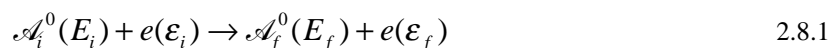

ADAS108: Electron impact excitation of neutral atoms and molecules

The program is for entry of electron impact excitation cross-section data for neutral atoms and molecules, examination and comparison with approximate forms, display and conversion to Maxwell averaged rate coefficients 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 ADAS108 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:

For electron impact with ions the collision strength is finite at threshold and in the high high energy asymptotic limit displays logarithmic, constant or inverse square behaviour with energy depending on whether the transition is of dipole, non-dipole non-spin change or spin change type. The code ADAS101 provides analysis of these cases in both a strict interpolative approach (called the 'ADAS' method) and an optimised economised spline fit approach (called the Burgess C-plot method). The present code is a development designed to handle the zero threshold behaviour of neutral collisions and to give adequate weighting and critical focus to the threshold region as ADAS101 did for the high energy region. Consider the reaction



with

$$\varepsilon_i + E_i = \varepsilon_f + E_f \quad 2.8.2$$

where E_i (E_f) is the excitation energy of the state i (f) denoted by \mathcal{A}_i^0 (\mathcal{A}_f^0) from the lowest level of the atom \mathcal{A}^0 and ε_i (ε_f) is the energy of the incident (scattered) electron. Let ω_i and ω_f be the statistical weights of the states i and f . The reaction is described by a *cross-section* for the process denoted by $\sigma_{i \rightarrow f}(\varepsilon_i)$. Energetically the reaction can only take place if the incident electron energy $\varepsilon_i \geq \Delta E_{if} = E_f - E_i$. It is convenient to introduce the threshold parameter $X = \varepsilon_i / \Delta E_{if} = \varepsilon_f / \Delta E_{if} + 1$, with $X \in [1, \infty]$. The cross-section can therefore be expressed in terms of the incident electron energy ε_i , the scattered electron energy ε_f , or the threshold parameter X . Also, introduce the *collision strength* Ω_{if} , such that

$$\Omega_{if} = \omega_i (E_i / I_H) (\sigma_{i \rightarrow f}(\varepsilon_i) / \pi a_0^2) = \omega_f (E_f / I_H) (\sigma_{f \rightarrow i}(\varepsilon_f) / \pi a_0^2) \quad 2.8.3$$

Working in energies E_f relative to the threshold energy, let E_0 mark the division between the threshold region and the high energy region. We seek to treat the high energy region $[E_0, \infty]$ in the manner of ADAS101 and introduce new methods for the low energy region $[0, E_0]$. The threshold behaviour is expected to be a power law $\sim (X - 1)^B$ with the power determined by the dominant partial wave, l , of the incident electron ($B \sim l + 1/2$). If the s-wave dominates then a square root behaviour occurs. Without access to the detailed cross-section calculations, this information is not generally available with collision data.

An extended Burgess-Tully approach

We seek mappings of the independent energy variable, x_- , from final energies $[0, E_0]$ to $[-1, 0]$ and x_+ , from $[E_0, \infty]$ to $[0, 1]$ and compatible transformations of the collision strengths. Introduce a scale parameter, B , for the threshold region and C , for the asymptotic region. C is the usual Burgess-Tully parameter. The transformations are given below indexed by Burgess-Tully type and a letter for the threshold.

Type 1a: dipole allowed

$$\begin{aligned}
 x_+ &= 1 - \ln(C) / \ln((E_f - E_0) / E_{if} + C) \\
 x_- &= 2(E_f / E_0)^B / ((E_f / E_0)^B + 1) - 1 \\
 y_+ &= \Omega / \ln((E_f - E_0) / E_{if} + e) \\
 y_- &= \Omega / ((E_f / E_0)^B \exp(-(B - E_0 / eE_{if})((E_f / E_0) - 1))) \\
 y_+(0) &= \Omega(E_0) \\
 y_+(1) &= 4\omega_i f_{i \rightarrow f} / E_{if}
 \end{aligned} \tag{2.8.4}$$

S_{if} is the line strength and $f_{i \rightarrow f}$ the absorption oscillator strength.

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

$$\begin{aligned}
 x_+ &= ((E_f - E_0) / E_{if}) / ((E_f - E_0) / E_{if} + C) \\
 x_- &= 2(E_f / E_0)^B / ((E_f / E_0)^B + 1) - 1 \\
 y_+ &= \Omega \\
 y_- &= \Omega / ((E_f / E_0)^B \exp(-B((E_f / E_0) - 1))) \\
 y_+(0) &= \Omega(E_0)
 \end{aligned} \tag{2.8.5}$$

Type 3a: spin change

$$\begin{aligned}
 x_+ &= ((E_f - E_0) / E_{if}) / ((E_f - E_0) / E_{if} + C) \\
 x_- &= 2(E_f / E_0)^B / ((E_f / E_0)^B + 1) - 1 \\
 y_+ &= ((E_f - E_0) / E_{if} + 1)^2 \Omega \\
 y_- &= \Omega / ((E_f / E_0)^B \exp(-(B + 2E_0 / E_{if})((E_f / E_0) - 1))) \\
 y_+(0) &= \Omega(E_0)
 \end{aligned} \tag{2.8.6}$$

Type 4a: weak dipole

$$\begin{aligned}
 x_+ &= 1 - \ln(C) / \ln((E_f - E_0) / E_{if} + C) \\
 x_- &= 2(E_f / E_0)^B / ((E_f / E_0)^B + 1) - 1 \\
 y_+ &= \Omega / \ln((E_f - E_0) / E_{if} + C) \\
 y_- &= \Omega / (\ln(C)(E_f / E_0)^B \\
 &\quad \exp(-(B - E_0 / C(C)E_{if})((E_f / E_0) - 1))) \\
 y_+(0) &= \Omega(E_0) / \ln(C)
 \end{aligned} \tag{2.8.7}$$

An alternative transformation of the independent variable in the threshold region is also provided which is of exponential rather than power law type.

Type b

$$x_- = \exp(-B[\sqrt{(E_{if} / E_f)} - \sqrt{(E_{if} / E_0)}]) - 1 \tag{2.8.8}$$

These transformations introduce three parameters, B , C and E_0 . We impose a requirement of continuity on the derivative of $x(E_f)$ at $x = 0$ which determines E_0 in

terms of B and C . For example, for type 1a and 4a, $E_0 = E_{if} BC \ln(C)/2$; for types 2a and 3a, $E_0 = E_{if} BC/2$; for types 1b and 4b, $E_0 = E_{if} (BC \ln(C)/2)^{2/3}$; for types 2b and 3b, $E_0 = E_{if} (BC)^{2/3}$. Thus the Burgess-Tully parameter allows the usual distortion of the high energy x scale while the B parameter allows stretching or contraction of the threshold region. Note that the transformations maintain continuity of value and derivative of x_- and x_+ at $E = E_0$ and also of y_- and y_+ . The stretching enabled by B and C variation allows convergence on best matching and fit of threshold and asymptotic regions.

In the spirit of Burgess and Tully, it is appropriate to seek an optimised least squares spline to the data and that this should now be based on the nine fixed knot positions $[x_i = i/4 : i = -4, \dots, +4]$. The spline is specified with constant curvature at both ends. The spline evaluation routine takes as input the x value and the spline values at the nine knot positions. The least square algorithm for optimally determining the knot values follows the same pattern as that of Burgess and Tully. The special cases of under-determined splines, that is when the number of data values $N \leq 9$ were tedious to prepare but use Lagrangian inverse interpolation of the de-activated knots as before. Fig. 2.8.1a. shows the B-C plot for electron impact excitation of He I ($1s^2 \ ^1S - 1s2p \ ^1P$). The data are from the assessment by De Heer et al. (1998) and they have been analysed as type 1a. Fig.2.8.2a. shows the He I ($1s^2 \ ^1S - 1s2p \ ^3P$) electron impact excitation from the same source, analysed as type 3a.

The ADAS strict interpolative approach

We seek an approximate form $\Omega^{(approx)}$ for the collision strength which can act as a comparator for the actual data. A graph of the ratio $[\Omega(X_i)/\Omega_i^{(approx)}; i = 1, \dots, N]$ exposes errors and the interpolating spline through the data values (which do not differ substantially from unity) is an accurate interpolant. We introduce the following parametrised approximate forms with constants $F_1, F_2, F_3, B, b', X_k$:

Type 1a: dipole allowed

$$\begin{aligned}\Omega_+^{(approx)} &= F_3 S_{if} \ln(X - X_k + F_2) \\ \Omega_-^{(approx)} &= F_1 ((X - 1)/(X_k - 1))^B \\ &\quad \exp(-(B - b')((X - X_k)/(X_k - 1)))\end{aligned}\tag{2.8.9}$$

where $b' = (X_k - 1)F_3 S_{if} / F_1 F_2$ and $F_1 = \Omega_k$.

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

$$\begin{aligned}\Omega_+^{(approx)} &= F_2 + F_3/(X - X_k + 1) \\ \Omega_-^{(approx)} &= F_1 ((X - 1)/(X_k - 1))^B \\ &\quad \exp(-(B - b')((X - X_k)/(X_k - 1)))\end{aligned}\tag{2.8.10}$$

where $b' = (X_k - 1)F_3 / F_1$ and $F_1 = \Omega_k$.

Type 3a: spin change

$$\begin{aligned}\Omega_+^{(approx)} &= F_3/(X - X_k + F_2)^2 \\ \Omega_-^{(approx)} &= F_1 ((X - 1)/(X_k - 1))^B \\ &\quad \exp(-(B - b')((X - X_k)/(X_k - 1)))\end{aligned}\tag{2.8.11}$$

where $b' = -2(X_k - 1)F_3 / F_1 F_2^3$ and $F_1 = \Omega_k$.

Type 4a: other

$$\begin{aligned}\Omega_+^{(approx)} &= 1 \\ \Omega_-^{(approx)} &= 1\end{aligned}\tag{2.8.12}$$

Note the inclusion of the line strength in the definition of type 1. If high energy data is correct and consistent with the line strength then F_3 should equal $4/3$. Burgess-Tully impose this condition on their optimised fit. Type 4 is the null case of no approximate form. There is no adjustable transformation of the independent variable X but, as in the Burgess-Tully case, it is convenient to transform to $X' = 1 - 2/X$ for displaying the ratio over the finite range $[-1,1]$ with balanced weighting between the threshold and asymptotic regions. The parameters of the approximate forms are determined by fixing $\Omega_-^{(approx)}(X_0) = \Omega_0$, $\Omega_+^{(approx)}(X_N) = \Omega_N$ and $\Omega_-^{(approx)}(X_k) = \Omega_+^{(approx)}(X_k) = \Omega_k$. Note that the Ω values at X_N and X_k fix F_2 and F_3 , explicitly for types 2a and 3a and implicitly for type 1a. Then b' is determined explicitly from continuity of the derivative at X_k , that is $\Omega_-^{(approx)'}(X_k) = \Omega_+^{(approx)'}(X_k)$, so that an implicit equation is left finally for determining B . The procedure requires $N \geq 3$. For $N = 2$, we force $F_3 = 4/3$, for type 1, $F_3 = 0$ for type 2 and $F_2 = 1$ for type 3. For $N = 1$, we additionally force $B = 0.5$. Also data which do not manifest the expected asymptotic behaviours can prevent solution for the approximate form. In such cases, the forced contractions are again imposed. For historical reasons, in the ADAS graphical user interface, the normal solution for the approximate form is called '2-point fitting' and the contracted problem cases, '1-point fitting'. For $N \geq 3$, there is a choice of matching position. We seek X_k with $2 \leq k \leq N - 1$ so that

$\sum_{i=1}^N (\Omega(X_i) - \Omega^{(approx)}(X_i))^2$ is a minimum. Figure 2.8.1b and figure 2.8.2b show the

interpolation of the $\Omega/\Omega^{(approx)}$ ratio graph. The data are for the same examples as in figures 2.8.1a and 2.8.2b respectively. The cases are again analysed as types 1a and 3a.

Quadratures over Maxwellian electron distributions

The production of Maxwell averaged collision strengths is straightforward. The Burgess-Tully Gauss-Laguerre based approach remains valid for the high energy region in the optimised nine-point spline case. The finite range of the low energy region is treated similarly. The Gaussian quadrature in this case is tuned to the usual $\sqrt{X-1}$ behaviour. In the ADAS approach, it is noted that the approximate forms are integrable in terms of known functions. Thus setting $ate = (E_{if}/I_H)(I_H/kT_e)$,

$$Y^{(approx)}(T_e) = Y_-^{(approx)}(T_e) + Y_+^{(approx)}(T_e)\tag{2.8.13}$$

Type 1a

$$\begin{aligned}Y_-^{(approx)} &= F_1(X_k - 1) \cdot ate \cdot \exp(B - b') \frac{1}{|A|^{B+1}} \gamma(B + 1, A) \\ Y_+^{(approx)} &= \exp(-(X_k - 1) \cdot ate) F_3 S_{if} \cdot \\ &\quad [\ln(F_2) + \exp(ate \cdot F_2) E_1(ate \cdot F_2)]\end{aligned}\tag{2.8.14}$$

where $A = (B - b') + (X_k - 1) \cdot ate$, γ is the incomplete gamma function and E_1 is the first exponential integral. Note that in γ , the principal value of the logarithm must be taken for negative values of the argument A .

Type 2a

$$Y_-^{(approx)} = F_1(X_k - 1) \cdot ate \cdot \exp(B - b') \frac{1}{|A|^{B+1}} \gamma(B + 1, A)$$

$$Y_+^{(approx)} = \exp(-(X_k - 1) \cdot ate) \cdot [F_2 + F_3 \exp(ate) E_1(ate \cdot)] \quad 2.8.15$$

Type 3a

$$Y_-^{(approx)} = F_1(X_k - 1) \cdot ate \cdot \exp(B - b') \frac{1}{|A|^{B+1}} \gamma(B + 1, A)$$

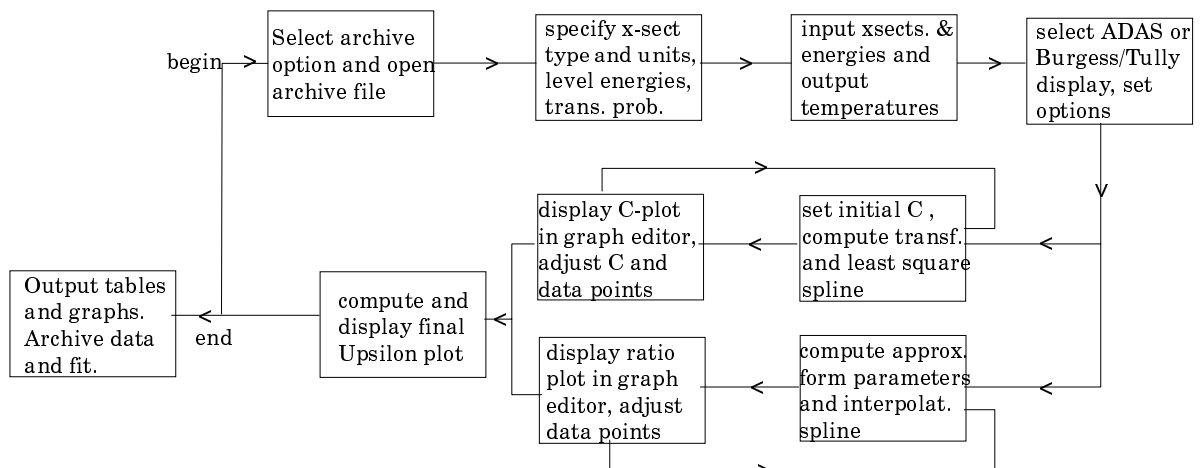
$$Y_+^{(approx)} = \exp(-(X_k - 1) \cdot ate) F_3 \cdot ate^2 \cdot \frac{1}{(ate \cdot F_2)} [1 - ate \cdot F_2 \cdot \exp(ate \cdot F_2) E_1(ate \cdot F_2)] \quad 2.8.16$$

Since the quadrature in the threshold region is tuned to $\sqrt{X - 1}$ behaviour, modest improvement of accuracy in the threshold region is achieved by numerical integration of the difference of the interpolated exact data and the approximate form and then completing with the analytic integral of the approximate form.

Program steps:

These are summarised in the figure 2.08.

Figure 2.08



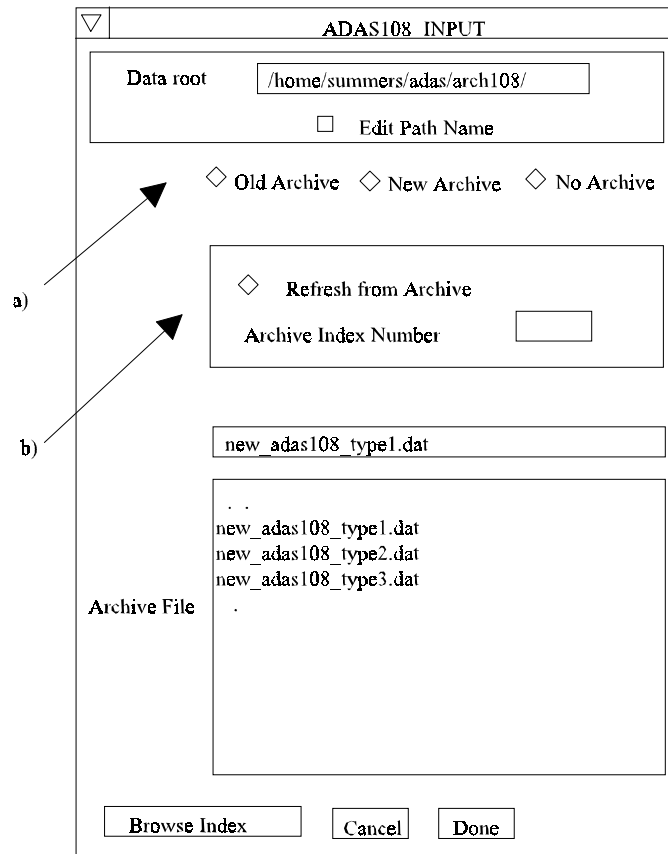
Interactive parameter comments:

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 button to activate ADAS108.

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 ADAS108 analysis is `.../uid/adas/arch108/` 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.

ADAS108 PROCESSING OPTIONS

Data file name : /home/summers/adas/arch108/new_adas108_type1.dat

Browse Index

Nuclear Charge: Ion Charge:

Transition Type: Transition Probability:

Form: S f A

Lower Level	Upper Level
Index : <input type="text"/>	Index : <input type="text"/>
Stat. Wt. : <input type="text"/>	Stat. Wt. : <input type="text"/>
Level Energy : <input type="text"/>	Level Energy : <input type="text"/>

Select Energy Form : cm-1 Rydbergs

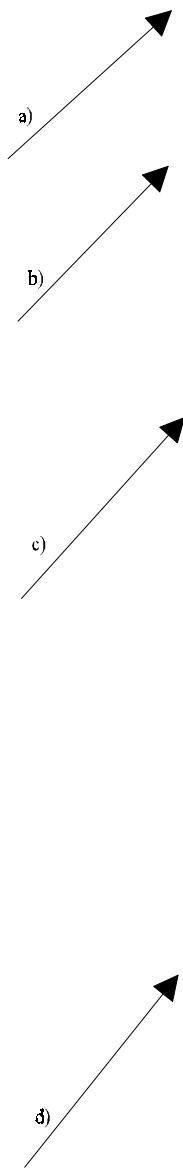
INDEX	Input Energy	Input X-sect	Output Temp.
1	1.000E+00	1.000E+00	1.000E+05
2	2.000E+00	2.000E+00	2.000E+05
3	5.000E+00	5.000E+00	3.000E+05
4	1.000E+01	1.000E+01	4.000E+05
5	2.000E+01	2.000E+01	7.000E+05
6	5.000E+01	5.000E+01	8.000E+05
7	1.000E+02	1.000E+02	1.000E+06
8	2.000E+02	2.000E+02	2.000E+06

Energy units : X. X-section units : Omega. Temperature units : Kelvin.

Edit Table

Default Temperature values

Edit the processing options data and press Done to proceed



7. Four types of collision cross-section 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 cross-sections, energies 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, energy, cross-section 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 Ω . If data is returned from archive it will be in these forms. Click the *Done* button if editing is completed satisfactorily.
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/Summers analysis option*. 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/Summers case.
14. Two graphs are presented. The first is a scaled comparative graph for assessing the cross-section 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 diamonds with a spline drawn through these tabular points in the ADAS analysis option case. In the Burgess/Summers analysis option case, the spline is drawn through the special nine knot points which are distinguished as crosses. The points can be modified by using the buttons b) beneath the graph in association with the mouse. In the Burgess/Summers analysis option case, the knot points may only be moved vertically and a special button is present for this case. Also in the Burgess/Summers case, the parameters 'B' and 'C' can be varied to seek an optimum fit. This is done with the sliders at a). Note that the RMS error of the least square fit is displayed and continuously updated at the top of the graph.
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. The coordinates of the moved point are displayed and continuously updated at the foot of the graph. 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.

ADAS108 OUTPUT OPTIONS

Data file name : /home/summers/adas/arch108/new_adas108_type1.dat

ADAS Analysis Option
 Burgess/Summers Analysis Option

Optimisation Level : 1 2 Optimisation Option : On Off

Bad Point Option : On Off Dipole X-sect. Fitting : Ratio Difference

Graphical Output

Graph Title Default Device

1st. Default Graph Scaling 2nd. Default Graph Scaling

X-min : X-max : X-min : X-max :

Y-min : Y-max : Y-min : Y-max :

Enable Hard Copy Replace

File name :

Text Output Replace

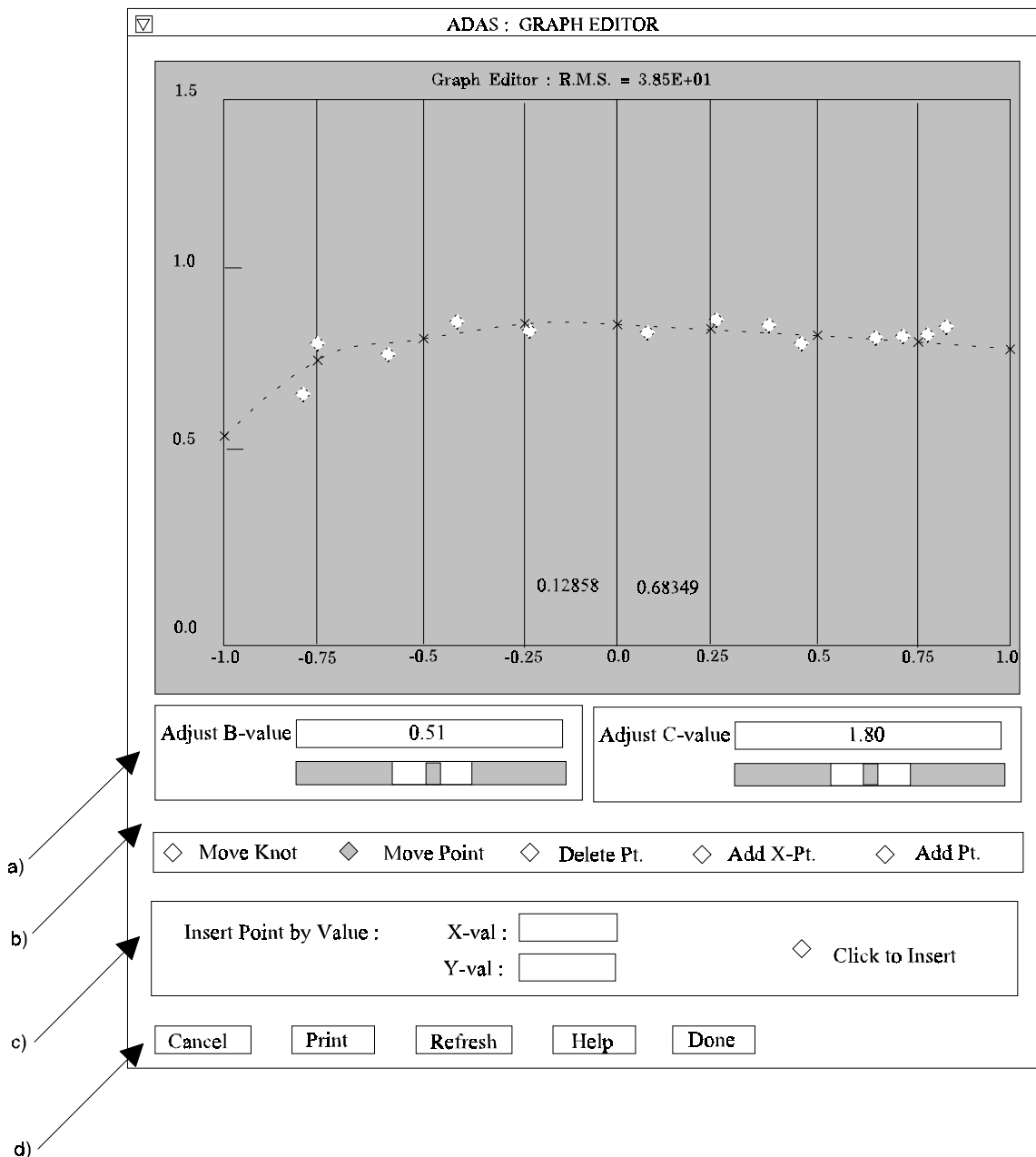
File name :

B-value C-value

Insert non-dipole point at infinity : Ω -value :

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.



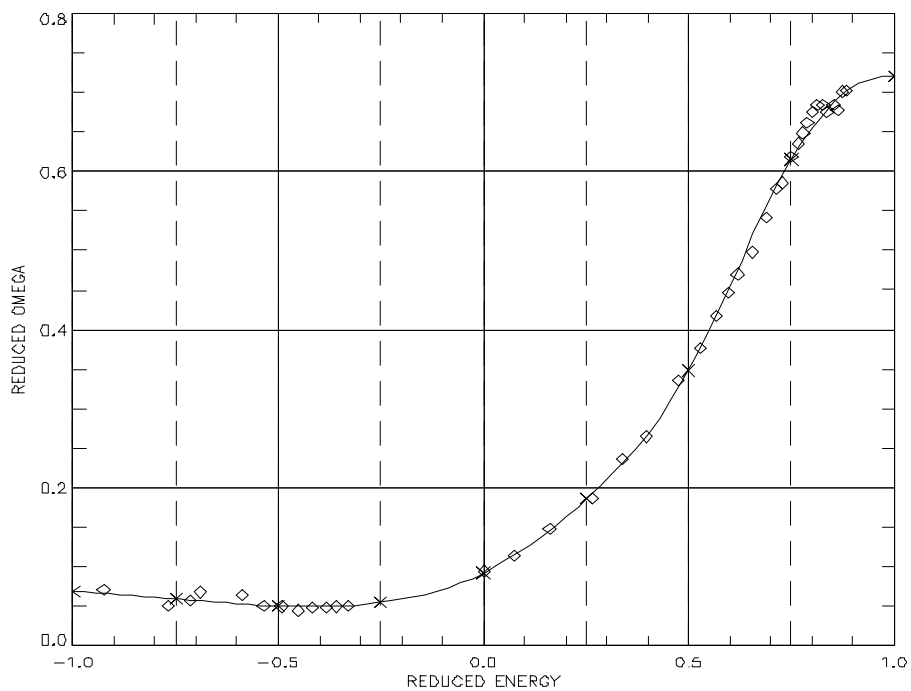
19. The Upsilon graph is displayed after graph editing. There is no option to modify this output graph. The graph may be printed, using the *Print* button. If the results of the analysis are acceptable and to be archived, click the *Archive* button.

Illustration:

Figure 2.8.1

- (a) Type 1a: B-C nine-knot spline least square fit to dipole allowed neutral atom collision strength, (b) Type 1a: ADAS ratio plot and interpolation spline for the same dipole-allowed neutral atom collision strength. Parameters are given in the ADAS specification above the plot. Note the variability of the tabular data which gives some grounds for adjustment of some values. The stated uncertainty of the data is ~10%.

OPTIMISED FIT TO OMEGA DATA POINTS : DE HEER (1998) HEI[1(1)S-2(1)P]
 ADAS : ADAS RELEASE: ADAS98 V2.2 PROGRAM: ADAS08 V1.1 DATE: 28/06/99 TIME: 07:54
 FILE : /home/summers/adas/arch108/new_test_adas_type1.dat R.M.S. = 2.7360E+01
 KEY : (DIAMONDS - INPUT DATA) (FULL LINE - BURGESS SPLINE FIT)(CROSSES - BURGESS KNOT POINTS)
 FIT : type = 1 b-val = 0.704 c-val = 1.870



COLLISION STRENGTH RATIO GRAPH : DE HEER (1998) HEI[1(1)S-2(1)P]
 ADAS : ADAS RELEASE: ADAS98 V2.2 PROGRAM: ADAS108 V1.1 DATE: 28/06/99 TIME: 07:52
 FILE : /home/summers/adas/arch108/new_test_adas_type1.dat
 KEY : (DIAMONDS - INPUT DATA) (FULL LINE - IDL SPLINE FIT)
 FIT : type = 1 b0 = 0.53828 bp0 = 1.70840 f1 = 0.34300 f2 = 1.62850 f3 = 0.00000 xk = 2.35670

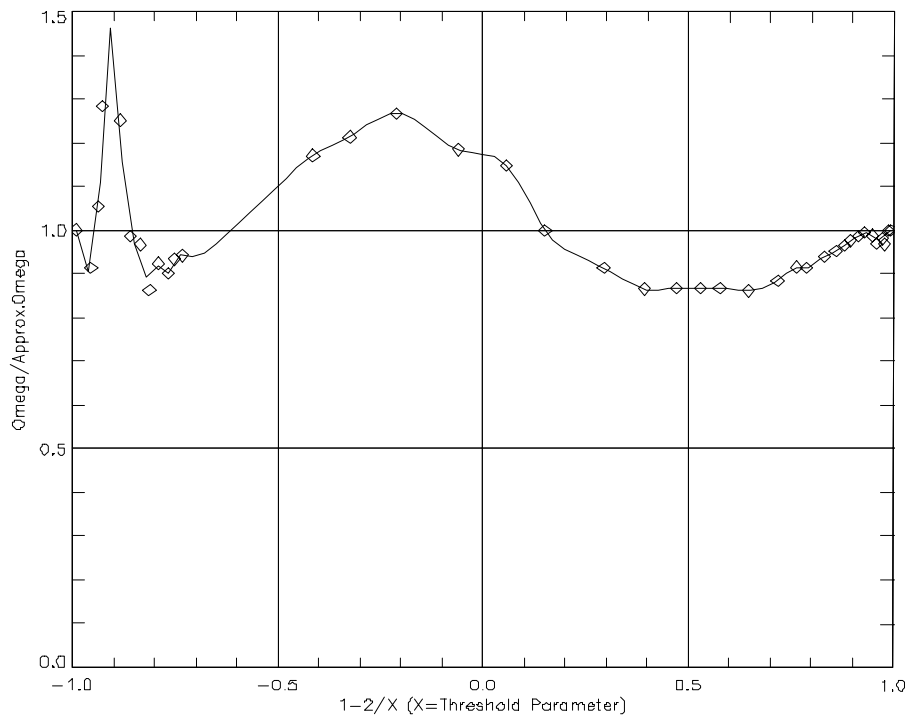
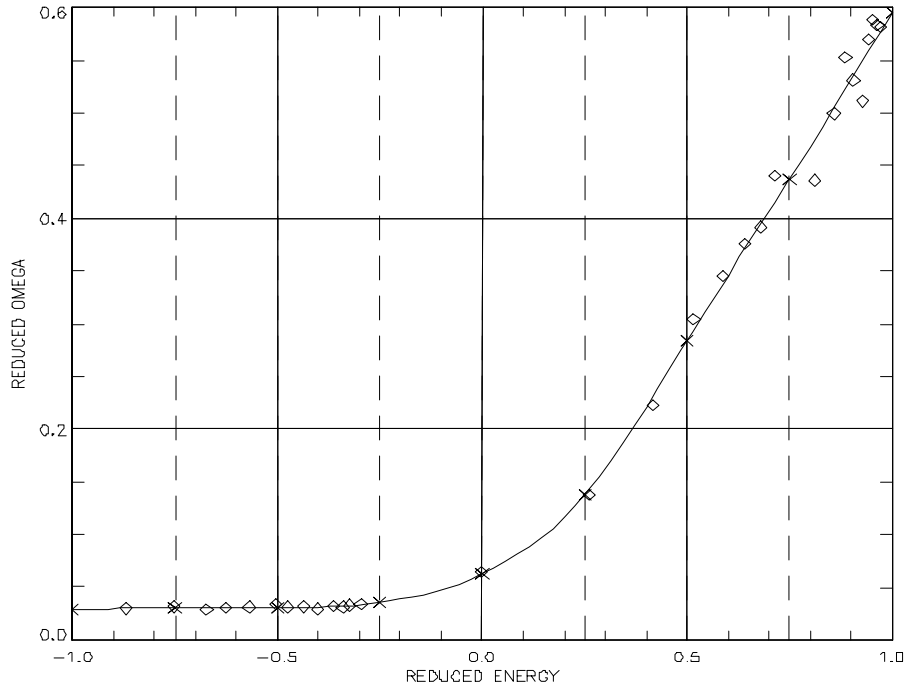


Figure 2.8.2

(a) Type 3a: B-C nine-knot spline least square fit to spin change neutral atom collision strength, (b) Type 3a: ADAS ratio plot and interpolation spline for the same spin change neutral atom collision strength. Parameters are given in the ADAS specification above the plot. Note again the variability of the tabular data which gives some grounds for adjustment of some values.

OPTIMISED FIT TO OMEGA DATA POINTS : DE HEER (1998) HEI[1(1)S-2(3)P]
 ADAS : ADAS RELEASE: ADAS98 V2.2 PROGRAM: ADAS108 V1.1 DATE: 28/06/99 TIME: 08:02
 FILE : /home/summers/adas/arch108/new_test_adas_type3.dat R.M.S. = 4.1670E+00
 KEY : (DIAMONDS - INPUT DATA) (FULL LINE - BURGESS SPLINE FIT)(CROSSES - BURGESS KNOT POINTS)
 FIT : type = 3 b-val = 0.64B c-val = 1.339



COLLISION STRENGTH RATIO GRAPH : DE HEER (1998) HEI[1(1)S-2(3)P]
 ADAS : ADAS RELEASE: ADAS98 V2.2 PROGRAM: ADAS108 V1.1 DATE: 28/06/99 TIME: 08:00
 FILE : /home/summers/adas/arch108/new_test_adas_type3.dat
 KEY : (DIAMONDS - INPUT DATA) (FULL LINE - IDL SPLINE FIT)
 FIT : type = 3 b0 = 0.56483 b1C = -1.21690 f1 = 0.04090 f2 = 3.84420 f3 = 0.60442 xk = 3.33900

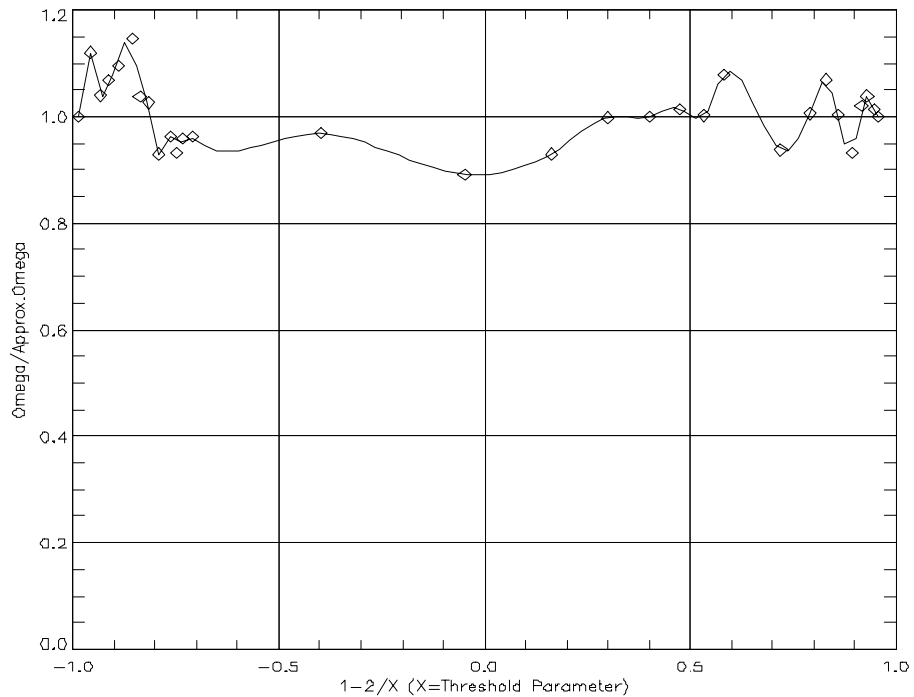
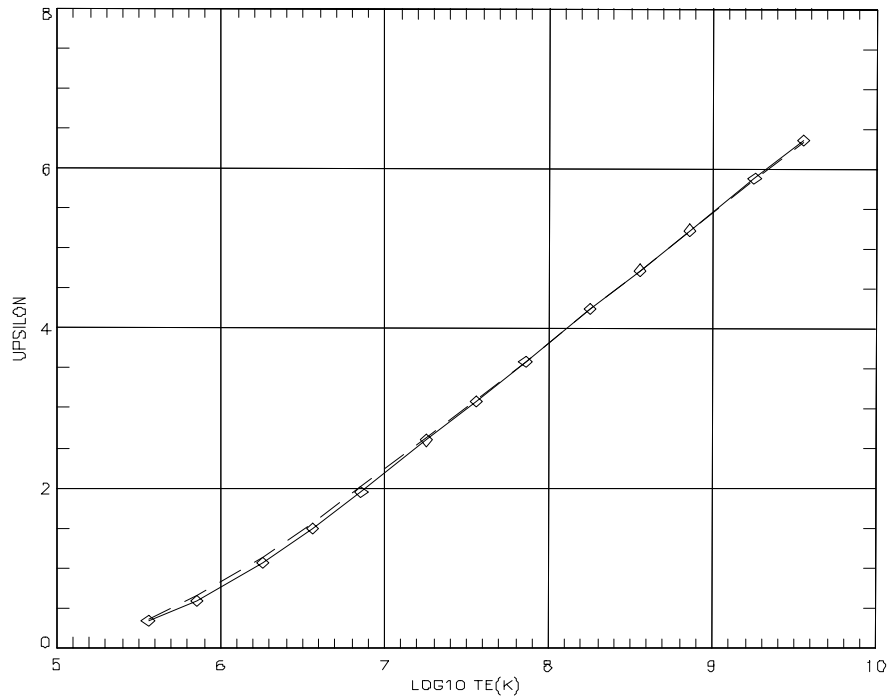


Figure 2.8.3.

The figures show the final Upsilon's for the dipole and spin change cases produced by the ADAS interpolative analysis. The solid straight lines connect the tabular output values. The dashed line is the optimised approximate form. In the present cases, it provides a remarkably accurate representation of the Maxwell integral over the exact data.

UPSILON GRAPH : DE HEER (1998) HE[[1(1)S-2(1)P]]
 ADAS : ADAS RELEASE: ADAS98 V2.2 PROGRAM: ADAS108 V1.1 DATE: 28/06/99 TIME: 07:54
 FILE : /home/summers/adas/arch108/new_test_adas_type1.dat
 KEY : (DIAMONDS + FULL LINE - OUTPUT DATA) (DASHED LINE - APPROXIMATE FORM)



UPSILON GRAPH : DE HEER (1998) HE[[1(1)S-2(3)P]]
 ADAS : ADAS RELEASE: ADAS98 V2.2 PROGRAM: ADAS108 V1.1 DATE: 28/06/99 TIME: 08:01
 FILE : /home/summers/adas/arch108/new_test_adas_type3.dat
 KEY : (DIAMONDS + FULL LINE - OUTPUT DATA) (DASHED LINE - APPROXIMATE FORM)

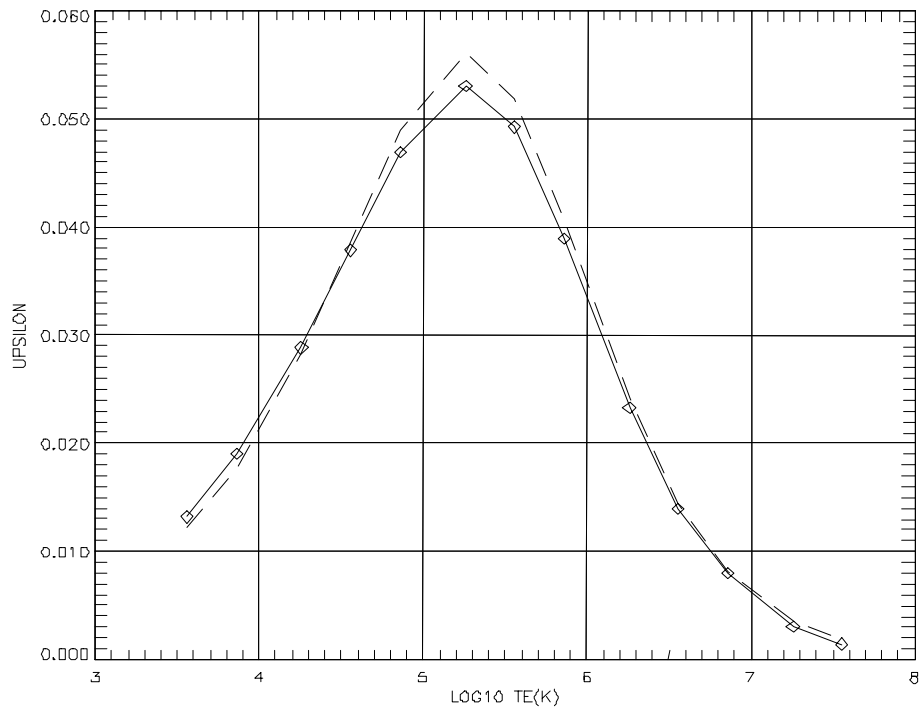


Table 2.8

The table shows the standard printed output for the example of ADAS interpolative analysis of the dipole example of figure 2.8.1a. The archive is of the same structure. The Burgess/Summers nine-point spline archive record is in the economised form used by Burgess-Tully.

```

ADAS RELEASE: ADAS98 V2.2 PROGRAM: ADAS108 V1.1 DATE: 28/06/99 TIME: 07:54
I 0 HE+ 0 1S2(1S)-1S2P(1P) KVI(1998)28/06/99 A
NUCLEAR CHARGE = 2.00 ION CHARGE = 0.00 EFFECTIVE ION CHARGE = 1.00
LOWER INDEX = 1 UPPER INDEX = 4
LOWER ENERGY = 0.000000 UPPER ENERGY = 1.559639
LOWER WEIGHT = 1.0 UPPER WEIGHT = 3.0
ACOEFF = 1.8000E+09 S = 5.3162E-01 FABS = 2.7638E-01 ENERGY DIFFERENCE = 1.559639
XSECT TYPE= 1 XSECT OPT. FACTORS, FXC2 = 1.6285E+00 FXC3 = 1.3231E+00 IXOPS = 1 IBPTS = 0 IFPTS = 2 IDIFF = 0
BO = 5.3828E-01 BPO = 1.7084E+00 FXC1 = 3.4300E-01 XK = 2.3567E+00

X OMEGA APPROX. OMEGA DIFFERENCE
1.0040E+00 4.6400E-03 4.6400E-03 0.0000E+00
1.0228E+00 1.1000E-02 1.2035E-02 -1.0347E-03
1.0322E+00 1.5400E-02 1.4610E-02 7.8985E-04
1.0370E+00 2.0300E-02 1.5810E-02 4.4899E-03
1.0605E+00 2.6300E-02 2.1023E-02 5.2772E-03
1.0747E+00 2.3500E-02 2.3840E-02 -3.3950E-04
1.0888E+00 2.5600E-02 2.6485E-02 -8.8498E-04
1.1029E+00 2.5000E-02 2.9022E-02 -4.0223E-03
1.1171E+00 2.9100E-02 3.1497E-02 -2.3972E-03
1.1312E+00 3.0500E-02 3.3895E-02 -3.3947E-03
1.1407E+00 3.3100E-02 3.5484E-02 -2.3840E-03
1.1548E+00 3.5600E-02 3.7813E-02 -2.2129E-03
1.4140E+00 9.4000E-02 8.0297E-02 1.3703E-02
1.5083E+00 1.1800E-01 9.7274E-02 2.0726E-02
1.6497E+00 1.5900E-01 1.2541E-01 3.3588E-02
1.8854E+00 2.1500E-01 1.8155E-01 3.3454E-02
2.1211E+00 2.9000E-01 2.5261E-01 3.7389E-02
2.3567E+00 3.4300E-01 3.4300E-01 0.0000E+00
2.8281E+00 4.7700E-01 5.2182E-01 -4.4824E-02
3.2994E+00 5.7500E-01 6.6425E-01 -8.9248E-02
3.7708E+00 6.7800E-01 7.8266E-01 -1.0466E-01
4.2421E+00 7.6600E-01 8.8395E-01 -1.1795E-01
4.7135E+00 8.4400E-01 9.7250E-01 -1.2850E-01
5.6561E+00 9.6600E-01 1.1218E+00 -1.5583E-01
7.0702E+00 1.1500E+00 1.2993E+00 -1.4928E-01
8.4842E+00 1.3200E+00 1.4409E+00 -1.2085E-01
9.4269E+00 1.3900E+00 1.5215E+00 -1.3154E-01
1.1784E+01 1.5900E+00 1.6902E+00 -1.0019E-01
1.4140E+01 1.7400E+00 1.8261E+00 -8.6073E-02
1.6497E+01 1.8700E+00 1.9399E+00 -6.9950E-02
1.8854E+01 1.9900E+00 2.0379E+00 -4.7933E-02
2.3567E+01 2.1700E+00 2.2005E+00 -3.0502E-02
2.8281E+01 2.3200E+00 2.3325E+00 -1.2487E-02
3.7708E+01 2.5100E+00 2.5395E+00 -2.9470E-02
4.7135E+01 2.6200E+00 2.6992E+00 -7.9190E-02
7.0702E+01 2.9300E+00 2.9881E+00 -5.8052E-02
9.4269E+01 3.0900E+00 3.1922E+00 -1.0223E-01
1.4140E+02 3.4800E+00 3.4792E+00 7.7053E-04
2.3567E+02 3.8400E+00 3.8400E+00 3.2419E-14
TE (K) GAMMA APPROX. GAM EX. RATE DEXC. RATE GBARF
3.6100E+05 3.4286E-01 3.6509E-01 2.4897E-09 1.6416E-09 3.6852E-02
7.2200E+05 5.9152E-01 6.5001E-01 4.2719E-09 2.0027E-09 6.3579E-02
1.8050E+06 1.0596E+00 1.1394E+00 5.9384E-09 2.2688E-09 1.1389E-01
3.6100E+06 1.4908E+00 1.5639E+00 6.3252E-09 2.2572E-09 1.6024E-01
7.2200E+06 1.9522E+00 2.0153E+00 6.0602E-09 2.0902E-09 2.0983E-01
1.8050E+07 2.5991E+00 2.6351E+00 5.2083E-09 1.7599E-09 2.7936E-01
3.6100E+07 3.0903E+00 3.1134E+00 4.4087E-09 1.4796E-09 3.3215E-01
7.2200E+07 3.5870E+00 3.5958E+00 3.6309E-09 1.2144E-09 3.8554E-01
1.8050E+08 4.2434E+00 4.2369E+00 2.7222E-09 9.0863E-10 4.5609E-01
3.6100E+08 4.7297E+00 4.7233E+00 2.1469E-09 7.1613E-10 5.0837E-01
7.2200E+08 5.2308E+00 5.2101E+00 1.6795E-09 5.6004E-10 5.6223E-01
1.8050E+09 5.8755E+00 5.8542E+00 1.1934E-09 3.9785E-10 6.3152E-01
3.6100E+09 6.3632E+00 6.3416E+00 9.1397E-10 3.0468E-10 6.8395E-01

```

Notes:

Neutral atoms and molecules are usually present in low temperature plasmas with significant deviations of the electron distribution function from Maxwellian. It is planned to incorporate non-Maxwellians more closely with this code in the future.