

ADAS103: Dielectronic recombination - graphing and interpolation

The program is for entry of total zero density dielectronic recombination coefficient data, examination, comparison with approximate forms, optimising of approximate form fits, display and interpolation to arbitrary electron temperatures.

Background theory:

Consider the reactions



where

$$\begin{aligned} E_{p_\rho} + \epsilon &= E_{p_i, nl} = E_{p_\rho, nl} + h\nu_s \\ E_{p_\rho, nl} &\approx E_{p_\rho} - I_{nl} \end{aligned} \quad 2.3.2$$

The initial state of the recombining ion X^{+z+1} is denoted by p_ρ and is called the *parent* state. $I_{nl} = (z+1)^2 I_H / (n - \mu_{nl})^2$ is the ionisation energy of the nl electron with μ_{nl} its *quantum defect*. Parent states whose populations are of sufficient abundance in a plasma to be relevant starting points for recombination events are only the ground state of the $z+1$ ion and the lowest metastable states (the latter need to be included in a complete picture). Metastable and ground parents are labelled by the index ρ . Dielectronic recombination proceeds via a *resonant capture* process whereby the parent (or core) state is excited (usually to a non-metastable, that is an *excited* state) and the initially free electron enters a bound orbital labelled by nl quantum numbers forming a *doubly excited state*. The excited parent state is labelled by i . Such states readily breakup again via the inverse process, called the *Auger* (or *autoionisation*) process, releasing the electron again. There is, however, a possibility of a radiative transition before this whereby a photon is emitted of sufficient energy to leave the residual z -times ionised ion stable against autoionisation. The combined capture/stabilisation process is dielectronic recombination. The energy of the emitted photon $h\nu_s$ is generally close to the parent (core) transition energy $\Delta E_{p_\rho, p_i} = E_{p_i} - E_{p_\rho}$ and the associated spectrum line is called a *satellite line*.

The dielectronic recombination rate coefficient from initial state $X_{p_\rho}^{+z+1}$ to state $X_{p_\rho, nl}^{+z}$, via doubly excited state $X_{p_i, nl}^{+z}$, may be denoted by $\alpha(p_\rho; p_i; p_\rho, nl)$ where it is assumed that the distribution of free electron energies is Maxwellian. The zero density total dielectronic recombination coefficient via the parent transition $p_\rho \rightarrow p_i$ and the total zero density dielectronic recombination coefficient via any parent transition are given by

$$\alpha(p_\rho; p_\rho) = \sum_i \alpha(p_\rho; p_i; p_\rho) = \sum_{i, nl \geq n_0 l_0} \alpha(p_\rho; p_i; p_\rho, nl) \quad 2.3.3$$

The sum over nl begins with the lowest accessible levels energetically, namely, $n_0 l_0$ and extends to infinity. The approximate value of n_0 is given by the solution of equation 2.3.2 with $\epsilon=0$. Very many highly excited states contribute to the sums in general. More highly excited states contribute when the parent transition energy $\Delta E_{p_\rho, p_i}$ is small (typical for $\Delta n=0$ transitions, where Δn denotes the change in principal quantum number of the active core electron) and fewer for larger parent transition energies (that is for ' $\Delta n \geq 1$ ' transitions). The summed coefficient for a particular parent transition $p_\rho \rightarrow p_i$ can be represented approximately as a product of an exponential factor $\exp(\bar{\epsilon}/kT_e)$ (where $\bar{\epsilon}$ is close to $\Delta E_{p_\rho, p_i}$ and sometimes written as $\bar{\epsilon} = \Delta E_{p_\rho, p_i} / a$ with $a \approx 1$) and a temperature independent factor.

The coefficient $\alpha(p_\rho; p_i; p_\rho, nl)$ may be evaluated from the Auger transition probability $A_{p_i, nl \rightarrow p_\rho}^a$ and the radiative transition probability $A_{p_i, nl \rightarrow p_\rho, nl}^r$ as

$$\alpha(p_\rho; p_i; p_\rho, nl) = 8(\pi\alpha_0^2)^{3/2} (I_H/kT_e) (\omega_{p_i, nl} / \omega_{p_\rho}) \exp(-\varepsilon/kT_e) A_{p_i, nl \rightarrow p_\rho, nl}^r b_{p_\rho; p_i, nl} \quad 2.3.4$$

where

$$b_{p_\rho; p_i, nl} = \frac{A_{p_i, nl \rightarrow p_\rho}^a}{A_{p_i, nl \rightarrow p_\rho}^a + A_{p_i, nl \rightarrow p_\rho, nl}^r} \quad 2.3.5$$

and ω_{p_ρ} and $\omega_{p_i, nl}$ are the statistical weights of the states $X^{+z+1}(p_\rho)$ and $X^{+z}(p_i, nl)$ respectively. $b_{p_\rho; p_i, nl}$ is sometimes called the *b-factor* of the doubly excited state.

There are three complications. Firstly, the equation 2.3.5 is an over simplification in that the denominator should be a sum over all Auger and radiative pathways. A particularly important case is when an Auger transition to a different, higher energy parent, can occur. That is

$$X^{+z}(p_i, nl) \rightarrow X^{+z+1}(p_j) + e \quad 2.3.6$$

Such an *alternative Auger channel* can strongly reduce the b-factor above some critical n_c where the Auger channel is open. Note also that outer electron radiative stabilisations can contribute.

Secondly, the expression for the b-factor in equation 2.3.5 assumes that no other processes than the Auger breakup and radiative stabilisation disturb the double excited state. However, plasma microfields, Lorentz motional electric fields and further collisions can cause such disturbance. This is called *doubly excited state redistribution* and in general it serves to increase the 'effective' total dielectronic recombination coefficient. Such effects can also disturb the stabilised, *singly excited* states $X^{+z}(p_\rho, nl)$, the main effect being to decrease the 'effective' total dielectronic recombination coefficient, primarily by reionising the state. Note that a recombination event is only effective if the captured electron cascades (by multiple radiative steps) to the ground state. Only at zero density are all captures 'effective' and the simple sum 2.3.3 gives a meaningful unique total coefficient. Normally dielectronic data are given as the zero density totals, but a strategy is necessary to allow for the finite density effects in realistic application to plasmas.

Thirdly, the most satisfactory picture requires consideration of metastable parent states. In this 'generalised picture', recombination can begin with one metastable parent and end up with a state built on a different parent, that is with a coefficient such as $\alpha(p_\rho; p_i; p_\sigma, nl)$. If stabilisation to a final state built on a metastable parent with energy above the lowest parent energy occurs, a secondary autoionisation to a lower energy parent is energetically allowed above some some critical n_s . The effect is that sums in expressions 2.3.3 should be terminated at n_s when describing non-ground metastable parent to metastable parent built final state recombination coefficients.

Approximate forms:

The 'General Formula' for zero density dielectronic recombination developed by Burgess has been very influential in plasma physics applications. It applies to an individual parent transition, is easily evaluated, and may be written symbolically as $\alpha^{GF}(p_\rho; p_i; p_\rho)$ where the final state parent must be the same as the initial state. The formula can be improved in specific cases by adjusting the $\exp(-\Delta E_{p_\rho, p_i} / akT_e)$ and using a simple multiplier on the temperature independent factor. Let the set of relevant parent transitions be divided into two groups (corresponding in principle to $\Delta n = 0$ and $\Delta n \geq 1$ classes), then an approximate form for comparison with zero density total dielectronic data and for adjustment to fit the data as well as possible is

$$\alpha^{approx}(p_p; p_p) = scale_1 \exp(-edisp_1/akT_e) \sum_{i_1 \in grp_1} \alpha^{GF}(p_p; p_{i_1}; p_p) + scale_2 \exp(-edisp_2/akT_e) \sum_{i_2 \in grp_2} \alpha^{GF}(p_p; p_{i_2}; p_p) \quad 2.3.7$$

In optimising, adjustment is made for each group as a whole. There are at most two groups allowed. $scale_1$ and $scale_2$ are the adjustable parameters, $edisp_1$ and $edisp_2$ being preset by the user on input. Also, for each parent transition, the transition energy and oscillator strength are required.

However the General Formula only represents the zero density total rate coefficient and does not indicate how the total should be split up into n or nl -shell components. Such information is necessary for finite density studies in real plasmas. To achieve this, use is made of a second approximate form in parallel with the one based on the General Formula. The second approximate form is an algorithm based on the 'General Program' for nl -resolved dielectronic coefficients prepared by Burgess. The numerical results from this program were used in developing the General Formula. A zero density total coefficient for a particular parent transition is obtained from the General Program by summing over the nl component coefficients. The General Program can be used as an approximate form. There is one adjustable parameter $corfac$ but its precise action depends on details of the n and l quantum numbers of the active core electron in the initial and excited parent. This adjustable parameter is in addition to the parent transition energy and transition probability. The program also allows for termination of the sum through alternative Auger channels of secondary autoionisation by the parameter $ncut$ ($\equiv n_s$ or n_c).

The general program computes Auger rate coefficients by a Correspondence Principle argument with partial wave excitation collision strengths. Bethe approximation partial waves are extrapolated below threshold in the program. However, the lowest partial waves in general give a severe overestimate. This situation is put right by introducing correction factors for the lowest partial waves. These are deduced from high quality collision strength data and they depend on the particular type of transition. The implementation of the general program used as an approximate form here sets correction factors according to the active core electron transition as given in table 2.3.

Table 2.3

Type	parent electronic transition	$cor'_l : l=0,1,\dots, l_{max}$	DF
1	$n_p=1, n_i=2, l_i=l_p+1$	0.05, 0.30, 0.50, 0.90, 1.0	2.0
2	$n_p=2, n_i=3, l_i=l_p+1$	0.01, 0.02, 0.20, 0.40, 0.70, 0.90, 1.00	1.0
3	$n_p=2, n_i=3, l_i=l_p-1$	0.01, 0.01, 0.01, 0.08, 0.30, 0.70, 1.00	1.0
4	$n_p=n_i, l_i=l_p+1$	0.30, 0.35, 0.40, 0.45, 0.70, 0.90, 1.00	0.5
5	$n_p=n_i, l_i=l_p-1$	0.30, 0.35, 0.40, 0.45, 0.70, 0.90, 1.00	0.5
6	$n_p > n_i, l_i=l_p+1$ excl. types 1,2,3	0.01, 0.02, 0.20, 0.40, 0.70, 0.90, 1.00	1.0
7	$n_p > n_i, l_i=l_p-1$ excl. types 1,2,3	0.01, 0.01, 0.01, 0.08, 0.30, 0.70, 1.00	1.0

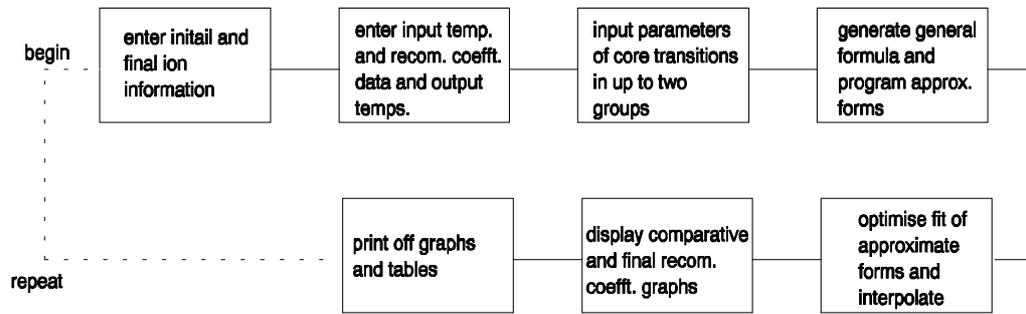
The adjustable parameter $corfac$ alters the correction factors cor'_l to

$$cor'_l = \exp(-corfac/(l^{DF} + 0.5)) cor'_l \quad 2.3.8$$

Program steps:

These are summarised in the figure 2.3.

Figure 2.3



Interactive parameter comments:

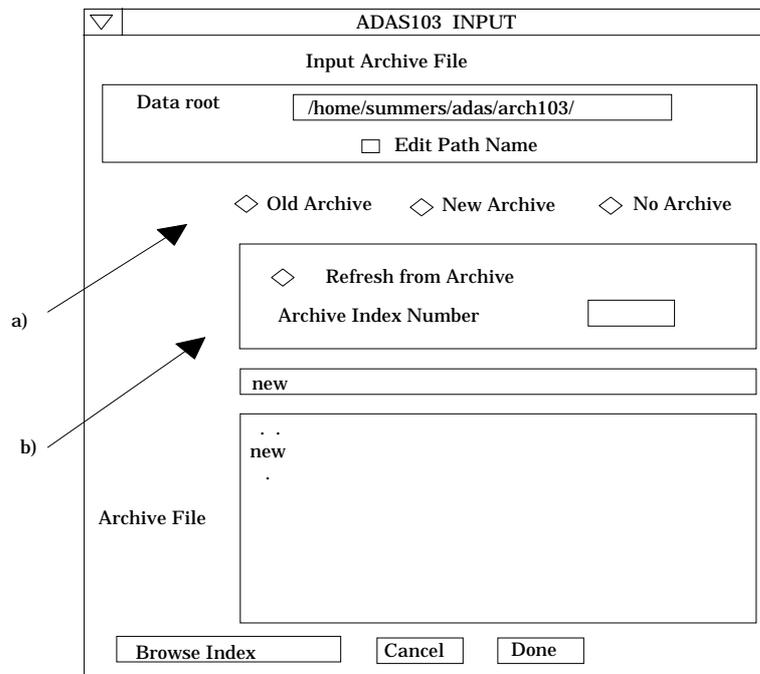
Remember to ensure you have a defaults directory allocated. This should have the pathway */.../uid/adas/defaults* where *uid* is your user identifier. The defaults directory records the parameters you set the last time you ran each ADAS code.

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 third button to activate ADAS103.

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 ADAS103 analysis is */.../uid/adas/arch103/* 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* remains available at the top of the window to display the archive index list.
7. ADAS103 follows the usual pattern of ADAS series 1 codes in that it seeks to match an approximate form to the input data as an aid to interpolation. Also the optimised approximate form is useable in its own right. ADAS103 is complex in that two approximate forms are used, namely the *Burgess General Formula* and the *Burgess General Program*. Parameters are required to prepare both forms. Details are in the ADAS User Manual.
8. At a), the primary data on the nuclear and initial and final ion charges are entered. The parameters to the right at b) are concerned with the Burgess General Program and obtaining a reasonable approximation to the dielectronic capture to the lowest accessible level. The *Effective principal quantum number* entry allows its energy to be precise and therefore ensures correct low temperature behaviour. The *Phase space occupation factor* makes allowance for equivalent electrons in the lowest accessible level.
9. The entries at c) pertain to the recombining (parent) ion transitions or 'core transitions'. The parent transitions are treated in up to two groups which can be separately scaled. Usually the so called ' $\Delta n=0$ ' and ' $\Delta n>0$ ' division is made. Click on the *Group* button to show the transitions in the selected group in the table window below. There are two adjustable parameters for each group, namely a *mean energy displacement* (designed to improve temperature behaviour of the fit) and *Mean scale factor* to improve the absolute fit. Click on *Edit Table* to bring up the ADAS Table Editor widget in the usual manner.
10. Each parent core transition is represented by the initial and final orbital quantum numbers of the active electron together with initial and final statistical weights of the parent states. Then the core transition energy (Rydberg energy units) and oscillator strength are given. The last two entries are associated with optimising the Burgess General Program fit with a 'Bethe approx. adjustment factor' *Corfac* and a 'secondary autoionisation cut-off', *Ncut*. Set these to 0.0 and 1000 if unfamiliar with the program. More detail is in the ADAS User Manual.

ADAS103 PROCESSING OPTIONS

Data file name : /home/summers/adas/arch103/new.dat

Browse Index

Nuclear charge z0 Lowest accessible level params. for diel. recomb. :

Initial ion charge z1 Principal quantum number

Final ion charge z Effective principal quantum number

Phase space occupation factor

No. of core transition groups : Group

Initial mean energy disp. Mean scale factor

INDEX	NI	LI	WI	NJ	LJ	WJ	EIJ(RYD)	TR. PROB.	CORFAC	NCUT
1	1	0	2.0	2	1	6.0	3.655E+02	0.41600	0.0000	1000
2										

Edit Table

INDEX	Input Temp.	Input Coefft.	Output Temp.
1	1.000E+05	5.530E-15	1.000E+05
2	2.000E+05	3.710E-15	2.000E+05
3	5.000E+05	1.400E-14	3.000E+05
4	1.000E+06	2.500E-14	4.000E+05
5	2.000E+06	7.230E-14	7.000E+05
6	5.000E+06	1.240E-13	8.000E+05
7	1.000E+07	1.200E-13	1.000E+06
8	2.000E+07	1.010E-13	2.000E+06

Input Temp. units : K. Input Rate Form :Diel (zero e-dens. rate). Output Temp. units : K.

Edit Table

Default Temperature values

Edit the processing options data and press Done to proceed

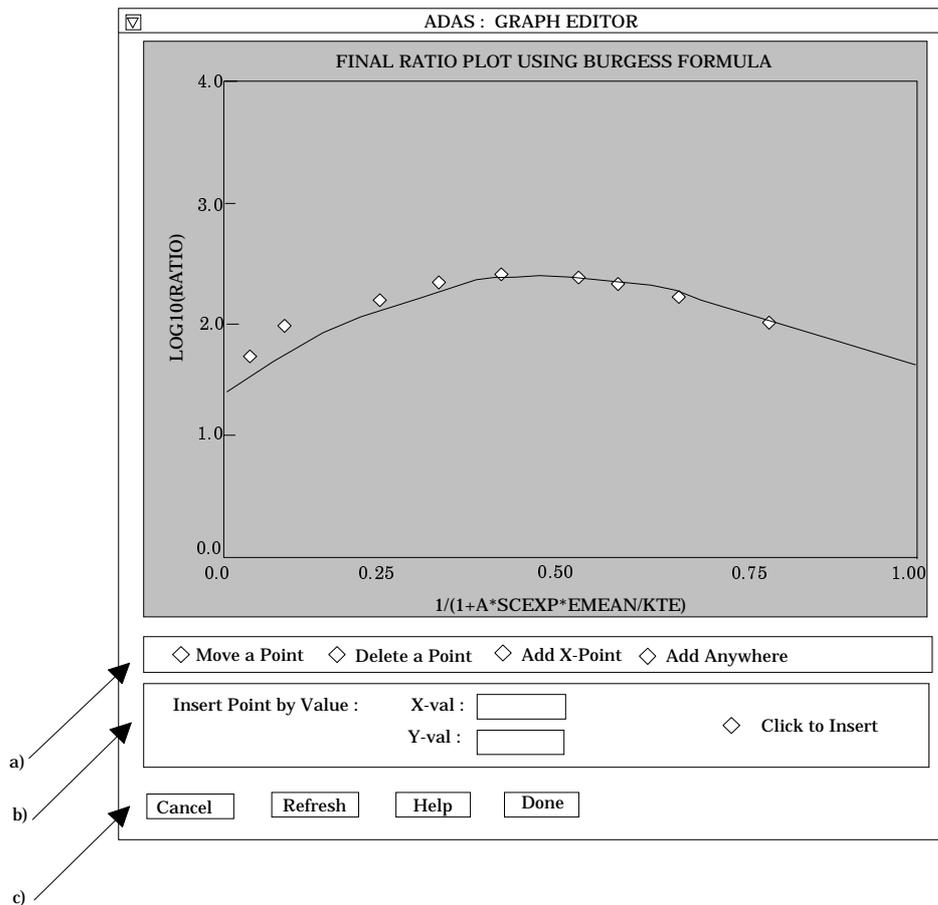
11. User input temperatures, rate coefficients and required output temperatures are entered at d) with the currently selected units shown below at e). Click the *Edit table* button to 'drop down' the ADAS Table Editor for data input.
12. If an archive data set is opened, temperature, rate coefficients and output temperature values are filled from this. Otherwise the fields are empty. Pressing the *Default Temperature values* button inserts a default set of output temperatures.
13. 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.
14. 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 shown below.

15. Since ADAS103 manipulates both the Burgess General Formula and Burgess General Program there is a number choices on optimising strategy and graph display. The primary options are at a) and are mostly presented as choices on 'drop-down' menus. Select FIT TO FORMULA to match the general program to the general formula otherwise FIT TO INPUT DATA. Select independently *Optimise Burgess formula fit* and *Optimise general program fit*.

16. An editable ratio graph will be presented first. At a), select *Graph to edit*. The choice here implies whether you plan to assess source data and possibly make adjustments with respect to the Burgess formula or Burgess program.

17. The *Switch to bad point distribution* is usually made retrospectively if the displayed interpolating spline on the editable graph shows severe 'overshoot'. The switch is to a 'safe' linear interpolation.
18. Two graphs are presented. The first is a comparative ratio graph for assessing the rate coefficient data and making adjustments if appropriate. The second graph displays the recombination rate coefficients at the user's temperatures.
19. At b) select *Graphical Output* and insert a *Graph Title*. The latter appears as the index entry if you save the results of your analysis to archive. A graphic scaling parameter should be entered. This allows some movement in the x-direction on the comparative display along the lines of the Burgess 'C parameter'. Zero is a good initial choice.
20. Make the required choices of graph scaling and axes choices at c) for the ratio graph and at d) for the recombination coefficient graph.
21. After making your choices on hard copy and text output click *Done* to show the ratio graph.
22. The ratio graph is displayed in the Graph Editor window as shown below. The graph displays the ratio of input rate coefficient to approximate form as circles with a spline drawn through these tabular points. The points can be modified by using the buttons a) beneath the graph in association with the mouse.



23. 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.
24. To insert a point by value use sub-window b).
25. The buttons at c) provide the usual *Cancel* 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, if any points are modified, the program cycles back to the Output Options window for reanalysis.
26. Click *Done* to display the final graphical output. The window appearance is as shown below.
27. Both the ratio plot and the final plot of recombination coefficients may be displayed at a). at b), click *Show Plot 1* for the ratio plot and *Show Plot 2* for the recombination coefficient plot.

28. To store the results in the archive file, click *Archive*. To make a hard copy of the graph, click *Print*.

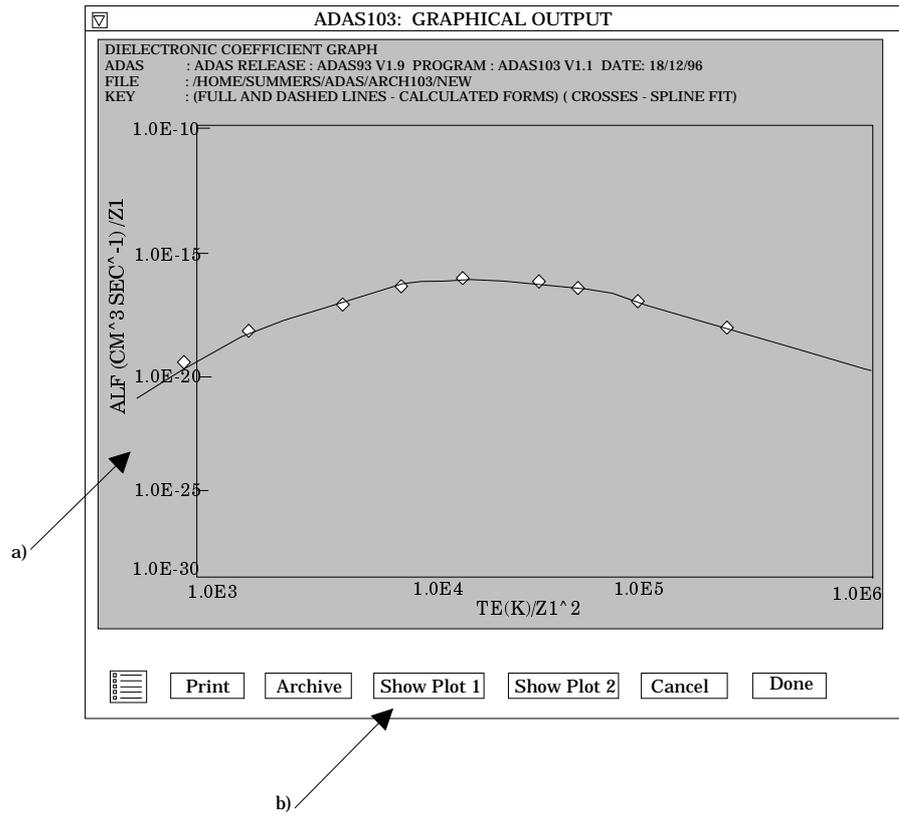
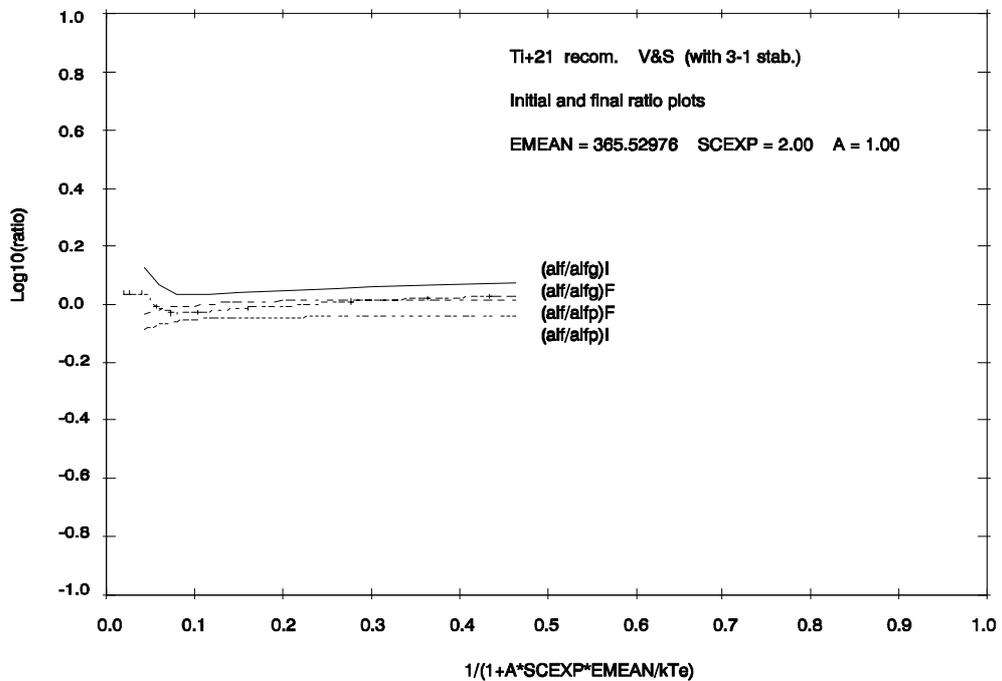


Illustration:

Figure 2.3a



The output from the program is illustrated for the recombination reaction

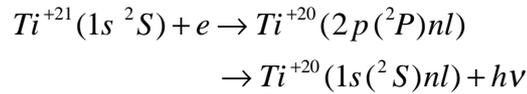
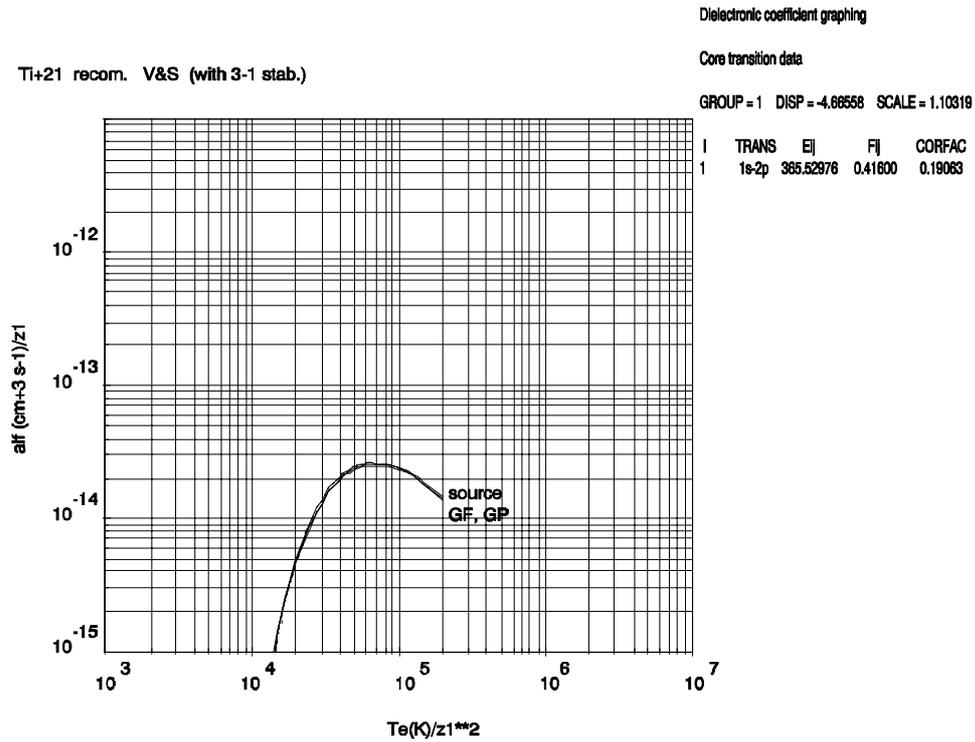


Figure 2.3a shows comparative ratio plots of the source dielectronic data to the initial and then optimised general formula and general program. Spline interpolated values used in forming the final interpolated data are shown as crosses. Source data values are connected by straight lines.

Figure 2.3b shows the z-scaled dielectronic recombination coefficients plotted as a function of z-scaled temperatures. Curves are given for the interpolated source data and for the fitted approximate form.

Figure 2.3b



The tabular output is shown in table 2.3. Energies are in units of I_H , recombination rate coefficients are in units of $cm^3 s^{-1}$. ALFG and ALFP denote the Burgess general formula and general program respectively. EMEAN is a mean core transition energy for the various core transitions which contribute to the group formed as an oscillator strength weighted mean. The two values of EDISP and SCALE are the initial and final (adjusted) settings of the Burgess general formula approximate form. CORFAC(I) and CORFAC(F) are the initial and final (adjusted) values of the *corfac* parameter. The type, ITYPE, is selected automatically according to the initial and final quantum numbers of the transition (see table 2.3). IXOPT=1 indicates that the fit of the Burgess general formula is optimised (0 otherwise), IBPOPT=1 indicates optimisation of the general program to fit the general formula (IBFSEL=0) or to fit the source data (IBFSEL=1). The latter is only possible for a single core transition. Otherwise the summed general formula values for the core transitions belonging to a group are optimised collectively and then the general program is optimised to each (adjusted) general formula component separately. This requires IBFSEL=0 which is forced in this case. Cubic spline interpolation in temperature is used if IBPTS=0 and linear interpolation if IBPTS=1. SCEXP is the scale expansion factor used in the graphical display. Final results are at the selected output temperatures with the interpolated source data, general formula and general program values all given. The parameter X is $((z+1)^2 I_H / v_0^2) / kT_e$.

Table 2.3.

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TI+21 RECOM. V&S (WITH 3-1 STAB.)

NUCLEAR CHARGE = 22.00  RECOMBINING ION CHARGE = 21.00  RECOMBINED ION CHARGE = 20.00
NO = 2  V0 = 1.973  PHFRAC = 0.750
GROUP 1  EMEAN = 365.53000  EDISP = 0.00000  SCALE = 1.00000
        -4.66558  1.10319

NI  LI  NJ  LJ  WI  WJ  EIJ  FIJ  CORFAC(I)  CORFAC(F)  NCUT  ITYPE
1  0  2  1  2.  6.  365.53000  0.41600  0.00000  0.19062  1000  1

<-----INITIAL VALUES-----> <-----FINAL ADJUSTED VALUES----->
TE(K)  ALF  X  ALF/ALFG  ALF/ALFP  X  ALFG  ALFP  ALF/ALFG  ALF/ALFP
5.0000D+06  5.5304D-15  2.3085D+01  1.3466D+00  8.2179D-01  2.3085D+01  5.0802D-15  5.9742D-15  1.0886D+00  9.2571D-01
7.0000D+06  3.7084D-14  1.6490D+01  1.1535D+00  8.4659D-01  1.6490D+01  3.8490D-14  3.8859D-14  9.6348D-01  9.5432D-01
1.0000D+07  1.3964D-13  1.1543D+01  1.0853D+00  8.7021D-01  1.1543D+01  1.5031D-13  1.4224D-13  9.2902D-01  9.8170D-01
1.5000D+07  3.3682D-13  7.6951D+00  1.0787D+00  8.8901D-01  7.6951D+00  3.5787D-13  3.3559D-13  9.4117D-01  1.0037D+00
2.0000D+07  4.6746D-13  5.7714D+00  1.0916D+00  8.9746D-01  5.7714D+00  4.8614D-13  4.6117D-13  9.6157D-01  1.0136D+00
3.0000D+07  5.4932D-13  3.8476D+00  1.1161D+00  9.0462D-01  3.8476D+00  5.5344D-13  5.3741D-13  9.9256D-01  1.0222D+00
4.0000D+07  5.2627D-13  2.8857D+00  1.1329D+00  9.0757D-01  2.8857D+00  5.1985D-13  5.1307D-13  1.0123D+00  1.0257D+00
5.0000D+07  4.7605D-13  2.3085D+00  1.1445D+00  9.0910D-01  2.3085D+00  4.6414D-13  4.6326D-13  1.0257D+00  1.0276D+00
7.0000D+07  3.7609D-13  1.6490D+00  1.1592D+00  9.1060D-01  1.6490D+00  3.6084D-13  3.6533D-13  1.0422D+00  1.0294D+00
1.0000D+08  2.6972D-13  1.1543D+00  1.1713D+00  9.1157D-01  1.1543D+00  2.5549D-13  2.6170D-13  1.0557D+00  1.0307D+00

IXOPT = 1  IBPOPT = 1  IBFSEL = 1  IBPTS = 0  SCEXP = 2.000
TE(K)  ALF  ALFG  ALFGP
2.2050D+06  2.5229D-19  2.3176D-19  7.5305D-19
3.0870D+06  4.7206D-17  4.3363D-17  8.1019D-17
4.4100D+06  2.0422D-15  1.8760D-15  2.4097D-15
6.6150D+06  2.8493D-14  2.8996D-14  2.9789D-14
8.8200D+06  9.3485D-14  1.0036D-13  9.6285D-14
1.3230D+07  2.7209D-13  2.9110D-13  2.7233D-13
2.2050D+07  5.0000D-13  5.1591D-13  4.9164D-13
4.4100D+07  5.0699D-13  4.9774D-13  4.9337D-13
6.6150D+07  3.9342D-13  3.7861D-13  3.8219D-13
8.8200D+07  3.0632D-13  2.9070D-13  2.9643D-13
    
```

Notes: