

ADAS106: Electron impact ionisation rate - graphing and interpolation

The program is for entry of Maxwell averaged ionisation rate coefficient data, examination, comparison with and approximate form, optimising of approximate form fits, display and interpolation to selectable electron temperatures.

Background theory:

The theoretical background is the same as that for program ADAS205. In this case however data are provided as Maxwell averaged ionisation rate coefficients or equivalent forms so there is no requirement for Maxwell averaging.

Approximate forms:

The Maxwell averaged approximate forms follow from expressions 2.5.5, 2.5.6 and 2.5.7 in ADAS105. Hence

$$S^{BCHID}(z, \chi_i, \zeta_i, T_e) = 2\sqrt{\pi}\alpha c a_0^2 C \zeta_i (I_H / \chi_i)^{3/2} (\chi_i / kT_e)^{1/2} E_1(\chi_i / kT_e) w(\chi_i / kT_e) \quad 2.6.2$$

$$w(\chi_i / kT_e) = \{\ln(1 + kT_e / \chi_i)\}^{\beta / (1 + kT_e / \chi_i)}$$

$$\beta = 0.25 \{[(100z + 91) / (4z + 3)]^{1/2} - 5\}$$

where $2\sqrt{\pi}\alpha c a_0^2 = 2.17 \times 10^{-8} \text{ cm}^3 \text{ s}^{-1}$ and $E_1(x)$ is the first exponential integral. In basing an adjustable approximate form on this expression, it is supposed that the shells may be combined into at most two *shell groups*. Then the approximate form for the shell direct ionisation rate coefficient is

$$S_{shd}^{approx}(T_e) = \sum_I c_I \sum_{i \in I} S^{BCHID}(z, \chi_i, \zeta_i, T_e) \quad 2.6.3$$

c_I is an adjustable multiplier for the shell group I .

In a similar manner large autoionising resonances may be identified and combined into at most two *resonance groups*. The resulting approximate form for the excitation-autoionisation part is

$$S_{excit}^{approx}(T_e) = \sum_R c_R \sum_{r \in R} 1.45 \frac{8\pi}{\sqrt{3}} 2\sqrt{\pi}\alpha c a_0^2 W T_r (I_H / kT_e)^{1/2} (I_H / \Delta E_r) e^{-\Delta E_r / kT_e} \quad 2.6.4$$

where $\frac{8\pi}{\sqrt{3}} 2\sqrt{\pi}\alpha c a_0^2 = 3.15 \times 10^{-7} \text{ cm}^3 \text{ s}^{-1}$ and c_R is an adjustable multiplier for the shell group R . The expression for each resonance is an excitation rate coefficient obtained by averaging the excitation cross-section given in equation 2.5.7 of ADAS105. $W T_r$ is a preset weight factor input by the user.

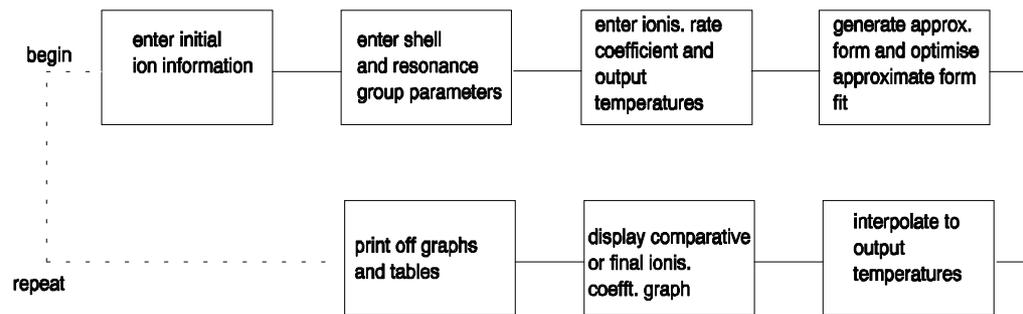
It is sometimes convenient to define an effective collision strength (gamma or Upsilon) for ionisation equivalent to that used for excitation which is finite at threshold as

$$Y = S / (2\sqrt{\pi}\alpha c a_0^2 [I_H / kT_e]^{1/2}) \quad 2.6.5$$

Program steps:

These are summarised in figure 2.6.

Figure 2.6

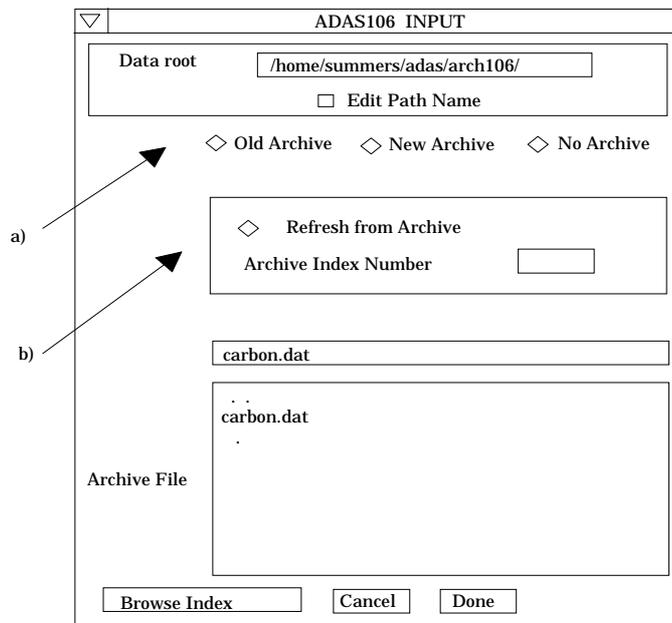


Interactive parameter comments:

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 sixth button to activate ADAS106.

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 ADAS106 analysis is `/.../uid/adas/arch106/` 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. As described in the ADAS User Manual, the examination of input ionisation rate coefficients is based on the generation of an approximate form for the rate coefficient variation with temperature with which the input is compared. The approximate form is built from 'shell groups' and 'resonance groups' designed to represent direct ionisation and autoionisation respectively. Scaling factors can be varied to attempt to optimise the fit of the approximate form to the input data.
8. At a), the primary data on the nuclear and ion charges are entered. Make an appropriate choice at *Use default scaling parameters* if you wish the scaling parameters to be frozen at your initial settings (YES) or allowed to vary (NO). Click on the appropriate diamond button to display the parameters of either the *Shell groups* or *Resonance groups* in the sub-window to the right at b).
9. Up to two shell or resonance groups may be prepared. Make this choice at *No. of shell groups* at the top of the sub-window at b). Then click on the button for the *1st* or *2nd. Group* to display its parameter settings below. Enter the group parameters in the editable table. The definitions of the various parameters are given in the ADAS User Manual. Remember to enter a *Default scaling parameter*. 1.0 is a good first choice. Click on *Edit Table* to bring up the ADAS Table Editor widget in the usual manner.
10. User input temperatures, rate coefficients and required output temperatures are entered at c) with the currently selected units shown below at d). Click the *Edit table* button to 'drop down' the ADAS Table Editor for data input.
11. 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.
12. 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.

ADAS106 PROCESSING OPTIONS

Data file name : /home/summers/adas/arch106/carbon.dat

Browse Index

Nuclear charge z0

Initial ion charge z

Final ion charge z1

Use default scaling parameters NO

If 'NO' then optimised scaling will be used

Display groups : Shell Resonance

No. of shell groups : Group 1 2

Default scaling parameter

INDEX	n	1	EION(RYD)	IZETA
1	2	1	1.2345e+00	4

Edit Table

INDEX	Input Temp.	Input Coefft.	Output Temp.
1	1.000E+05	1.000E+00	1.000E+05
2	2.000E+05	2.000E+00	2.000E+05
3	5.000E+05	5.000E+00	3.000E+05
4	1.000E+06	1.000E+01	4.000E+05
5	2.000E+06	2.000E+01	7.000E+05
6	5.000E+06	5.000E+01	8.000E+05
7	1.000E+07	1.000E+02	1.000E+06
8	2.000E+07	2.000E+02	2.000E+06

Temp. units : Kelvin. Rate coefft. units : cm3 sec-1. Temp. units : Kelvin .

Edit Table

Default Temperature values

Edit the processing options data and press Done to proceed

13. 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.

14. There is only one system of comparative display for ADAS106 at the moment.
15. Two graphs are presented. The first is a scaled comparative graph for assessing the rate coefficient data and making adjustments if appropriate. The second graph displays the final ionisation rate coefficient at the user's temperatures.
16. At a) 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.
17. Make the required choices of graph scaling and axes choices at b) for the comparative graph and at c) for the ionisation rate coefficient graph.

ADAS106 OUTPUT OPTIONS

Data file name : /home/summers/adas/arch106/carbon.dat

Browse Index

Graphical Output

Graph Title :

Graphic scaling parameter :

Select Device

Post-script

Post-script

HP-PCL

HP-GL

Ratio Graph Scaling

X-min : X-max :

Y-min : Y-max :

Ionis. Coefft. Graph Scaling

X-min : X-max :

Y-min : Y-max :

Enable Hard Copy Replace

File name :

Text Output Replace

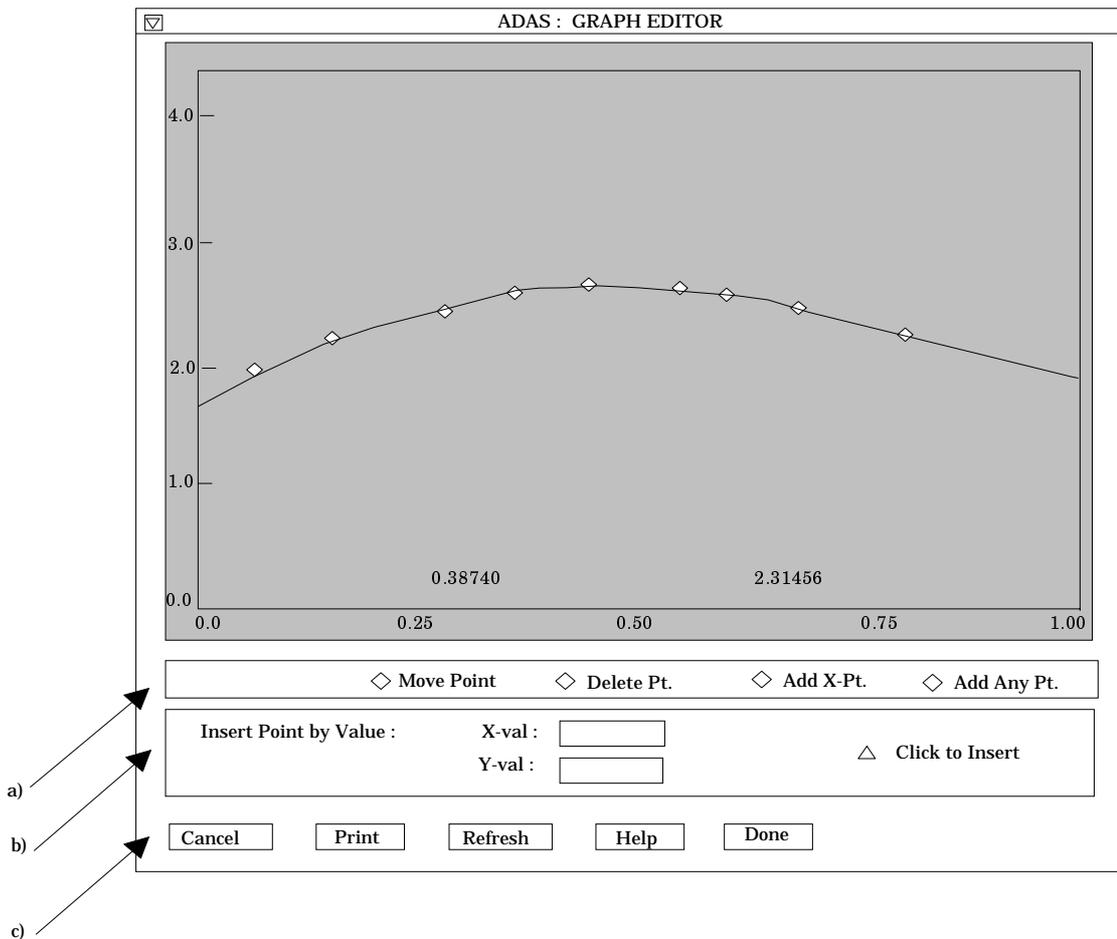
File name :

a)

b)

c)

18. After making your choices on hard copy and text output click *Done* to show the comparative graph.
19. The comparative 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.
20. 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.



21. To insert a point by value use sub-window b).
22. The buttons at c) 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, if any points are modified, the program cycles back to the Output Options window for reanalysis.
23. Click Done to display the final graphical output. The window appearance is as shown below.
24. Both the comparative plot and the final plot of ionisation rate coefficients may be displayed at a). Click *Show Plot 1* for the comparative plot and *Show plot 2* for the ionisation coefficient plot.
25. To store the results in the archive file, click *Archive*. To make a hard copy of the graph, click *Print*.

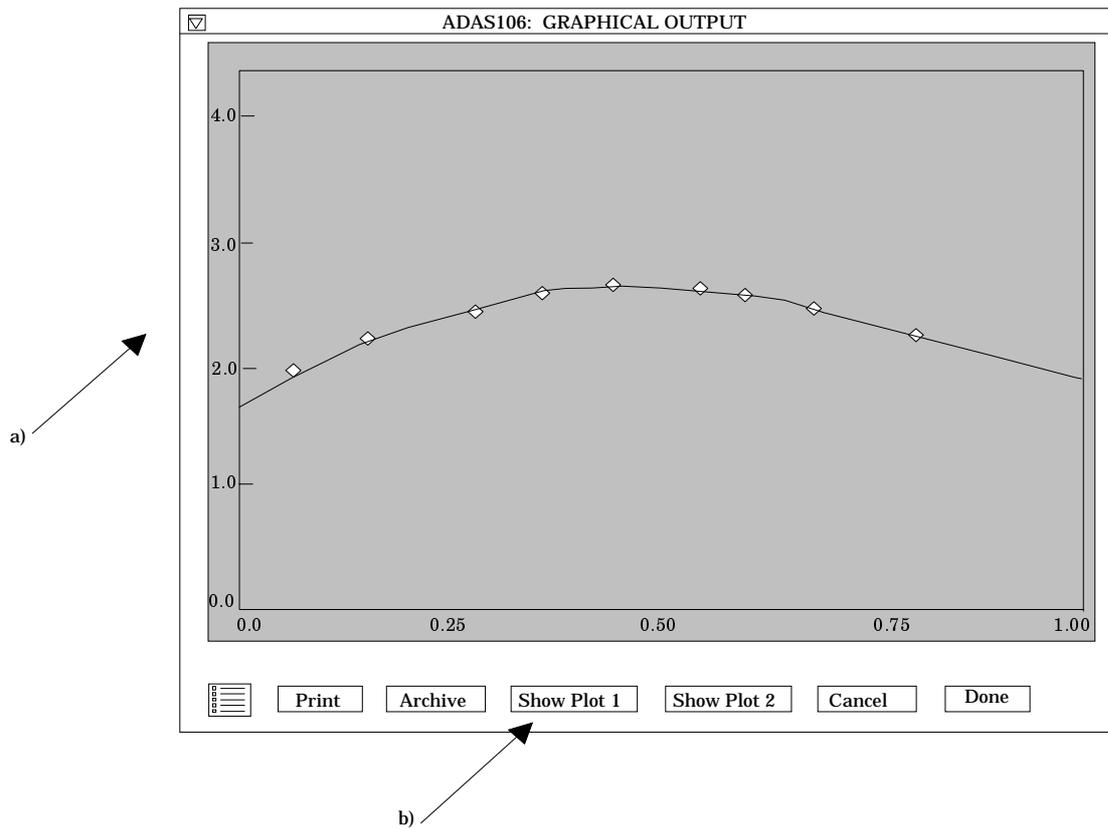


Illustration:

The output from the program is illustrated for the ionisation reaction

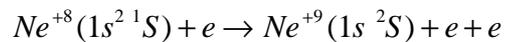
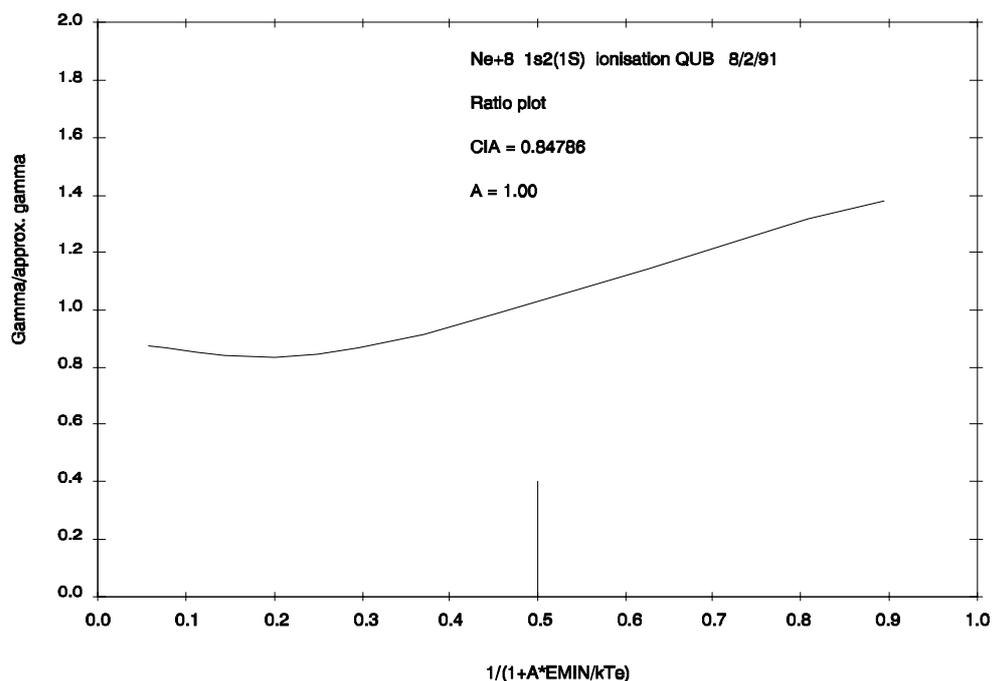


Figure 2.6a shows a comparative ratio plot of the source ionisation rate data, expressed in gamma (upsilon) form, to the optimised approximate form. The solid vertical line shows the position of the ionisation threshold energy. There is only a single shell group in this case. A is a graphing parameter which allows some shift of emphasis in the x-direction.

Figure 2.6a



In figure 2.6b, the solid line shows the final interpolated ionisation rate coefficient. The dashed line shows the optimised approximate form, denoted by Bchid. The graphs are presented as a function of z-scaled temperature.

The tabular output is given in table 2.6. Energies are in units of I_H , temperatures in K and the ionisation rate coefficient in $cm^3 s^{-1}$. S is the final ionisation rate coefficient and SEM the approximate form ionisation rate coefficient.

Figure 2.6b

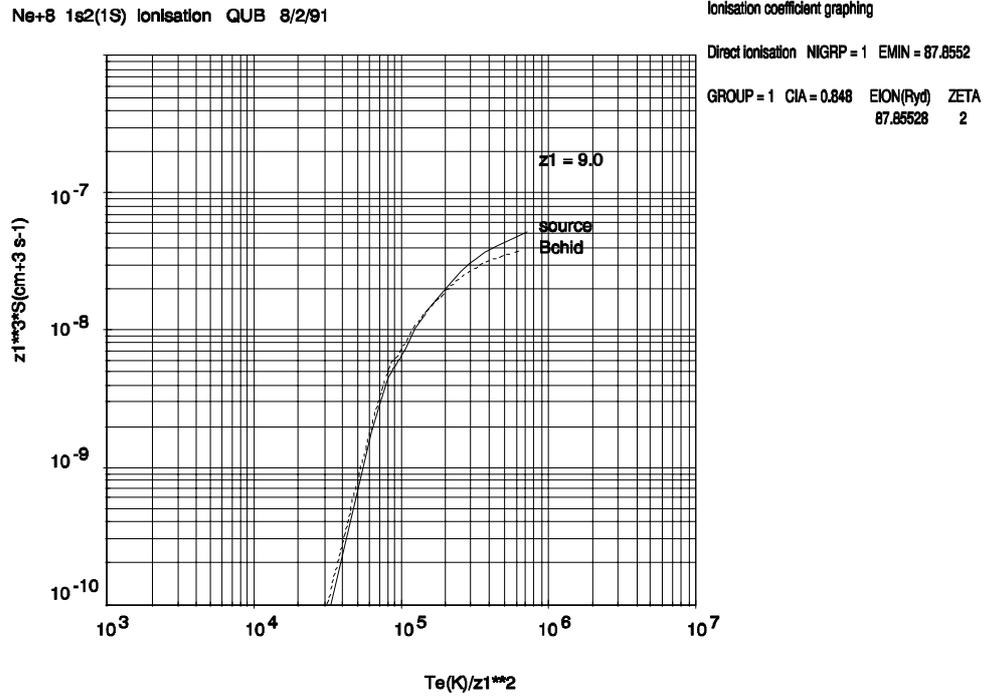


Table 2.6.

NE+8 1S2(1S) IONISATION QUB 8/2/91				
NUCLEAR CHARGE = 10.0 INITIAL ION CHARGE = 8.0 FINAL ION CHARGE = 9.0				
DIRECT IONISATION NIGRP = 1 EMIN = 87.85530				
GROUP 1 CIA = 0.848 EION(RYD) ZETA				
87.85530 2				
TE(K)	S(CM3 SEC-1)	GAMMA	GAM(EMP.)	GAM/GAM(EMP.)
8.12D+05	7.89997D-19	2.14877D-03	2.46287D-03	8.72463D-01
1.16D+06	1.53999D-16	2.98429D-03	3.44542D-03	8.66161D-01
1.74D+06	9.60996D-15	4.24398D-03	5.00233D-03	8.48399D-01
2.32D+06	7.78997D-14	5.41874D-03	6.47145D-03	8.37330D-01
3.48D+06	6.59997D-13	7.66994D-03	9.19102D-03	8.34504D-01
4.64D+06	1.98999D-12	9.86260D-03	1.16723D-02	8.44960D-01
5.80D+06	3.96998D-12	1.21014D-02	1.39608D-02	8.66812D-01
8.12D+06	9.08996D-12	1.65595D-02	1.80817D-02	9.15816D-01
1.16D+07	1.76999D-11	2.30908D-02	2.34127D-02	9.86253D-01
2.32D+07	4.15998D-11	4.22208D-02	3.68431D-02	1.14596D+00
4.64D+07	6.55997D-11	6.98359D-02	5.43833D-02	1.28414D+00
5.80D+07	7.14997D-11	8.01643D-02	6.08547D-02	1.31731D+00
1.16D+08	8.15997D-11	1.14808D-01	8.32006D-02	1.37989D+00
TE(K)	S	SEM		
1.1605D+05	1.0026D-63	1.1492D-63		
2.3211D+05	1.2674D-37	1.4526D-37		
5.8027D+05	7.3227D-22	8.3931D-22		
1.1605D+06	1.5400D-16	1.7780D-16		
2.3211D+06	7.7900D-14	9.3034D-14		
5.8027D+06	3.9700D-12	4.5800D-12		
8.1238D+06	9.0900D-12	9.9256D-12		
1.1605D+07	1.7700D-11	1.7947D-11		

2.3211D+07	4.1600D-11	3.6301D-11
5.8027D+07	7.1500D-11	5.4278D-11

Notes: