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# ADAS102: Electron impact excitation rate - graphing and interpolation

The program is for entry of electron impact excitation rate coefficient data, examination and comparison with approximate forms, display and interpolation to arbitrary electron temperatures for permanent storage in the ADAS database. There is no central ADAS data class associated with input to this program, since new data is entered by hand in the program. However a mechanism is provided for storage and retrieval of the output from the ADAS102 analysis. The output from a case may be stored in an archive file. Such files are present only on the user's own space. Storage is sequential with an index

## Background theory:

The theoretical background is the same as for the program ADAS101. In this case however data are provided as Maxwell averaged excitation rate coefficients or equivalent forms so there is no requirement for Maxwell averaging.

Three distinct types of rate coefficient are recognised, namely, dipole, non-dipole and spin change. The variant of rate coefficient used as standard in ADAS is the rate parameter (*Upsilon*), also called the Maxwell averaged collision strength or effective collision strength. All rate coefficients are converted to this form.

*Approximate forms:*

Simple approximate forms for the rate parameter which show correct asymptotic behaviour are

$$\begin{aligned} \text{dipole :} \quad Y_{ij} &\approx F_3 S_{ij} [\ln(1 + F_2) + EEI((1 + F_2)\Delta E_{ij} / kT_e)] \\ \text{non - dipole :} Y_{ij} &\approx F_3 + F_2 (\Delta E_{ij} / kT_e) EEI(\Delta E_{ij} / kT_e) \quad 2.2.1 \\ \text{spin change :} \quad Y_{ij} &\approx \frac{F_3 (\Delta E_{ij} / kT_e)}{1 + F_2} EE2((1 + F_2)\Delta E_{ij} / kT_e) \end{aligned}$$

where  $F_2, F_3$  are constants.  $EEI(x) = \exp(x)E_1(x)$  and  $EE2(x) = \exp(x)E_2(x)$  with  $E_1$  and  $E_2$  the first and second exponential integrals. The three forms are the Maxwell averages of the approximate forms given for  $\Omega_{ij}$ , the collision strength, in ADAS101.

To obtain rate parameters at temperatures intermediate between tabular values or in extrapolation, two distinct approaches are useful. Firstly, the source values may be treated as exact and an attempt made at optimum interpolation. Alternatively, a least squares fit can be made to the source values. In either case, control of the behaviour of the fit function especially in extrapolation is necessary. The two approaches are implemented in ADAS102 as described below.

### ADAS comparative plots:

The parameters  $F_2$  and  $F_3$  of the three approximate form 2.2.1 are determined from  $Y_1$  and  $Y_m$ , where  $\{(X_i, Y_i): i = 1, \dots, m\}$  are the input data with  $X = \Delta E_{ij} / kT_e$ , according to the type of cross-strength. Optionally the parameter  $F_3$  may be imposed and then  $F_2$  obtained from  $Y_1$ . The input data are ratioed to the approximate form and an interpolating spline put through the values. The ratio spline end conditions are imposed as zero gradient at the endpoints and extrapolation of the ratio is as a constant. Generally, the ratio is close to unity and so the interpolating spline provides a small correction only to the approximate form. Also extrapolation is stable and safe. The interpolating spline and approximate form are used to produce the final Upsilon's.

### Burgess C-plots:

Burgess & Tully (1992) examined the behaviour of  $Y$  as a function  $T_e$ , and defined reduced variables appropriately so that the whole variation of  $Y$  and  $T_e$  could be mapped onto a

finite range. They introduced a reduced temperature,  $x$ , and reduced Upsilon,  $y$ , for four types of transition. These are given below together with their limiting values when known. Burgess & Tully vary the parameter  $C$  to balance the spread of  $x$ -values across the range  $[0,1]$  and so optimise a five point, fixed knot, least squares spline through the data. This gives a compact representation of the data and a good control or check of the limiting high energy behaviour of the rate coefficient.

*Type 1 - dipole:*

$$x = 1 - \frac{\ln C}{\ln\left(\frac{kT_e}{E_{ij}} + C\right)}, \quad y(x) = \frac{Y}{\ln\left(\frac{kT_e}{E_{ij}} + e\right)} \quad 2.2.2$$

$$\text{with } y(0) = \Omega(0), \quad y(1) = \frac{4\omega_i f_{i \rightarrow j}}{E_{ij}}$$

*Type 2 - non-dipole, non-spin change:*

$$x = \frac{\left(\frac{kT_e}{E_{ij}}\right)}{\left(\frac{kT_e}{E_{ij}} + C\right)}, \quad y(x) = Y \quad 2.2.3$$

$$\text{with } y(0) = \Omega(0), \quad y(1) = \text{high energy Born limit of } \Omega.$$

*Type 3 - spin change:*

$$x = \frac{\left(\frac{kT_e}{E_{ij}}\right)}{\left(\frac{kT_e}{E_{ij}} + C\right)}, \quad y(x) = \left(\frac{kT_e}{E_{ij}} + 1\right)Y \quad 2.2.3$$

$$\text{with } y(0) = \Omega(0), \quad y(1) = \int_0^\infty \Omega d\left(\frac{E_j}{E_{ij}}\right).$$

*Type 4 - weak oscillator strength:*

$$x = 1 - \frac{\ln C}{\ln\left(\frac{kT_e}{E_{ij}} + C\right)}, \quad y(x) = \frac{Y}{\ln\left(\frac{kT_e}{E_{ij}} + C\right)} \quad 2.2.4$$

$$\text{with } y(0) = \frac{\Omega(0)}{\ln C}, \quad y(1) = \text{as for type 1.}$$

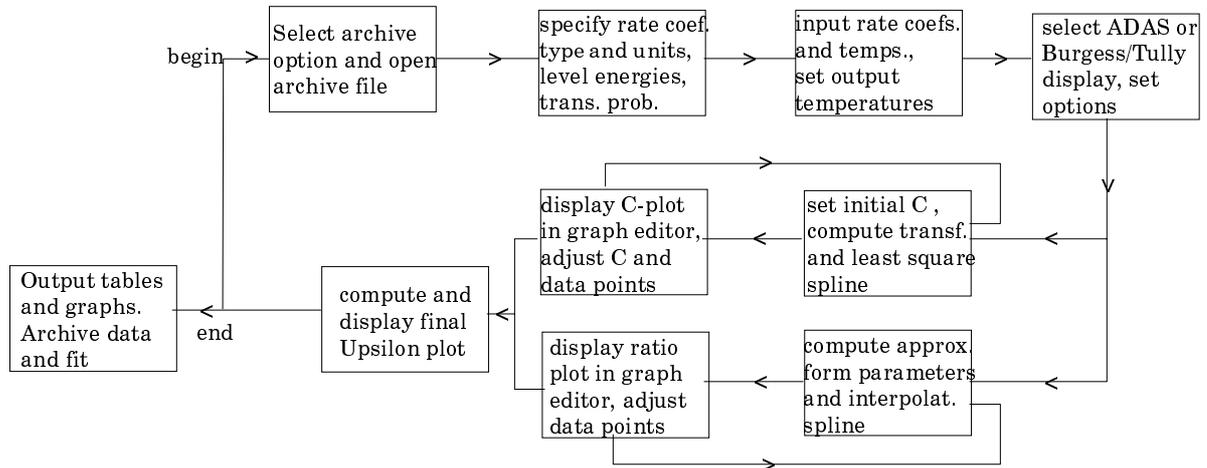
For the present code, the Burgess & Tully transformations are used as an aid to interpolation and extrapolation. That is an interpolating spline rather than a least squares optimising spline is passed through the Upsilon data for a transition. The collision data from the adf04 file does not in general have all the information ideally required for assigning to type and to specify threshold and high energy limits. For an LS-coupled data set, the total spin quantum numbers are available and so assignment to type 3 is possible. For intermediate coupling data sets, this is less clear and the categorisation has to be supported by the manifest decreasing behaviour of

Upsilon at high temperature. Since the *adf04* file includes the A-value for the transition, identification of type 1 and separation from type 2 is possible. The switch from type 1 to type 4 and from type 3 to type 4 is less clear and somewhat subjective.

## Program steps:

These are summarised in the figure 2.02.

Figure 2.02



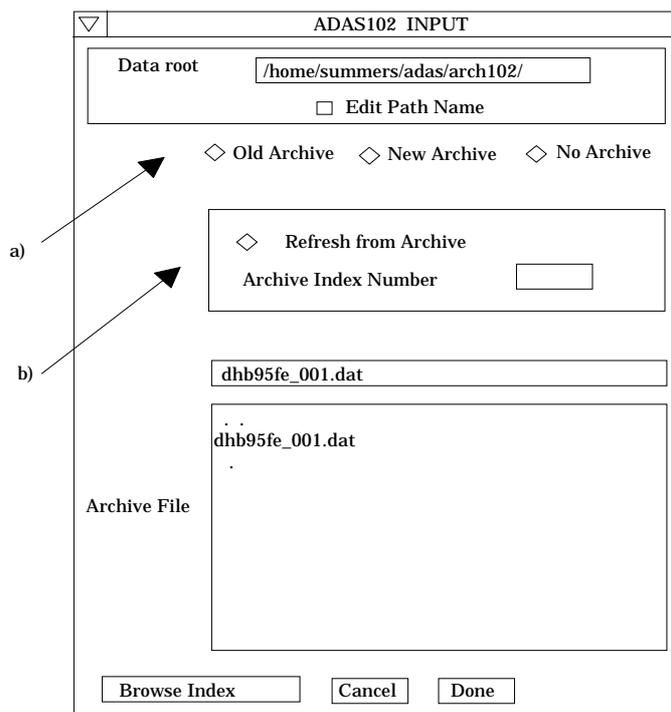
## Interactive parameter comments:

Remember to ensure you have a defaults directory allocated. This should have the pathway *.../uid/adas/defaults*

where *uid* is your user identifier. The defaults directory records the parameters you set the last time you ran each ADAS code. Move to the directory in which you wish ADAS created output text file (*paper.txt* is the default) and graphic files (e.g. *graph.ps* if a postscript file) to be placed. Initiate ADAS, move to the series 1 menu and click on the first button to activate ADAS101.

The **archive selection window** appears first. It is slightly different in operation than the usual file selection window.

1. The recommended root path for user archiving for ADAS102 analysis is *.../uid/adas/arch102/* which may be edited in the usual manner.
2. Click the appropriate button at a) for opening an old archive file, starting a new archive file or ignoring archiving. In the first case, the usual file display window shows existing archive files from which selection may be made. The selected file is displayed in the selection window. In the second case, the file display window is the same, but the selection window is editable for entry of a new archive file name. **Remember to press the *return* key on the keyboard to record an entered value.**
3. The capability is given for reworking or re-displaying the results of an earlier analysis stored in an archive file. At b) click on the *Refresh from archive* button. Then give the *Archive index number*. The selected data will be used as the default data in the subsequent processing and output windows. Archiving is strictly sequential. A new analysis is simply appended at the end of the archive file and the index updated. There is no data replacement or substitution.
4. Clicking on the *Browse Index* button displays the index list for the selected archive file. The possibility of browsing the index appears in the subsequent main window also.
5. 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

6. The button *Browse Index* at a) again allows display of the archive index list.
7. As described in the ADAS Manual, four types of rate parameter are allowed, namely 1-dipole, 2-non-dipole, 3-spin change and 4-other. Enter the *transition type* number at b). For dipole transitions the transition probability is required. Either the line strength (*S*), absorption oscillator strength (*f*) or Einstein A-value (*A*) forms are accepted. Click the appropriate button and enter the value.
8. At c) details of the upper and lower levels of the transition are entered. The energies of levels are measured upwards from the lowest level of the ion. Click on the *Select energy form* button to indicate which units are being used for these energies. Note that full statistical weights (including spin parts in the case of terms) are required.
9. User input *Upsilon*s, input temperatures and required output temperatures are displayed at d) with the currently selected units shown below. Click the *Edit table* button to 'drop down' the ADAS Table Editor for data input.
10. If an archive data set is opened, rate parameter and temperature values are filled from this. Otherwise the fields are empty. Pressing the *Default Temperature values* button inserts a default set of temperatures.
11. The ADAS Table Editor window follows the same pattern of operation as described previously. Note however the fairly wide selection of units in which data can be entered. This is to ease the problem of unit conversion for data from the general literature. Click on the buttons for the units with which you wish to work. The program internally converts to the threshold energy parameter *X* and the collision strength *Omega*. If data is returned from archive it will be in these forms. Click the *Done* button if editing is completed satisfactorily.

ADAS102 PROCESSING OPTIONS

Data file name : /home/summers/adas/arch102/dhb95fe\_001.dat

Browse Index

Nuclear Charge: 26.00 Ion Charge: 18.00

Transition Type: 1 Transition Probability: 5.40E+10

Form:  S  f  A

Lower Level Upper Level

Index : 1 Index : 4

Stat. Wt. : 9.0 Stat. Wt. : 9.0

Level Energy : 0.347841 Level Energy : 8.705277

Select Energy Form :  cm-1  Rydbergs

INDEX	Input Temp.	Input Coefft.	Output Temp.
1	1.000E+00	1.000E+00	1.000E+05
2	2.000E+00	2.000E+00	2.000E+05
3	5.000E+00	5.000E+00	3.000E+05
4	1.000E+01	1.000E+01	4.000E+05
5	2.000E+01	2.000E+01	7.000E+05
6	5.000E+01	5.000E+01	8.000E+05
7	1.000E+02	1.000E+02	1.000E+06
8	2.000E+02	2.000E+02	2.000E+06

Input Temp. units : Reduced. Input Rate Coefft.: Upsilon. Output Temp. units : Kelvin.

Edit Table

Default Temperature values

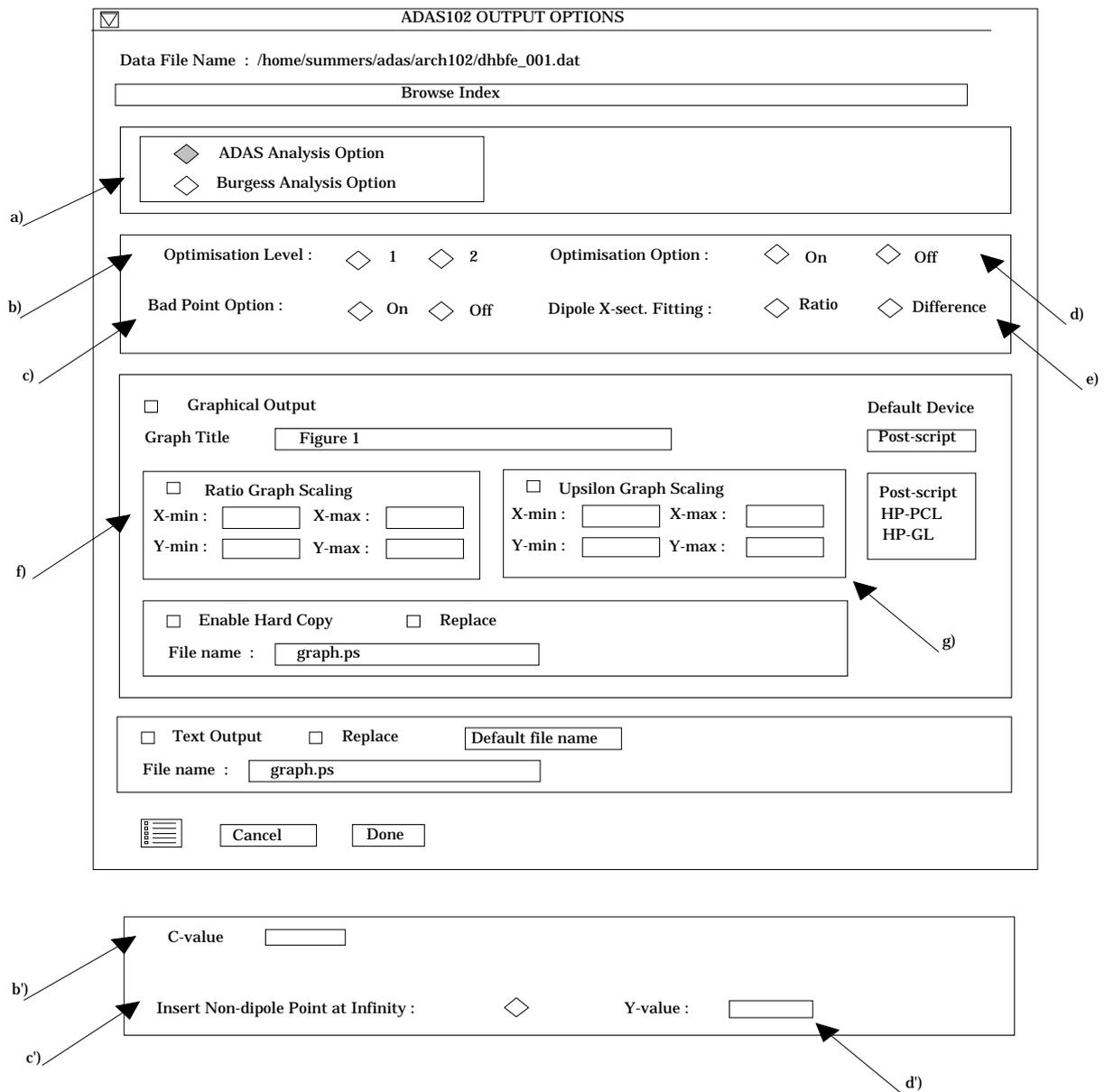
Edit the processing options data and press Done to proceed

Cancel Done

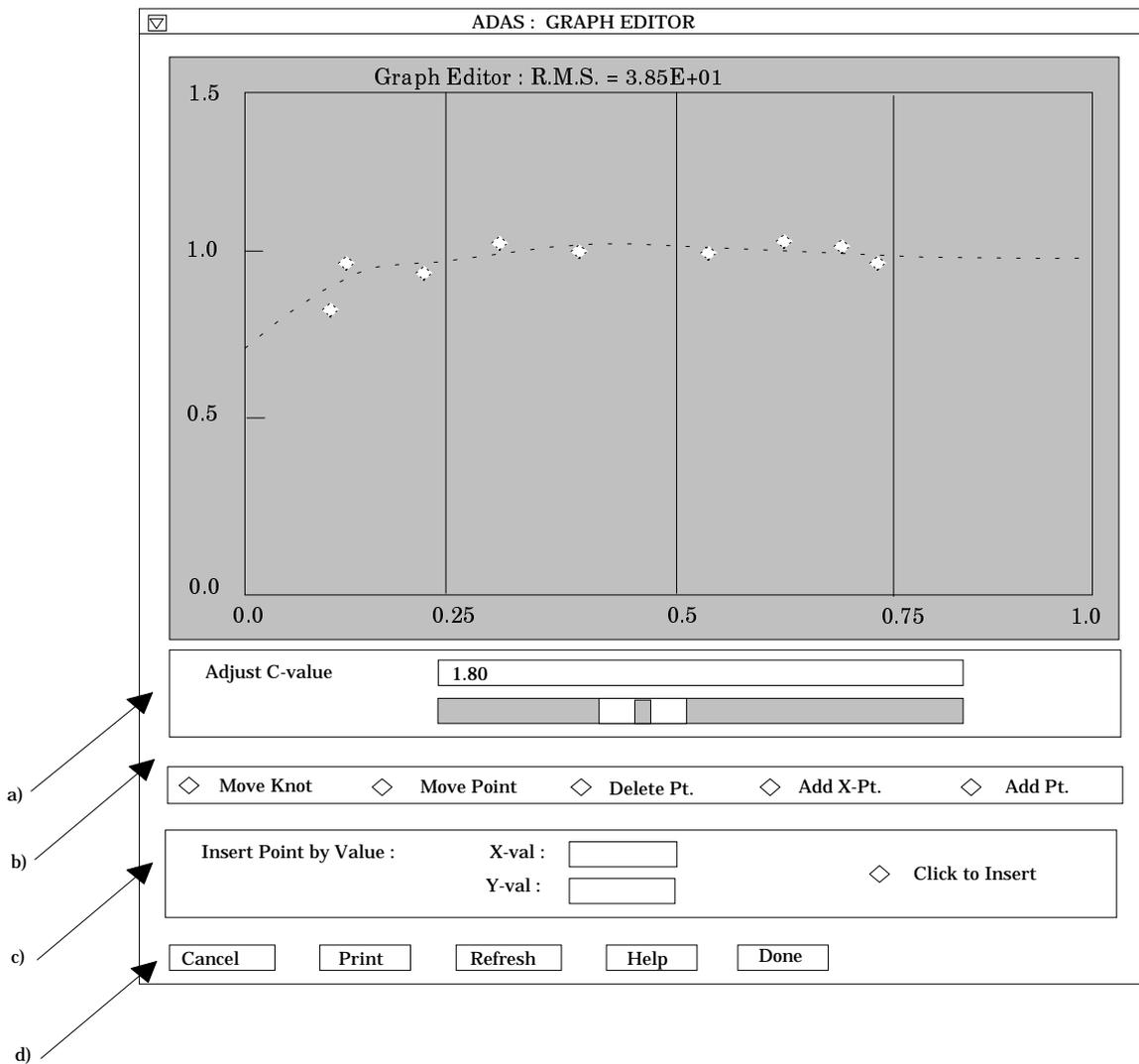
12. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window. The *Escape to Menu* icon is also available for a quick exit at the bottom left hand corner.

The **output options window** is more complex than in previous programs. It is shown below.

13. There is a choice of method for examination and display of the input data. At a), click either the *ADAS analysis option* which corresponds to the JET analysis or the *Burgess analysis option*. The latter is an implementation of the technique developed by Burgess and Tully which is popular in astrophysics. The sub-window at b) varies depending on this choice. Make the appropriate choices at b), c), d) and e) in the ADAS case or at b'), c') and d') in the Burgess case.



14. Two graphs are presented. The first is a scaled comparative graph for assessing the *Upsilon* data and making adjustments if appropriate. The second graph displays the final *Upsilon*s at the user's temperatures. Make the required choices of graph scaling and axes choices at f) for the comparative graph and at g) for the *Upsilon* graph.
15. The comparative graph is displayed in the Graph Editor window as shown below. The graph displays the scaled input values as circles with a spline drawn through these tabular points in the ADAS analysis option case. In the Burgess analysis option case, the spline is drawn through the special five knot points which are distinguished. The points can be modified by using the buttons b) beneath the graph in association with the mouse. In the Burgess analysis option case, the knot points may only be moved vertically and a special button is present for this case. Also in the Burgess case, the parameter 'C' can be varied to seek an optimum fit. This is done with the slider at a).



16. To move a point, click the *move a point* button. Then use the *left* mouse button to pick and drag a point to a new position. Note that the x-ordering of points should be maintained although not forced by the editor. Each point has a small active zone around it for picking by the mouse. Terminate point moving operations by pressing the *right* mouse button. To delete a point, click the *delete a point* button. Then click the *left* mouse button with the pointer over the point to be deleted. Terminate point deletion operations by pressing the *right* mouse button. To add a new point in the x-ordered position between two existing points, click the *add X-point* button. Then click the *left* mouse button with the pointer at the position where the new point is to be inserted. Terminate point insertion operations by pressing the *right* mouse button. For completeness, the capability for adding a point anywhere is given although physically unreasonable. The operation is slightly different. Click the *add anywhere* button. With the *left* mouse button pick a point after which you wish the new point added. Press the *left* mouse button with the pointer at the insertion point. Multiple insertions may be made by continuing to click the *left* mouse button. Click the *right* mouse button to terminate this particular insertion. Press the *right* mouse button a second time to terminate insertion operations.
17. To insert a point by value use sub-window c).
18. The buttons at d) provide the usual *Cancel*, *Print* and *Done* options. In addition the *Help* button displays some information on using the graph editing facilities. The original data and graph can be restored by clicking the *Refresh* button. Note that after leaving the graph editor window with the *Done* button, the modified and or additional points replace the original user input data. Note that with the ADAS analysis option, if any points are modified, the program cycles back to the Output Options window for

reanalysis. With the Burgess analysis option, movement only of the spline knots does not force reanalysis.

19. The Upsilon graph is displayed after graph editing. There is no option to modify this output graph. The graph may be printed, using the *Print* button. If the results of the analysis are acceptable and to be archived, click the *Archive* button.

### Illustration:

The output from the program is illustrated for the transition

$$Fe^{+18} : 2p^4 \ ^3P - 2p^5 \ ^3P$$

The figure 2.1a shows a comparative ratio plot of the source collision strength data to the optimised approximate form collision strengths. Spline interpolated values used in forming the Maxwell averages are marked as crosses. These indicate the reliability of the spline and whether a switch to the bad point option is advisable. Source data values are connected by straight lines.

Figure 2.2a

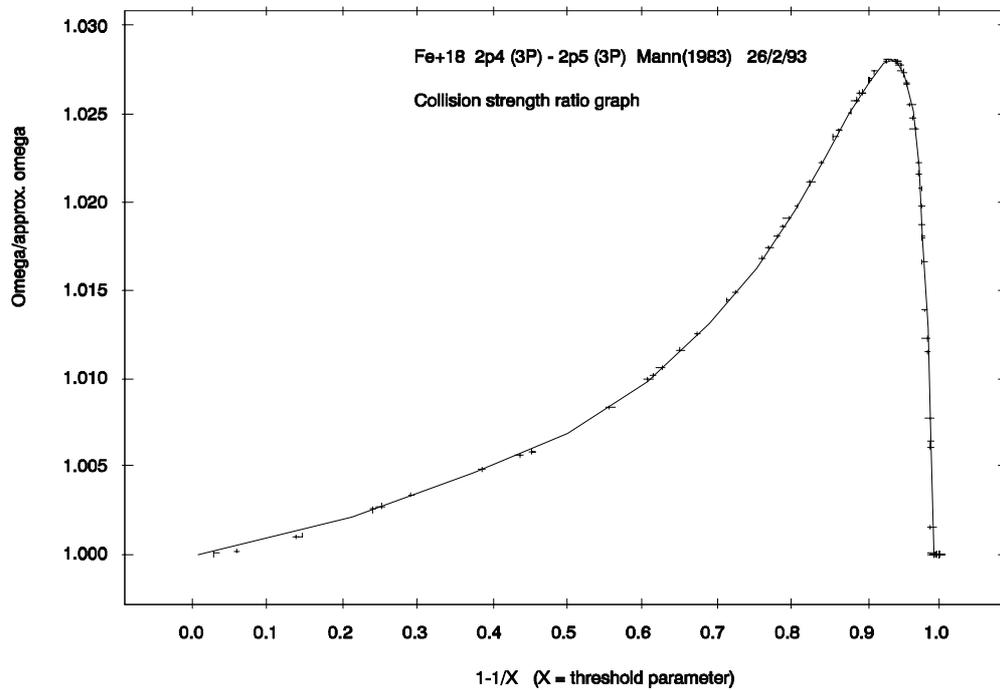
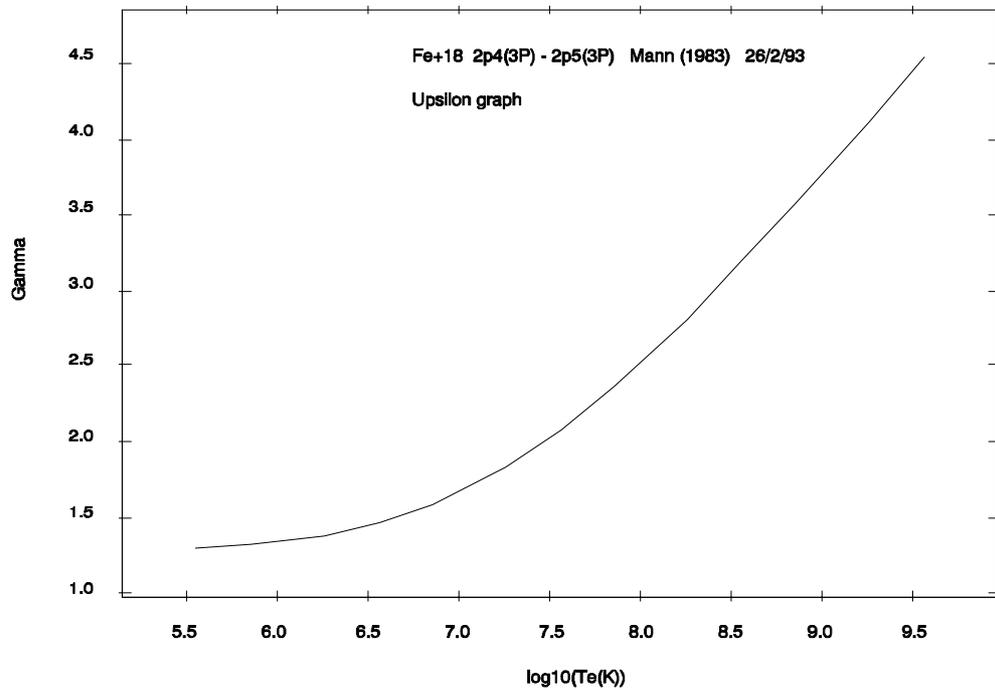


Figure 2.2b shows the Upsilon (gamma) parameter versus electron temperature (K) for the set of output temperatures. Straight lines are drawn between the output values.

Figure 2.2b



The tabular output is shown in table 2.2. Energies are in units of  $I_H$ , excitation and de-excitation rate coefficients are in units of  $cm^3 s^{-1}$  and the A-coefficient is in units of  $s^{-1}$ . IFPTS indicates the optimising level with FXC2 and FXC3 the optimised parameters. IBPTS = 1 if the bad point options is chosen, otherwise 0. IDIFF = 1 if the difference option is chosen, otherwise 0.

Table 2.2.

FE+18 2P4(3P)-2P5(3P) MANN(1983) 26/2/93					
NUCLEAR CHARGE = 26.00 ION CHARGE = 18.00 EFFECTIVE ION CHARGE = 19.00					
LOWER INDEX = 1		UPPER INDEX = 4			
LOWER ENERGY = 0.347841		UPPER ENERGY = 8.705277			
LOWER WEIGHT = 9.0		UPPER WEIGHT = 9.0			
ACOEFF = 5.4000E+10 S = 3.1095E-01 FABS = 9.6251E-02 ENERGY DIFFERENCE = 8.357436					
XSECT TYPE= 1 XSECT OPTIMISATION FACTORS , FXC2 = 6.9706E+00 FXC3 = 1.9825E+00 IBPTS = 0 IFPTS = 2 IDIFF = 0					
X	OMEGA	APPROX. OMEGA	DIFFERENCE		
1.0100E+00	1.2804E+00	1.2804E+00	2.2204E-16		
1.2710E+00	1.3030E+00	1.3002E+00	2.7617E-03		
1.5990E+00	1.3304E+00	1.3243E+00	6.1033E-03		
2.0120E+00	1.3626E+00	1.3533E+00	9.2875E-03		
2.5320E+00	1.4017E+00	1.3880E+00	1.3695E-02		
3.1860E+00	1.4477E+00	1.4290E+00	1.8665E-02		
4.0090E+00	1.5011E+00	1.4771E+00	2.4033E-02		
5.0440E+00	1.5625E+00	1.5326E+00	2.9900E-02		
6.3470E+00	1.6319E+00	1.5961E+00	3.5827E-02		
7.9870E+00	1.7093E+00	1.6677E+00	4.1635E-02		
1.0050E+01	1.7941E+00	1.7473E+00	4.6785E-02		
1.2646E+01	1.8860E+00	1.8348E+00	5.1177E-02		
1.5912E+01	1.9839E+00	1.9298E+00	5.4142E-02		
2.0022E+01	2.0868E+00	2.0316E+00	5.5211E-02		
2.5194E+01	2.1936E+00	2.1397E+00	5.3943E-02		
3.1702E+01	2.3030E+00	2.2532E+00	4.9751E-02		
3.9890E+01	2.4143E+00	2.3716E+00	4.2662E-02		
5.0194E+01	2.5262E+00	2.4942E+00	3.2035E-02		
6.3159E+01	2.6380E+00	2.6202E+00	1.7824E-02		
7.9472E+01	2.7491E+00	2.7491E+00	-1.6645E-07		
TE(K)	GAMMA	APPROX. GAM	EX. RATE	DEXC. RATE	GBARF
3.6100E+05	1.3027E+00	1.3001E+00	5.3754E-11	2.0791E-09	8.3365E-02
7.2200E+05	1.3244E+00	1.3194E+00	2.4034E-10	1.4947E-09	8.4758E-02
1.8050E+06	1.3828E+00	1.3715E+00	4.7512E-10	9.8696E-10	8.8490E-02

3.6100E+06	1.4642E+00	1.4451E+00	5.1272E-10	7.3897E-10	9.3700E-02
7.2200E+06	1.5906E+00	1.5619E+00	4.7283E-10	5.6765E-10	1.0179E-01
1.8050E+07	1.8376E+00	1.7991E+00	3.8554E-10	4.1478E-10	1.1760E-01
3.6100E+07	2.0819E+00	2.0447E+00	3.2034E-10	3.3227E-10	1.3323E-01
7.2200E+07	2.3705E+00	2.3420E+00	2.6268E-10	2.6752E-10	1.5170E-01
1.8050E+08	2.8120E+00	2.7975E+00	1.9925E-10	2.0071E-10	1.7995E-01
3.6100E+08	3.1888E+00	3.1758E+00	1.6035E-10	1.6094E-10	2.0407E-01
7.2200E+08	3.5771E+00	3.5729E+00	1.2743E-10	1.2766E-10	2.2892E-01
1.8050E+09	4.1157E+00	4.1157E+00	9.2829E-11	9.2897E-11	2.6339E-01
3.6100E+09	4.5342E+00	4.5342E+00	7.2341E-11	7.2367E-11	2.9017E-01

**Notes:**