

ADAS105: Electron impact ionisation cross-section - graphing and rate evaluation

The program is for entry of electron impact ionisation cross-section data, examination, comparison with an approximate form, optimising of approximate form fit, display and conversion to Maxwell averaged ionisation rate coefficients at selectable electron temperatures.

Background theory:

Consider the ionisation reaction

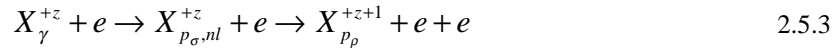


where the ion X^{+z} in initial state γ is ionised leaving the residual ion X^{+z+1} in the state p_p . Mostly ionisation from the ground state of the ion X^{+z} is presented in sources of atomic data. Also the particular final state of the ion X^{+z+1} is generally not specified, but rather a sum over all final states is given. It is assumed that this effectively leaves the final state ion in its ground state (possibly after some cascade steps). In practice, with initial target ions which have metastable states, experimental measurements are made on a mixed target and this mixture may not be easily resolvable. The reaction defined by equation 2.5.1 is called *direct ionisation* and if the initial state has an electronic configuration

$$\gamma \equiv n_1 l_1^{q_1} n_2 l_2^{q_2} \dots n_m l_m^{q_m} \quad 2.5.2$$

reference may be made to *shell direct ionisations*, that is from particular nl shells.

The ionisation can also proceed indirectly via an autoionisation reaction as

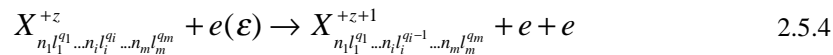


and this is called *excitation-autoionisation*. The excitation-autoionisation channels can contribute a very large part of the total ionisation cross-section and are responsible for the step-like structures seen on experimental ionisation cross-section data. Properly, there is a competition between autoionisation in the second step in equations 2.5.3 and radiative stabilisation (as in dielectronic recombination) which is not shown. For low charge states, the autoionisation is much more likely, but for high charge states, the radiative branch is expected to reduce the excitation-autoionisation contributions to the total cross-section progressively.

In examining and fitting total ionisation cross-section data with approximate forms is intended that the optimised approximate form should give some guidance to the resolution of the total cross-section into initial and final metastable state resolved parts. This ensures that resolved data is consistent with the best available totals. It is necessary therefore to describe the basis of the approximate forms in some detail.

Approximate forms:

There are a number of semi-empirical expressions for the ionisation cross-section Q . In these, it has been shown to be important to take account of the shell structure of the ionising ion as specified by the shell occupancies ζ_i and shell ionisation potentials χ_i . Such an expression is due to Burgess and Chidichimo (1983) which for the shell direct ionisation reaction



is written as

$$Q^{BCHID}(z, \chi_i, \zeta_i, \epsilon) = C \zeta_i (I_H / \epsilon) (I_H / \chi_i) \ln(\epsilon / \chi_i) w(\epsilon / \chi_i) \pi a_0^2$$

$$w(\epsilon / \chi_i) = \begin{cases} 0 & \epsilon \leq \chi_i \\ \ln(\epsilon / \chi_i)^{\beta(\chi_i / \epsilon)} & \epsilon > \chi_i \end{cases} \quad 2.5.5$$

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

The multiplier $C = 2.3$ was recommended by Burgess and Chidichimo. The factor W is designed to improve the behaviour near threshold for near neutral systems. 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 cross-section is

$$Q_{shd}^{approx}(\epsilon) = \sum_I c_I \sum_{i \in I} Q^{BCHID}(z, \chi_i, \zeta_i, \epsilon) \quad 2.5.6$$

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

$$Q_{excit}^{approx}(\epsilon) = \sum_R c_R \sum_{r \in R} 1.45 WT_r (I_H / \Delta E_r)(I_H / \epsilon) \pi a_0^2 \quad 2.5.7$$

c_R is an adjustable multiplier for the shell group R . The expression for each resonance is a simplified classical formula for the excitation cross-section multiplied by a weight factor WT_r . It is sometimes convenient to define a 'collisions strength' for ionisation equivalent to that used for excitation which is finite at threshold as

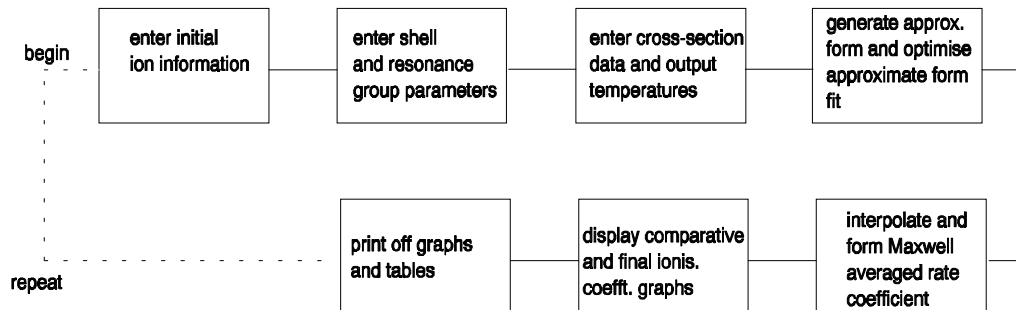
$$\Omega = Q / (1 - \chi_i / \epsilon) \quad 2.5.8$$

ADAS105 integrates the ionisation cross-section over a Maxwellian distribution of electron energies at a set of electron temperatures T_e .

Program steps:

These are summarised in the figure below.

Figure 2.5



Interactive parameter comments:

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

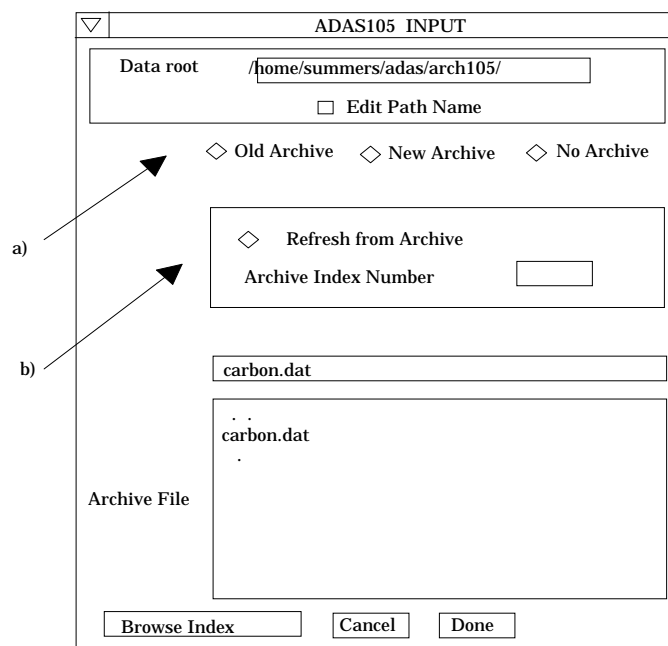
where *uid* is your user identifier. The defaults directory records the parameters you set the last time you ran each ADAS code. Move to the directory in which you wish ADAS created output text file (*paper.txt* is the default) and graphic files (e.g. *graph.ps* if a postscript file) to be placed. Initiate ADAS, move to the series 1 menu and click on the fifth button to activate ADAS105.

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 ADAS105 analysis is
`./.../uid/adas/arch105/`
 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 cross-sections is based on the generation of an approximate form for the cross-section variation with energy 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 energies, cross-sections 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, 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 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.

ADAS105 PROCESSING OPTIONS

Data file name : /home/summers/adas/arch105/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	l	EION(RYD)	IZETA
1	2	1	1.2345e+00	4

Edit Table

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 : Incident E (Ryd). X-section units : X-sect pi*a0^2. Temp. units : Kelvin .

Edit Table

Default Temperature values

Edit the processing options data and press Done to proceed

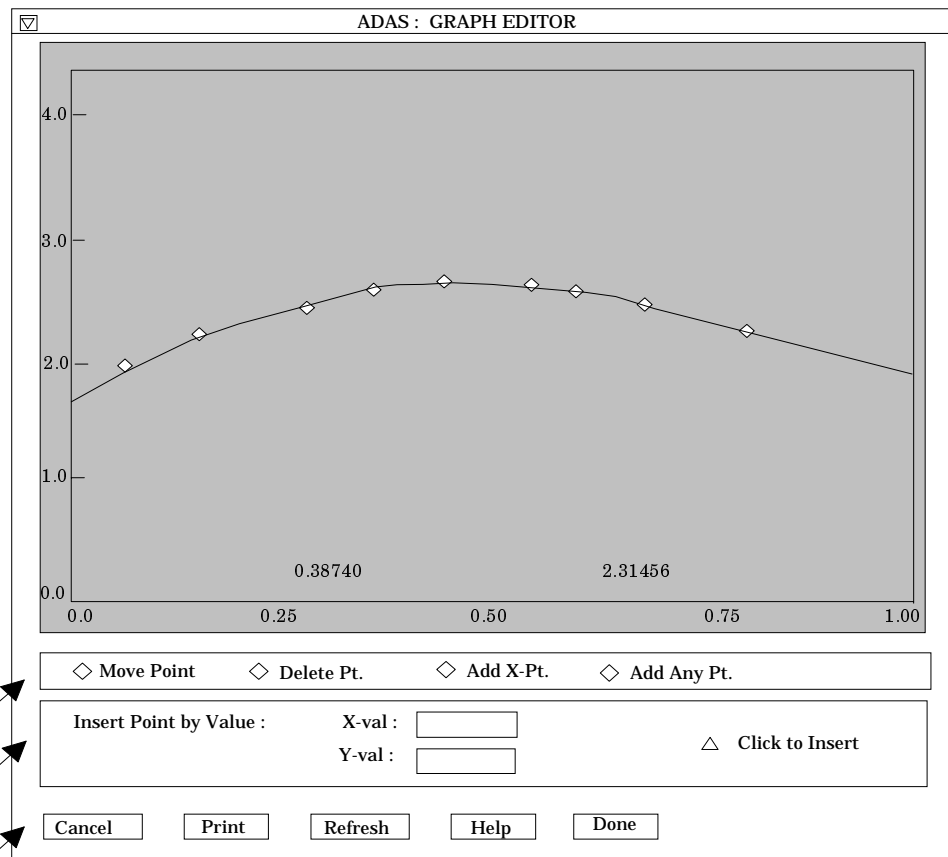
13. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window. The 'Escape to Menu' icon is also available for a quick exit at the bottom left hand corner.

The **output options window** is shown below.

14. There is only one system of comparative display for ADAS105 at the moment. Unlike ADAS101, a 'Burgess option' is not available.
15. 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 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. For default scaling the *Ratio Graph Scaling* and *Ionis. Coefft. Scaling* buttons should not be activated.

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 cross-section 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*.
26. Click *Done* to return to the Output Options window. The *Escape to Menu* icon is available. Click on it to quit the program and return to the ADAS series 1 menu.

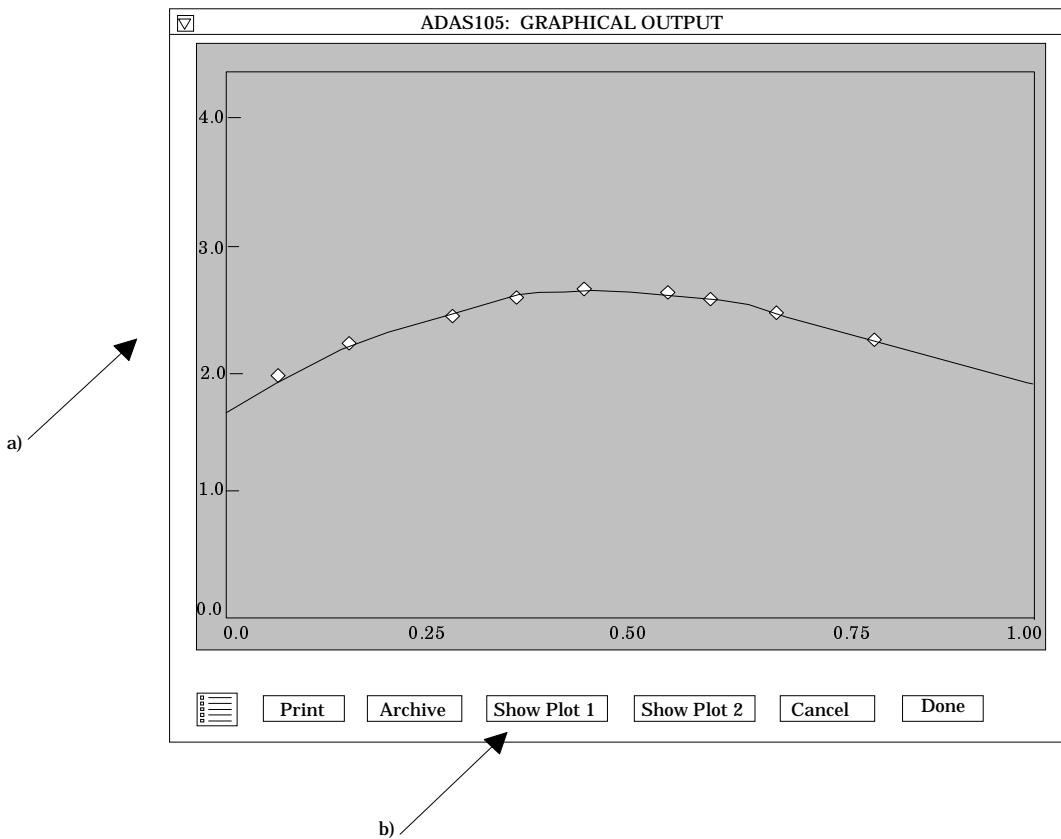


Illustration:

The output from the program is illustrated for the ionisation reaction

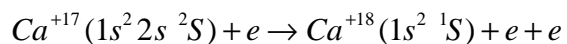


Figure 2.5a shows a comparative ratio plot of the source ionisation cross-section (expressed as a collision strength) data to an optimised one shell group + one resonance group. The position of the single resonance in the resonance group is marked by the vertical dashed line.

Figure 2.5a

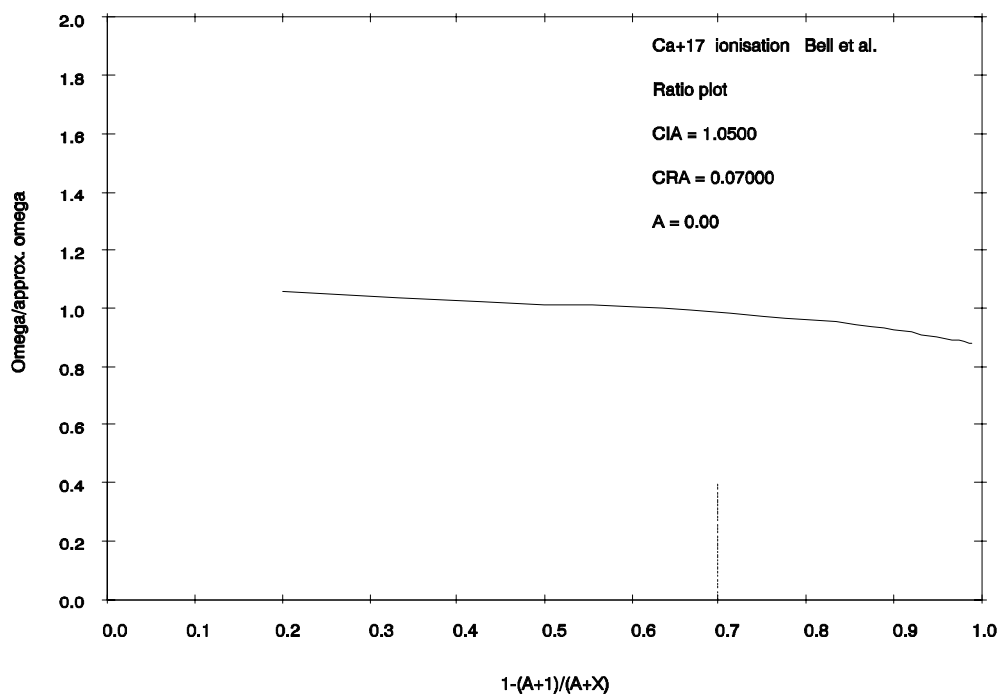


Fig. 2.5b shows the ionisation rate coefficient versus electron temperature (K) for the set of output temperatures. Solid lines are drawn between the tabular values of the final output data. The dashed line shows the optimised approximate form.

The tabular output is shown in table 2.5. Energies are in units of I_H . S is the final Maxwell averaged ionisation rate coefficient in units of $\text{cm}^3 \text{s}^{-1}$. QEM is the approximate cross-section and SEM the approximate rate coefficient. X is the threshold parameter relative to the first ionisation potential.

Figure 2.5b

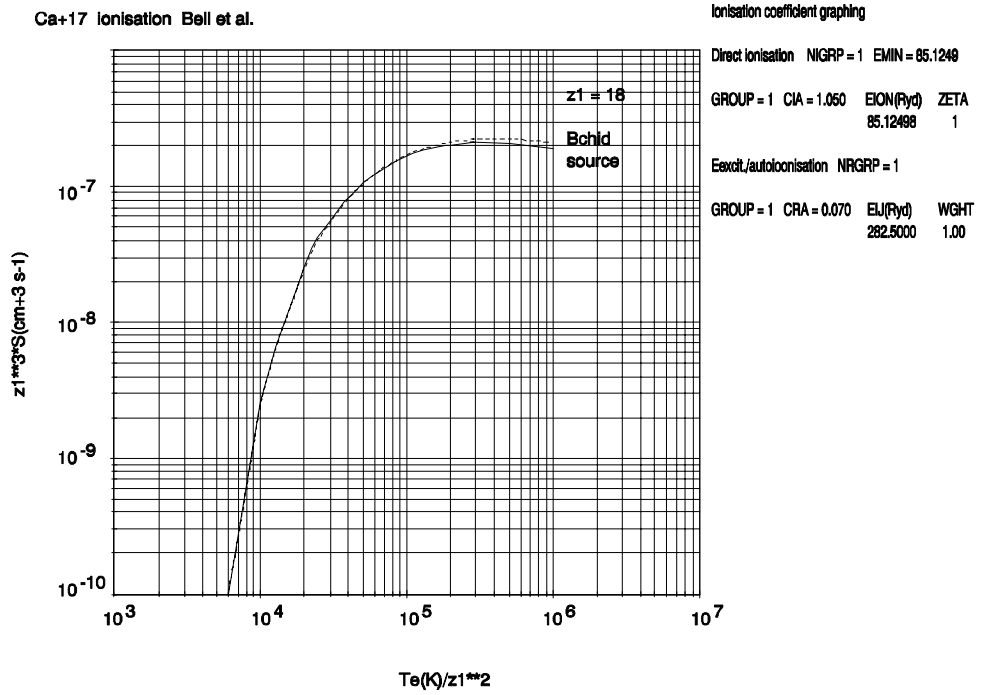


Table 2.5.

CA+17 IONISATION BELL ET AL.				
NUCLEAR CHARGE = 20.0 INITIAL ION CHARGE = 17.0 FINAL ION CHARGE = 18.0				
DIRECT IONISATION NIGRP = 1 EMIN = 85.12500				
GROUP 1 CIA = 1.050		EION(RYD) ZETA		
		85.12500 1		
EXCIT/AUTOIONISATION NRGRP = 1				
GROUP 1 CRA = 0.070		EIJ (RYD) WGHT		
		282.50000 1.000		
X	Q(PI*A0**2)	Q/(1-1/X)	QEM/(1-1/X)	Q/QEM
1.25000	6.29746D-05	3.14873D-04	2.97473D-04	1.05849D+00
1.50000	9.34388D-05	2.80316D-04	2.70263D-04	1.03720D+00
1.75000	1.09012D-04	2.54361D-04	2.48675D-04	1.02287D+00
2.00000	1.17083D-04	2.34166D-04	2.31009D-04	1.01367D+00
2.25000	1.21630D-04	2.18934D-04	2.16210D-04	1.01260D+00
2.50000	1.22766D-04	2.04610D-04	2.03585D-04	1.00504D+00
2.75000	1.22766D-04	1.92918D-04	1.92652D-04	1.00138D+00
3.00000	1.21630D-04	1.82445D-04	1.83070D-04	9.96586D-01
3.50000	1.18219D-04	1.65507D-04	1.68694D-04	9.81104D-01
4.00000	1.13445D-04	1.51260D-04	1.55413D-04	9.73279D-01
4.50000	1.08671D-04	1.39720D-04	1.44426D-04	9.67412D-01
5.00000	1.03897D-04	1.29871D-04	1.35152D-04	9.60930D-01
6.00000	9.53713D-05	1.14446D-04	1.20274D-04	9.51541D-01
7.00000	8.79825D-05	1.02646D-04	1.08791D-04	9.43520D-01
8.00000	8.16169D-05	9.32765D-05	9.96067D-05	9.36448D-01
9.00000	7.61606D-05	8.56807D-05	9.20626D-05	9.30678D-01

10.00000	7.15000D-05	7.94444D-05	8.57350D-05	9.26628D-01
12.50000	6.20652D-05	6.74622D-05	7.35638D-05	9.17057D-01
15.00000	5.50175D-05	5.89473D-05	6.47676D-05	9.10136D-01
20.00000	4.52417D-05	4.76228D-05	5.27697D-05	9.02466D-01
30.00000	3.38744D-05	3.50425D-05	3.92329D-05	8.93190D-01
40.00000	2.73951D-05	2.80975D-05	3.16316D-05	8.88274D-01
50.00000	2.31892D-05	2.36624D-05	2.66939D-05	8.86437D-01
75.00000	1.69372D-05	1.71661D-05	1.95018D-05	8.80231D-01
100.00000	1.35270D-05	1.36636D-05	1.55455D-05	8.78942D-01

TE(K)	TE(EV)	S	SEM
1.6200D+06	1.3959D+02	5.4925D-15	5.2105D-15
3.2400D+06	2.7918D+02	4.4829D-13	4.2970D-13
6.4800D+06	5.5836D+02	4.3631D-12	4.2473D-12
9.7200D+06	8.3754D+02	9.5298D-12	9.3779D-12
1.6200D+07	1.3959D+03	1.7965D-11	1.7960D-11
3.2400D+07	2.7918D+03	2.8603D-11	2.9304D-11
6.4800D+07	5.5836D+03	3.4699D-11	3.6473D-11
9.7200D+07	8.3754D+03	3.5929D-11	3.8312D-11
1.6200D+08	1.3959D+04	3.5543D-11	3.8525D-11
3.2400D+08	2.7918D+04	3.2741D-11	3.6141D-11

Notes: