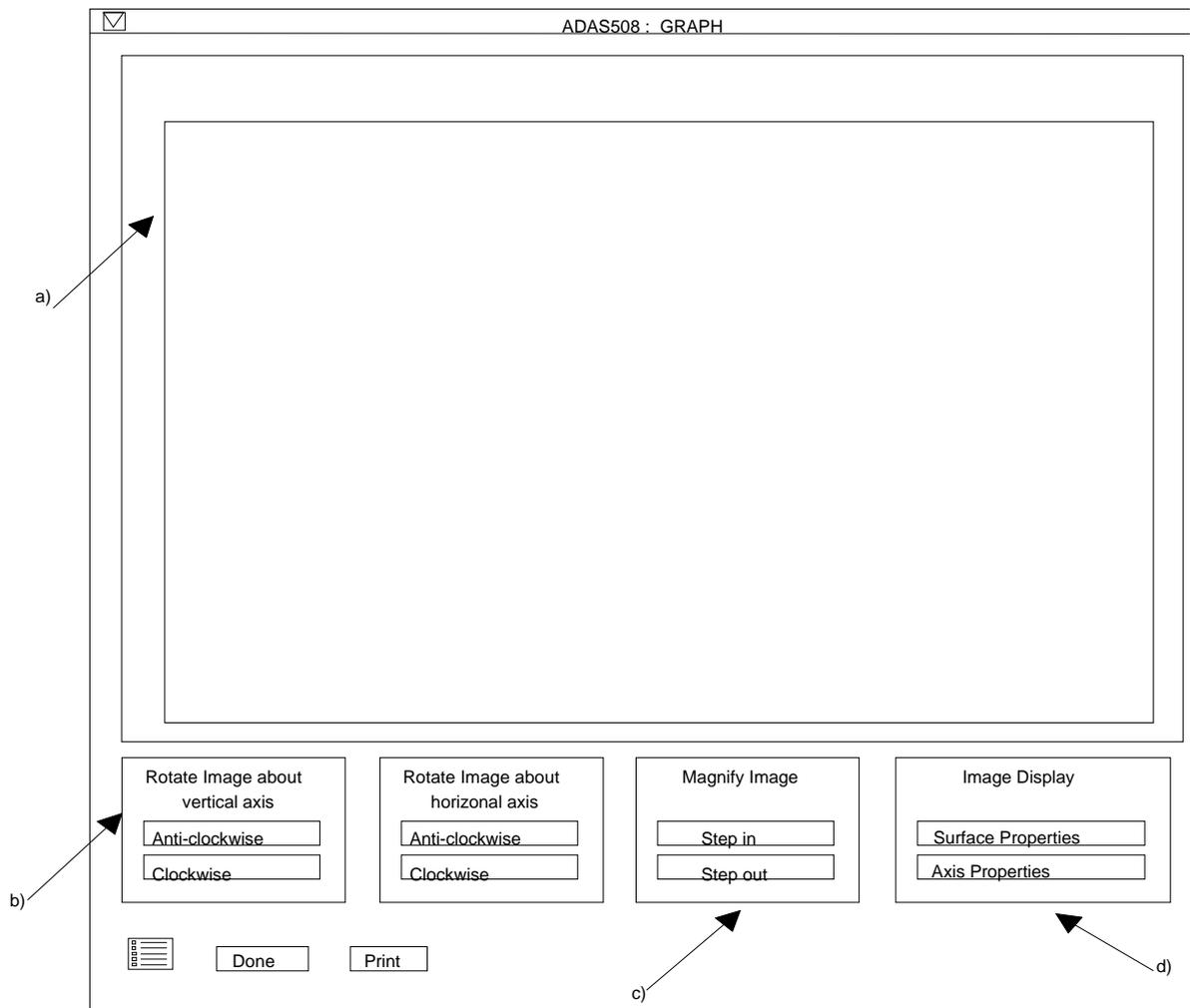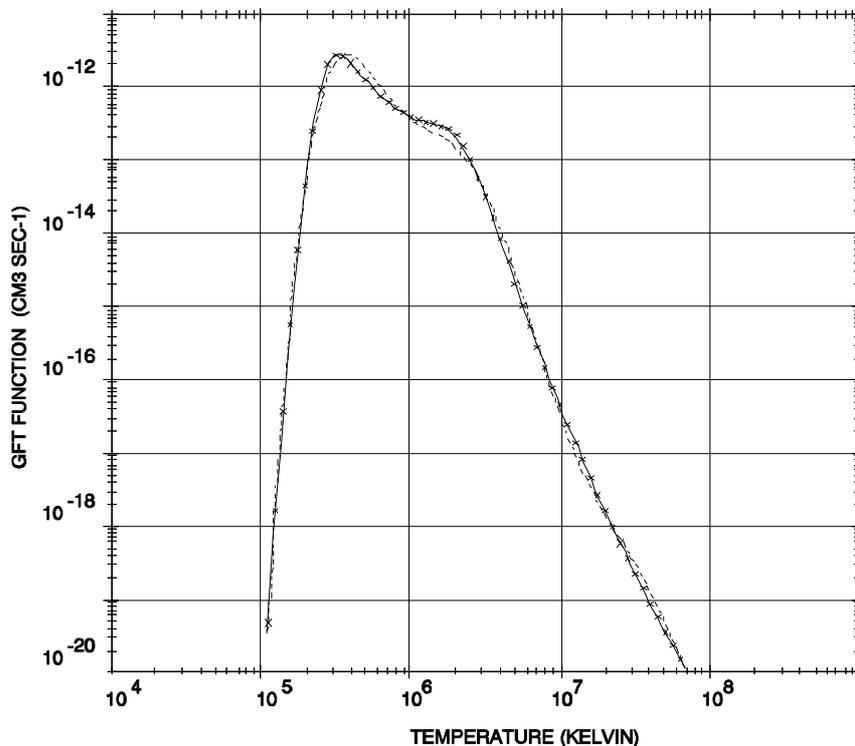
Lower right
Lower left

Upper right
Upper left

Hide axis

e)

Illustration:

Figure 6.8a shows the G(Te) function for 150.1 A line of OVI. The GFT data set was prepared for a constant pressure model at $3 \times 10^{+14}$ 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 6.8a

The tabulation is given in table 6.8a. For completeness, interpolation with temperature of the model electron density, electron pressure and N_H / N_e is given in the table.

Table 6.8a

```
ADAS RELEASE: ADAS91 V1.10  PROGRAM: ADAS506 V1.0   DATE: 10/04/94  TIME: 10:32
******** TABULAR OUTPUT FROM  G(TE) FUNCTION FILES INTERROGATION      PROGRAM: ADAS506 - DATE: 10/04/94
*******

------------------- TEST                             -------------------

        G(TE) CONTRIBUTION FUNCTIONS AS A FUNCTION OF TEMPERATURE
        ----------------------------------------------------------
                 DATA GENERATED USING PROGRAM: ADAS506
                 -------------------------------------

FILE: /JETSHP.GFT93#LI.DATA(SM#O5)   ELEM: O + 5  LINE: (01->05) WVLN:   150.1A

NUCLEAR CHARGE          (Z0) =   8
RECOMBINING ION CHARGE (Z1) =   6
RECOMBINED ION CHARGE  (Z)  =   5


   LEVEL       CONFIGURATION      QUANTUM NUMBERS
                                  2S+1  L  (WI-1)/2
-----------------------------------------------
 5 - UPPER     3p*  3P(J=0)        2    1    0.5
 1 - LOWER     2s   2S(J=0)        2    0    0.5


TRANSITION WAVELENGTH (APPROX.) =    150.1 A
TRANSITION WAVELENGTH (EXACT)   =    150.1 A


------------- TEMPERATURE ------------    GFT       DENS      PRESS      NH/NE
   KELVIN       EV     KELVIN/Z1**2 CM3 S-1     CM-3      KCM-3
------------------------------------------------------------------------------
  1.00D+05   8.62D+00    2.78D+03   8.46D-22   3.00D+09  3.00D+14  8.49D-01
  2.00D+05   1.72D+01    5.56D+03   4.52D-14   1.50D+09  3.00D+14  8.33D-01
  3.00D+05   2.59D+01    8.33D+03   2.56D-12   9.98D+08  3.00D+14  8.32D-01
  5.00D+05   4.31D+01    1.39D+04   1.27D-12   6.00D+08  3.00D+14  8.31D-01
  7.00D+05   6.03D+01    1.94D+04   6.31D-13   4.29D+08  3.00D+14  8.31D-01
  1.00D+06   8.62D+01    2.78D+04   3.87D-13   3.00D+08  3.00D+14  8.30D-01
  2.00D+06   1.72D+02    5.56D+04   2.14D-13   1.50D+08  3.00D+14  8.30D-01
  3.00D+06   2.59D+02    8.33D+04   4.24D-14   9.98D+07  3.00D+14  8.29D-01
  5.00D+06   4.31D+02    1.39D+05   2.04D-15   6.00D+07  3.00D+14  8.29D-01
  7.00D+06   6.03D+02    1.94D+05   2.97D-16   4.29D+07  3.00D+14  8.29D-01
  1.00D+07   8.62D+02    2.78D+05   4.38D-17   3.00D+07  3.00D+14  8.28D-01
------------------------------------------------------------------------------
```

```
0MINIMAX POLYNOMIAL - TAYLOR COEFFICIENTS: LOG10(GFT) vs. LOG10(TEMP<kelvin>)
 --------------------------------------------------------------------------------
           A( 1) =   7.392163053D+08        A( 2) =  -1.525818821D+09
           A( 3) =   1.445324362D+09        A( 4) =  -8.319180529D+08
           A( 5) =   3.246457026D+08        A( 6) =  -9.070529808D+07
           A( 7) =   1.866822456D+07        A( 8) =  -2.865755607D+06
           A( 9) =   3.281465908D+05        A(10) =  -2.768370818D+04
           A(11) =   1.672659108D+03        A(12) =  -6.854708225D+01
           A(13) =   1.707882983D+00        A(14) =  -1.954078669D-02

 LOGFIT - DEGREE=13  ACCURACY= 47.45%  END GRADIENT: LOWER= 120.01 UPPER= -14.19
 --------------------------------------------------------------------------------
```

Notes:

```
0MINIMAX POLYNOMIAL - TAYLOR COEFFICIENTS: LOG10(GFT) vs. LOG10(TEMP<kelvin>)
 --------------------------------------------------------------------------------
           A( 1) =   7.392163053D+08        A( 2) =  -1.525818821D+09
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 LOGFIT - DEGREE=13  ACCURACY= 47.45%  END GRADIENT: LOWER= 120.01 UPPER= -14.19
 --------------------------------------------------------------------------------
```