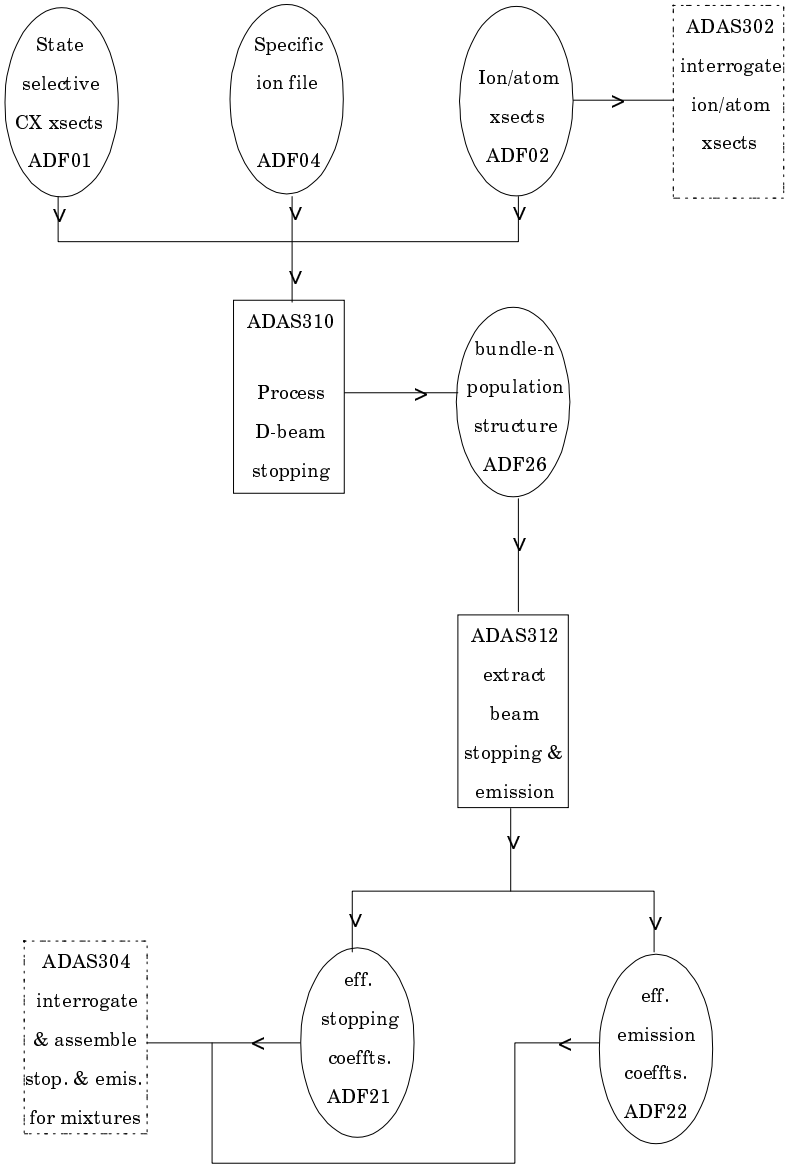
Atomic Data and Analysis Structure

Calculating beam stopping and emission

The chapter is concerned with the collisional-radiative population calculations for neutral deuterium beam atoms in interaction with thermal plasma and the delivery of appropriate derived data for the ADAS data-base. The primary program is ADAS310 which calculates the excited populations of principal quantum shells of deuterium (or other isotopes) in a beam. The population results are archived in ADAS data format adf26 together with associated collisional-radiative coefficients. The program ADAS312 is a post-processor which reviews the *adf26* data and extracts beam stopping and beam emission coefficients. The program assembles these coefficients and archives them in the compact forms used in experimental analysis namely ADAS data formats *adf21* for the beam stopping coefficient and *adf22* for the beam emission coefficients.

A schematic of the programs and data sets is shown in figure 3.0 below.

Figure 3.0


State selective CX xsects ADF01
Specific ion file ADF04
Ion/atom xsects ADF02
ADAS302 interrogate ion/atom xsects
ADAS310 Process D-beam stopping
bundle-n population structure ADF26
ADAS312 extract beam stopping & emission
ADAS304 interrogate & assemble stop. & emis. for mixtures
eff. stopping coeffts. ADF21
eff. emission coeffts. ADF22

ADAS310: Beam emission spectroscopy - process beam stopping and emission : H-beam

The program calculates the excited population structure, effective ionisation and recombination coefficients of hydrogen atoms or hydrogenic ions in an impure plasma. A very many n-shell bundle-n approximation is used. The hydrogen atoms may be part of the thermal plasma or may be in a beam. The latter case is the only one of relevance for this manual, however the full flexibility of the program has been retained.

Background theory:

For hydrogen or hydrogenic ions in a plasma, the largest collision cross-sections are those for which n=n' and l=l'±1. For these cases the transition energy is nearly zero and the cross-sections are so large for electron and ion densities of relevance for fusion that it is very good approximation to assume relative statistical population for the l-states. Thus for hydrogenic systems only populations of complete n-shells need be evaluated, the *bundle-n* approximation. The equilibrium populations of the n-shells, N_n, are the solution of the statistical balance equations

$$\begin{aligned}
&\sum_{n'>n}[A_{n'\to n}+u(\nu)B_{n'\to n}+N_e q^{(e)}_{n'\to n}+N_e q^{(p)}_{n'\to n}]N_{n'}\\
&+\sum_{n''<n}[u(\nu)B_{n''\to n}+N_e q^{(e)}_{n''\to n}+N_e q^{(p)}_{n''\to n}]N_{n''}\\
&+N_e N_+\alpha^{(r)}_n+N_e^2 N_+\alpha^{(3)}_n+N_e N_+\int u(\nu)B_{\kappa\to n}d\kappa\\
&=\{\sum_{n'>n}[u(\nu)B_{n\to n'}+N_e q^{(e)}_{n\to n'}+N_e q^{(p)}_{n\to n'}]\\
&+\sum_{n''<n}[A_{n\to n''}+u(\nu)B_{n\to n''}+N_e q^{(e)}_{n\to n''}+N_e q^{(p)}_{n\to n''}]\\
&+\int u(\nu)B_{n\to\kappa}d\kappa+N_e q^{(e)}_{n\to\varepsilon}+N_e q^{(p)}_{n\to\varepsilon}\}N_n
\end{aligned} \qquad 3.10.1$$

N_n is the population of the state $X^{+z_0-1}_n$ and N_+ of the parent ion X^{+z_0}. N_e is the free electron density and N_p the free proton density. A and B are the usual Einstein coefficients, $q^{(e)}$ and $q^{(p)}$ denotes collisional rates due to electrons and protons, $\alpha^{(r)}_n$ and $\alpha^{(3)}_n$ denote radiative and three-body recombination and $u(\nu)$ is the energy density of the radiation field. There is one such equation for each value of n from 1 to ∞. The equations may be extended by including reactions for other impurity ions additional to the protons. The radiation field presence in the equations is not of direct relevance to hydrogen population modelling in a fusion plasma, but it can be exploited in a purely technical manner to separate the influence of different driving populations in the collisional-radiative sense.

Gaunt factors

It is convenient to express the coefficients in terms of Gaunt factors. Thus

$$A_{n\to n'}=\left(\frac{16\alpha^4 c}{3\sqrt{3}\pi a_0}\right)\frac{z_0^4 g^I_{n,n'}}{n^3 n'(n^2-n'^2)} \qquad n'<n \qquad 3.10.2$$

and the Einstein B coefficients are given by

$$B_{n\to n'}=A_{n\to n'}\Big/\frac{8\pi h\nu^3}{c^3} \qquad B_{n'\to n}=\frac{n^2}{n'^2}B_{n\to n'} \qquad 3.10.3$$

where $\nu=(z_0^2 I_H/h)(1/n'^2-1/n^2)$ is the frequency of the $n\to n'$ photon. With a Planck radiation field of energy density $u(\nu)$ at temperature T_r and dilution W, the photo-excitation rate coefficient is given by

$$u(\nu)B_{n'\to n} = \left(\frac{16\alpha^4 c}{3\sqrt{3}\pi a_0}\right)\frac{Wz_0^4 g^I_{n,n'}}{nn'^3(n^2-n'^2)} / [\exp(h\nu/kT_r)-1] \quad 3.10.4$$

The stimulated emission rate coefficient is given by

$$u(\nu)B_{n'\to n} = \left(\frac{16\alpha^4 c}{3\sqrt{3}\pi a_0}\right)\frac{Wz_0^4 g^I_{n,n'}}{nn'^3(n^2-n'^2)} / [\exp(h\nu/kT_r)-1] \quad 3.10.5$$

The ADAS library contains subroutines for evaluation of the bound-bound Gaunt factors $g^I_{n,n'}$.

In a similar manner the bound-free rates are obtained. The photo-ionisation rate coefficient from the level n is

$$\int u(\nu)B_{n\to\kappa}d\kappa = \left(\frac{8\alpha^4 c}{3\sqrt{3}\pi a_0}\right)\frac{Wz_0^4}{n^5}\int_{I_n/kT_r}^{\infty}\frac{g^{II}_{n,\kappa}dx}{x(e^x-1)} \quad 3.10.6$$

The stimulated recombination coefficients is

$$\int u(\nu)B_{n\to\kappa}d\kappa = 8\left(\frac{\pi a_0^2 I_H}{kT_e}\right)^{3/2}\left(\frac{8\alpha^4 c}{3\sqrt{3}\pi a_0}\right)\frac{Wz_0^4}{n^3} \exp(I_n/kT_e)\int_{I_n/kT_r}^{\infty}\frac{g^{II}_{n,\kappa}\exp(-T_r x/T_e)dx}{x(e^x-1)} \quad 3.10.7$$

and the radiative recombination coefficient is

$$\alpha_n^{(r)} = 8\left(\frac{\pi a_0^2 I_H}{kT_e}\right)^{3/2}\left(\frac{8\alpha^4 c}{3\sqrt{3}\pi a_0}\right)\frac{z_0^4}{n^3} \exp(I_n/kT_e)\int_{I_n/kT_e}^{\infty}\frac{g^{II}_{n,\kappa}\exp(-x)dx}{x} \quad 3.10.8$$

where $I_n = z_0^2 I_H/n^2$, T_e is the Maxwellian free electron temperature. The ADAS library contains subroutines for evaluation of the bound-free Gaunt factors $g^{II}_{n,\kappa}$. The radiation dilution and radiation temperature are relevant only to hydrogen in astrophysical plasmas. Thus the general dilution factor for the beam case is set to zero. It is useful however to be able to artificially depopulate the ground level of hydrogen so as to isolate the contributions to populations of excited levels of hydrogen coming from recombination alone. This is achieved by having a separate dilution factor applying to photo-ionisation from the ground level which can be switched on and off. The only requirement here is that this dilution factor and the associated radiation field temperature be large. Pre-set values in ADAS310 are suitable for most purposes.

The de-excitation rate for hydrogenic ions by electrons is

$$q^{(e)}_{n'\to n} = \frac{2^8}{3}\left(\frac{2\sqrt{\pi}\alpha\, ca_0^2}{3}\right)\frac{n'^3 n^5}{(n'^2-n^2)^4}\frac{g^I_{n,n'}}{z_0^2}\left(\frac{I_H}{kT_e}\right)^{1/2} P(\Delta E_{n,n'}/kT_e) \quad 3.10.9$$

for $n' > n$ and the excitation rate is

$$q^{(e)}_{n\to n'} = \frac{2^8}{3}\left(\frac{2\sqrt{\pi}\alpha\, ca_0^2}{3}\right)\frac{n'^5 n^3}{(n'^2-n^2)^4}\frac{g^I_{n,n'}}{z_0^2}\left(\frac{I_H}{kT_e}\right)^{1/2} \exp(-\Delta E_{n,n'}/kT)\, P(\Delta E_{n,n'}/kT_e) \quad 3.10.10$$

Particularly simple expressions for P are given by Van Regemorter. In general an effective P-factor is deduced from more complex collision cross-section calculations or experimental cross-section measurements. similar formulation may be used for proton collision rates.

The electron collisional ionisation rate coefficient may be described by

$$q_{n\to\varepsilon}^{(e)} = 8\sqrt{\pi}\alpha\, c a_0^2 \left(\frac{I_H}{kT_e}\right)^{1/2} \frac{n^2}{z_0^2} \exp(-I_n / kT_e) \int_0^\infty G \exp(-\zeta) d\zeta \qquad 3.10.11$$

and the three-body recombination coefficient by

$$\alpha_n^{(3)} = 2^6 \pi^2 (\alpha\, c a_0^5) \left(\frac{I_H}{kT_e}\right)^2 \frac{n^4}{z_0^2} \int_0^\infty G \exp(-\zeta) d\zeta \qquad 3.10.12$$

with $\zeta = (W_n / I_n - 1) / kT_e$ and

$$G = \left[\left(\frac{W_n / I_n - 1}{W_n / I_n + 1} \right) - \frac{W_n / I_n}{(W_n / I_n + 1)^2} \ln(W_n / I_n) + \frac{1}{4} I^{IP}(W_n) \right] \qquad 3.10.13$$

in the Exchange Classical Impact Parameter ECIP approximation. I^{IP} is the impact parameter part.

b-factors and scaling

It is convenient to rewrite the statistical balance equations in terms of the deviations of the populations from those which would occur in thermodynamic equilibrium. The deviation b_n is defined by

$$N_n = N_e N_+ 8 \left(\frac{\pi a_0^2 I_H}{kT_e} \right)^{3/2} n^2 \exp(I_n / kT_e) b_n \qquad 3.10.14$$

Also it is convenient to introduce $c_n = b_n - 1$ and scaled temperatures and densities

$$t_e = \left(\frac{kT_e}{I_H}\right)\frac{1}{z_0^2},\ t_r = \left(\frac{kT_r}{I_H}\right)\frac{1}{z_0^2} \text{ and } \rho_e = 2^5 \sqrt{\frac{\pi}{3}} \frac{\pi a_0^2}{\alpha^3} \frac{N_e}{z_0^7} \qquad 3.10.15$$

with similar forms for the proton temperature and density. In these terms the statistical balance equations become particularly suitable for calculation.

Solution of the collisional-radiative equations

The general solution of the statistical balance equations to obtain collisional-radiative coefficients and populations is described in detail in the description of ADAS208. The methods of condensation, projection and expansion which give flexibility in the treatment of metastables and in the merging of low resolution and high resolution population models are also described there. For the case of hydrogen in beams entering fusion plasmas, the bundle-n level of resolution is appropriate for all n-shells (subject to refinements described below of the key transitions) provided the interest is in beam stopping and integral beam emission. Nonetheless, observations show that principal quantum shell radiative transitions by beam atoms are spectrally resolved into motional Stark multiplets. Using the methods of projection and expansion, the bundle-n solution can be expanded over low n-shell Stark manifolds for a fuller study. ADAS310 has some capability for supporting such studies which it does by accessing an '*expansion definition file'* and by archiving the '*condensed-projection matrices'*. These aspects have been de-activated for the present version of ADAS310 (although the expansion definition file is still requested).

Approximations for collision cross-sections

Internal routines calculate default values for electron and ion impact excitation and ionisation in a number of approximations. For electron impact excitation between nearby n-shells ($\Delta n \leq m \sim 2$), the impact parameter approximation (Burgess and Summers, 1976) is used. The order of the quadrature over the cross-section to produce the rate coefficients may be altered but the highest precision is generally used. For $\Delta n > m$ the formulae of Percival and Richard (1970) are available or the simpler Van Regemorter (1962) approximation may be used. For ion impact excitation, cross-sections are included for $\Delta n \leq m' \sim 2$ with the expressions of Lodge et al. (1976) or Vainshtein as alternatives..

Supplementary precision data

The general purpose routines described above are satisfactory for generating collision cross-section data at moderate accuracy for the very many n-shell atom population structure. However the precision may be improved for excitation, ionisation and charge transfer involving the ground level and possibly other low n-shells. Such improvement is particularly important for beam stopping coefficients and active or passive Lyman and Balmer line spectroscopy. Systematic improvement is implemented by drawing on the ADAS ion/atom and ion/electron collision database. A supplementation subroutine (SUPPH1 for H^0 (HI)), which is subject to periodic adjustment executes the data acquisition under the following classes

class	**returned data**	**source**
electron excit.	excit. & dexcit. maxwellian. rate coefficients	specific ion files (*adf04*) bundle-n form
electron ions.	ionis. maxwellian rate coefficient	*szd* files (*adf07*)
proton excit.	excit. & dexcit. displaced maxwell. rate coefficients	*sia#h* files (*adf02*)
proton ionis.	ionis.. displaced maxwell. rate coefficient	*sia#h* files (*adf02*)
impurity excit.	excit. & dexcit. displaced maxwell. rate coefficients	*sia#h* files (*adf02*)
impurity ionis.	ionis.. displaced maxwell. rate coefficient	*sia#h* files (*adf02*)

The supplementary data is introduced, for example as an effective P factor

$$P_{n,n'} = q^{(s)}_{n\to n'} / \{(2\sqrt{\pi}\alpha c a_0^2) \sqrt{I_H / kT}[(I_H / \Delta E_{n,n'}) f_{n\to n'}]\exp(-\Delta E_{n,n'} / kT)]\} \qquad 3.10.16$$

for excitation which replaces the moderate accuracy formulaic value if available. For the hydrogenic ion as a plasma species, state selective charge exchange recombination data to excited levels for hydrogen donors may be included and these data are accessed directly from the appropriate file (*adf01*)

Distinctions in analysis for hydrogen in beam or plasma

The program can apply to hydrogen atoms in a thermal plasma or to hydrogen atoms in a beam. The practical distinction is made by the assignment of a translational velocity for beam atoms. This velocity is incorporated in the integrals of beam particle / plasma particle cross-sections over the Maxwellian distributions in the thermal plasma. For hydrogen forming part of the thermal plasma, the translational velocity is set to zero. In the latter circumstance, ion impact collision rates are very small compared with electron impact rates. Also recombination (both free-electron capture and charge exchange capture) become significant processes. For the hydrogen atoms in a fast beam, recombination is not relevant and although formally present is ignored in the results. However the translational velocity can make ion impact collisions more important than electron collisions.

Multiple impurities and z_{eff}

In general several impurity species (nuclei) may be involved in collisionally inducing transitions. Of these the hydrogen nuclei are often the most important and because of better

availability of data and approximations for proton induced rates, the protons are usually treated as a special (plasma) species and the other species treated as the 'impurities'. Let the electron and proton number densities be N_e and N_p respectively. Let the set of impurities charges and fractions by number be $\{z_{0_i}^{(imp)}, f_i^{(imp)}; i = 1,..,I\}$ then the total impurity number density, z_{eff} and component impurity number densities are

$$\begin{aligned} N^{(imp)} &= (N_e - N_p) / (\sum_{i=1}^{I} z_{0_i}^{(imp)} f_i^{(imp)}) \\ z_{eff} &= (N_p + N^{(imp)} [\sum_{i=1}^{I} (z_{0_i}^{(imp)})^2 f_i^{(imp)}]) / N_e \\ N_i^{(imp)} &= f_i^{(imp)} N^{(imp)} \end{aligned} \qquad 3.10.16$$

In the case of single impurity, which is frequently used as a single 'effective' impurity, it is convenient to alter the definitions. Taking N_e, N_p and z_{eff} as prescribed

$$\begin{aligned} z_0^{(imp)} &= (z_{eff} N_e - N_p) / (N_e - N_p) \\ N^{(imp)} &= (N_e - N_p) / z_0^{(imp)} \end{aligned} \qquad 3.10.17$$

determines the effective charge for the single impurity and its number density.

The beam stopping coefficient is the collisional radiative ionisation coefficient. However there is sometimes confusion about its definition. Although hydrogen nuclei impact ionisation and charge transfer are the most efficient reactions causing beam stopping, it is usual in fusion to define the stopping coefficient with respect to the electron density. Thus the stopping rate (cm^{-3} s^{-1}) is $N_e N_B S^{(e)}$ with N_B the neutral beam density. For ADAS310, this applies even if the stopping is calculated for the case of a pure impurity with all the free electrons contributed by the impurity in charge balance. Thus for a pure impurity of number density N_I and nuclear charge Z, with effective ionisation coefficient, $S^{(I)}$, the stopping rate is $N_I N_B S^{(I)}$ and $S^{(e)} = S^{(I)} / Z$.

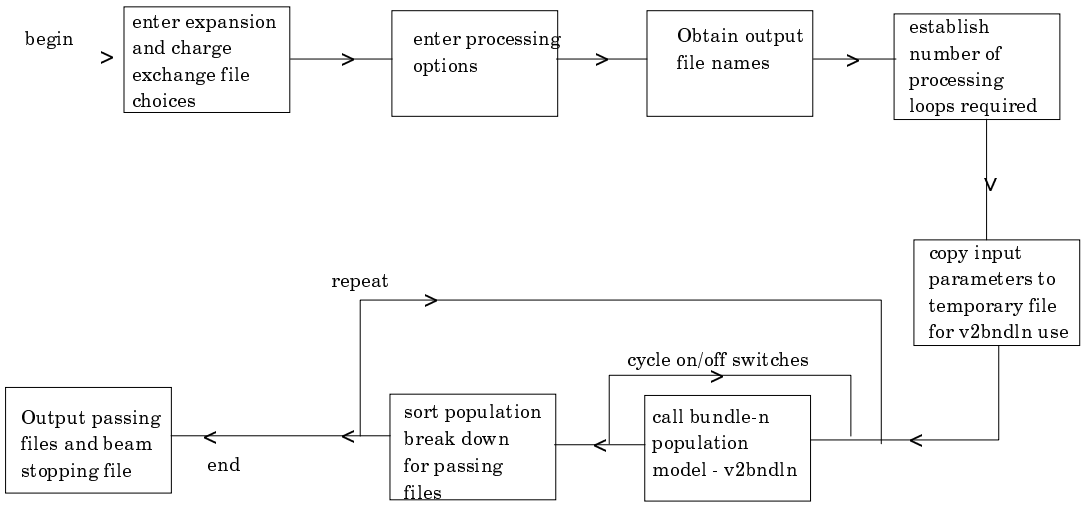
Population results and preparing tabulations

ADAS 310 is too slow in execution for a direct link to inter-pulse experiment analysis and so it is used to prepare tabulations of effective beam stopping and beam emission coefficients for subsequent look-up. The effective coefficients are most sensitive to the beam particle energy and the plasma ion density and less sensitive to plasma ion temperature and Z-effective. Suitable tabulations can therefore be built on a reference set of plasma and beam conditions, a two-dimensional array of coefficients as functions of beam energy and plasma density at the reference conditions of the other parameters and then one-dimensional vectors of the coefficients as functions of each minor parameter at the reference condition of all the other parameters. ADAS310 accepts as input the definition of these scans, establishes an extended list of cases required to achieve these scans and then executes repeated population calculations at each set of plasma conditions in the list. ADAS310 can compute the populations for any mixture of light impurities (hydrogen to neon) in the plasma. It is impractical to deal with all possible mixtures of impurities. It is our usual practice to execute ADAS310 in turn for each light impurity from hydrogen to neon treated as a pure species. The mixed species effective coefficients are constructed from these pure impurity solutions by the theoretical data acquisition routines. The main population output is very complete and in principle contains all information on possible emitted spectrum lines up to very high n-shells together with both ionisation and recombination collisional-radiative coefficients. It is archived as ADAS data format *adf26*. ADAS310 can also produce directly the final tabulations of beam stopping coefficient according to ADAS data format *adf21*, however this is normally done using the post-processor program ADAS312.

Program steps:

These are summarised in the figure below.

Figure 3.10



Interactive parameter comments:

The program which makes use of data from archived ADAS data-sets initiates an interactive dialogue with the user in three parts, namely, input data file selection, entry of user data and disposition of output. The primary calculations may be conducted in foreground or background.

Move to the directory in which you wish the ADAS created files to appear. These include the output text file produced after executing any ADAS program (*paper.txt* is the default), and up to four further output data files. There is no graphical output from this program Initiate ADAS310 from the program selection menus in the usual manner.

The **file selection window** appears first as illustrated below.

1. At a) enter the beam species (H for hydrogen and its isotopes) and the atomic charge of the beam species. Only data for neutral beam species is present in the central ADAS database at this time.

2. There are two data files to be selected, the expansion file and the charge exchange file. The procedure is the same in both cases.

3. Data root a) shows the full pathway to the appropriate data sub-directories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas,* to use this facility.

4. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing

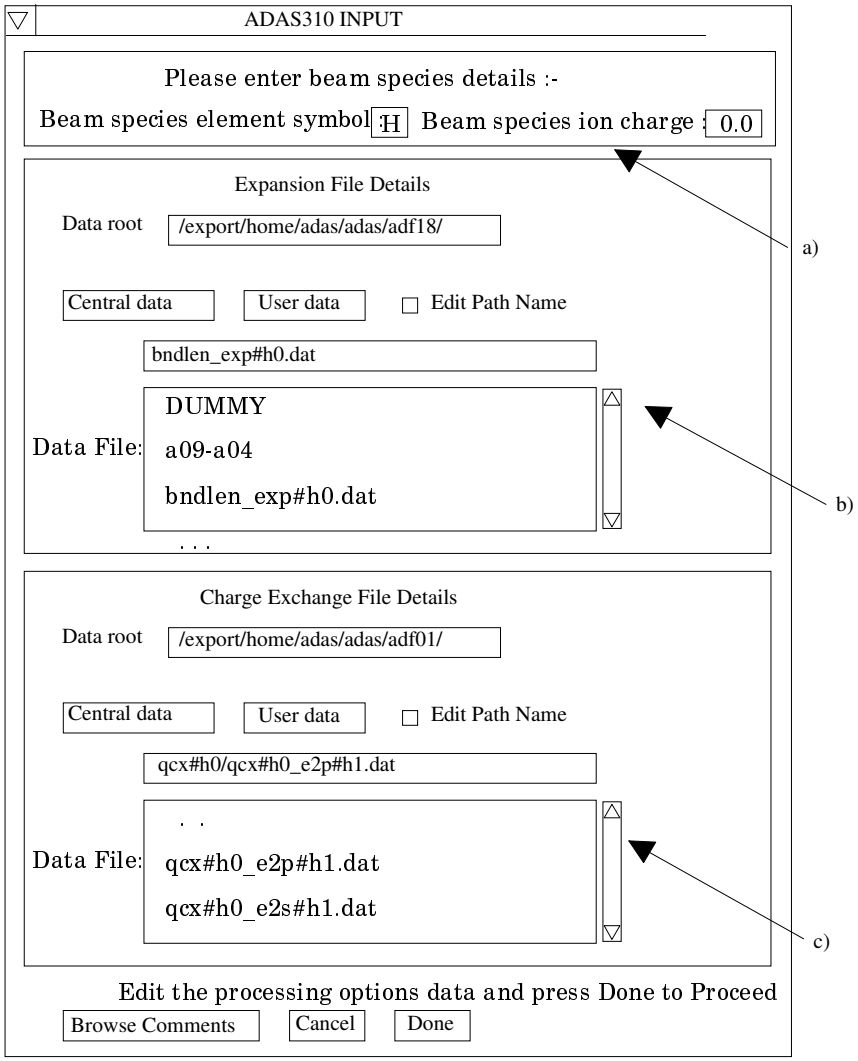
5. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.

6. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual data-files are presented for selection. Data-files all have the termination *.dat*.

7. The expansion file is selected at b). A special ADAS data type *adf18* is used for such 'expansion' and 'cross-referencing' files. They fall into various categories, kept in sub-directories, according to where they map from and to. Thus the sub-directory *a09_a04* contains data sets mapping from the *adf09* data type into the *adf04* data type. We shall deal with the purposes of these in the discussion of advanced population modelling in the next release. For the moment note that

bndlen_exp#h0.dat is the one needed here and it sits alone as shown in the illustration. Always select it.

8. The charge exchange file is selected at c). Again this is not of importance for neutral beam stopping. The charge exchange data set is required when hydrogen nuclei can act as electron receivers from other species. You will see no effect of your selection here on the beam stopping coefficient but the selection is kept in for the future. Once a charge exchange data file is selected, the set of buttons at the bottom of the main window become active.

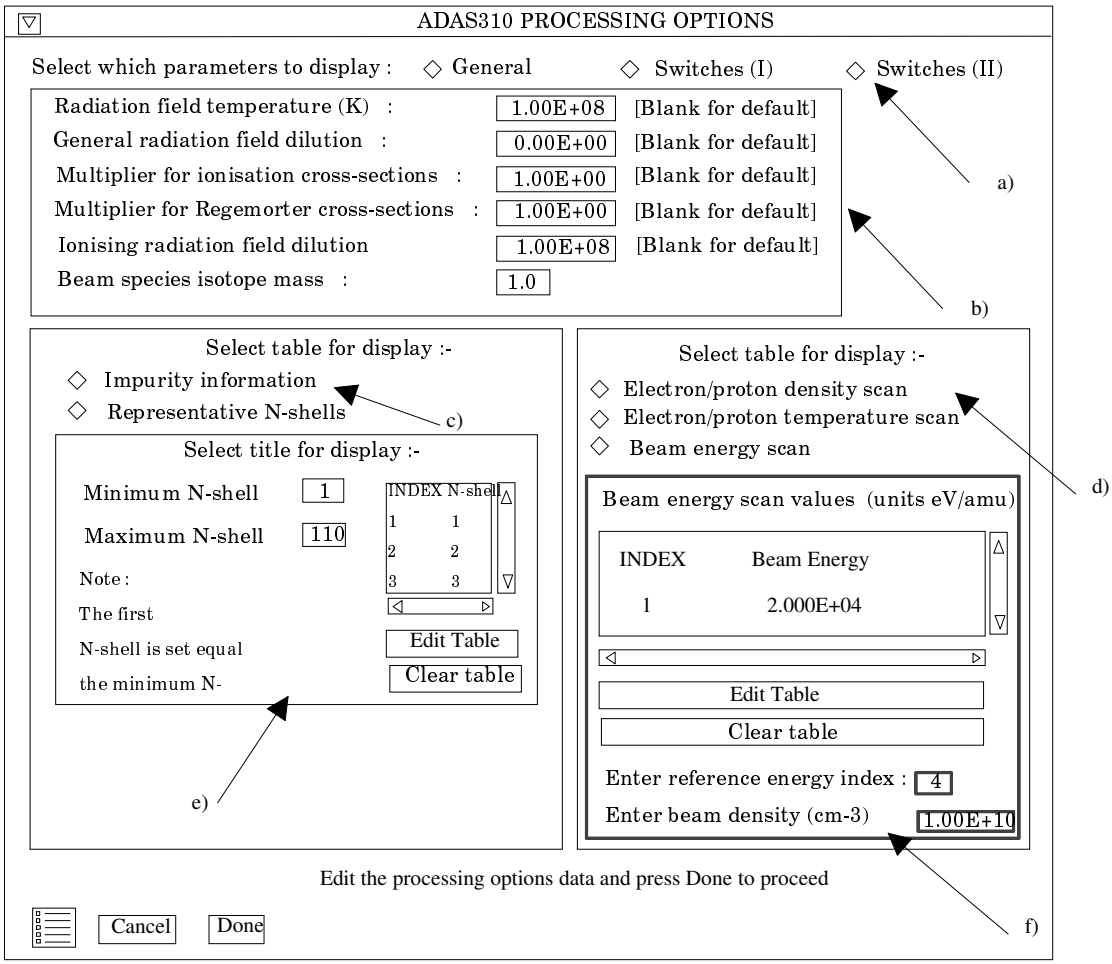


9. Clicking on the *Browse Comments* button displays any information stored in the selected charge exchange data-file. It is important to use this facility to find out what is broadly available in the data-set. The possibility of browsing the comments appears in the subsequent main window also.

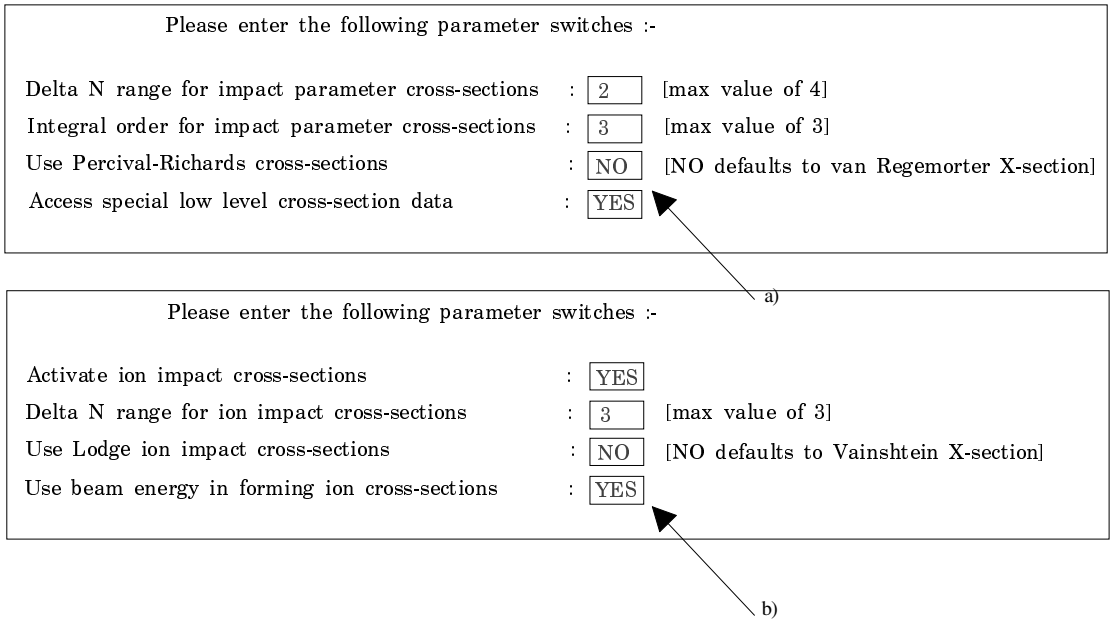
10. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

The **processing options window** has the appearance shown below

11. The various control parameters of the collisional-radiative population calculation are organised into three groups selected in turn by the buttons *General*, *Switches (I)* and *Switches (II)*. These cause the appropriate set of parameters to be displayed at b). The default settings are reasonable and they can be ignored as long as only beam stopping is the intent.



12. *Switches (I)* allow some choices to do with electron collision cross-sections and *Switches (II)* allow some choices to do with ion collision cross-sections. (see the corresponding sub-window inserts below Make sure that *Access to low level data* is chosen at a) and *Use beam energy informing cross-sections* at b). It is this latter piece of information that informs the calculation that the neutral hydrogen is in the beam and not in the plasma.



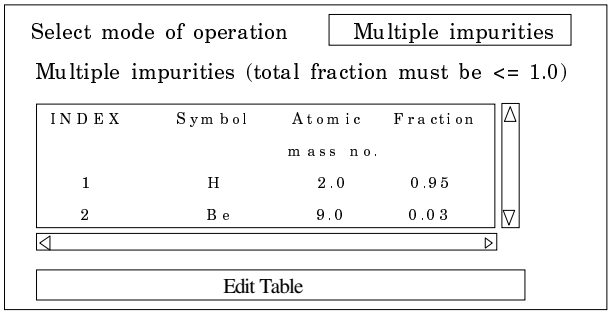
13. The choices at c) above must then be made. Click the *Impurity information* or *Representative N-shell* buttons. The appropriate sub-window is displayed at c).

14. The representative N-shells requires specification of the lowest N-shell, Highest N-shell and a set of sensibly spaced 'representative' N-shells spanning the range. Make sure the lowest is 1 for hydrogen. Make the highest around 110 and use about 20 representative levels. Use all levels up to N=10 and then start to space more widely.

15. The Impurity information sub-window is shown below. There are two modes of operation. Single impurity or Multiple impurities. Click the drop-down list button to make your choice.

16. The single impurity case has only one impurity nucleus in addition to protons present in the plasma. The single impurity case is used to build up such data sets in *adf21*. Note how the impurity and protons fit together (equations 3.10.16 and 3.10.17 in the ADAS User Manual). The proton and electron density choices to be made next influence this.

17. The multiple impurity choice enables us to investigate the influence of an impurity mixture on the stopping with greater precision. Edit in the fractions you wish in the usual manner. Note that the impurity density acts non-linearly in the stopping coefficient and so the linear superposition implied by the use of ADAS304 is imprecise. It is however very fast which is necessary in large scale experimental data analysis.



18. At d) the choice of plasma and beam parameters for the scans are made Click on the appropriate button to work on each scan in turn. Note that you edit in a set of values and then choose one to be the reference value of that parameter. The table may be edited by clicking on the *Edit Table* button.. The ADAS Table Editor window is then presented with the same set of editing operations available as are described in bulletin *nov18-94*. Values should be monotonic increasing. It has proved helpful to add a *Clear Table* button to remove all entries in the output field.

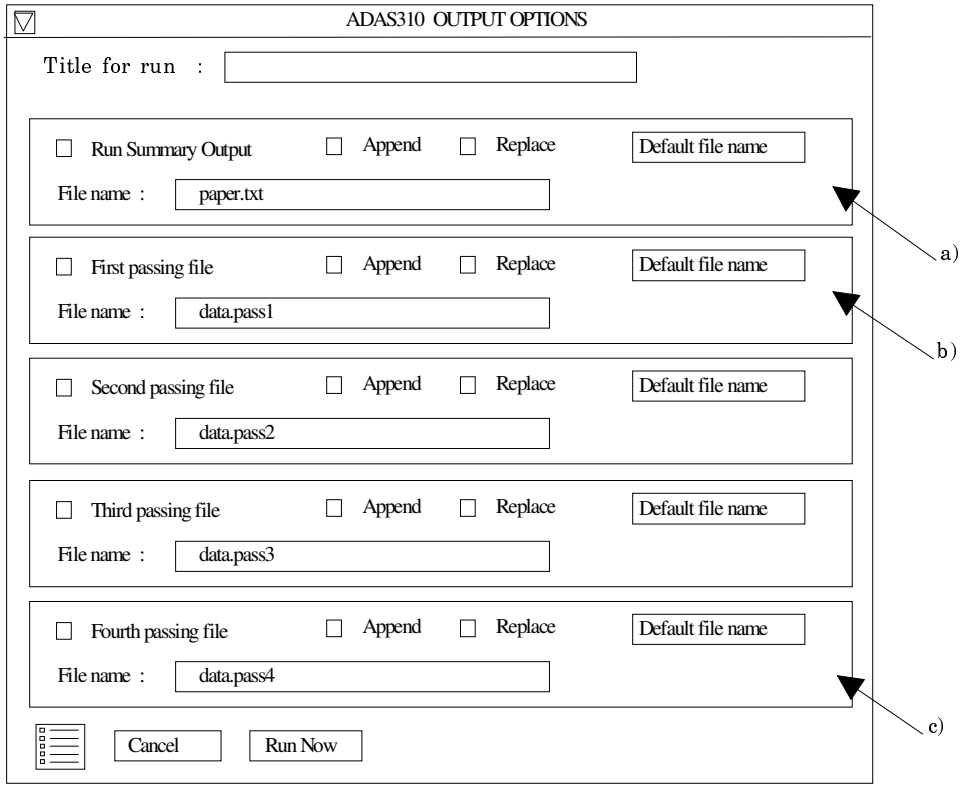
19. Note that a neutral hydrogen density in the beam is requested. This is necessary to allow a mathematical separation of the various influences on the neutral hydrogen population structure and is not an experimental beam density. A value of order 10^6 or greater is suitable for the program operation.

20. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

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

21. It follows the usual pattern except that there is no graphical output.

22. The Run Summary is given in the output file specified at a). The *Run Summary Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Run Summary Output* is on. If the file already exits a choice to *Replace* or *Append* may be made. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Append* or *Replace* button has not been activated.



23. Four additional passing files may be produced which are placed in your pass directory. The fourth is the assembled stopping coefficients structured according to an *adf21* file. The first passing file contains line printer formatted pages of data, one page for each individual population structure case run. The data held on these sheets is very comprehensive. By appropriate choice of the parameters mentioned in the processing section above and choice of input files, hydrogen in all its possible conditions in a fusion plasma can be obtained (beam and non-beam).

24. Click the *Run Now* button to initiate the calculations. These are run in fore-ground since they are of fairly modest duration. A thermometer widget illustrated below keeps you informed of the progress of the calculations.

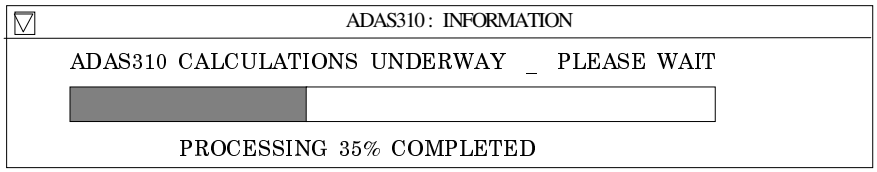


Illustration:

Table 3.10a.

```
 EFFECTIVE CONTRIBUTION TABLE FOR ION PRINCIPAL QUANTUM SHELL POPULATIONS IN THERMAL PLASMA

    HYDROGEN                Z0 = 1.00E+00               Z1 = 1.00E+00

    TRAD = 1.00E+08 K       TE = 5.80E+07 K             TP = 5.80E+07 K
       W = 0.00E+00         NE = 1.00E+12 CM-3          NP = 0.00E+00 CM-3

      EH = 5.00E+03 EV/AMU  NH = 1.00E+06 CM-3       NH/NE = 1.00E-06   FLUX = 9.78E+13 CM-2 SEC-1


CHARGE EXCHANGE OFF: N1/N+ = 3.96967E-10  RECOMB COEFF = 3.98614E-17 CM+3 SEC-1  IONIZ COEFF = 1.00415E-07 CM+3 SEC-1

CHARGE EXCHANGE ON : N1/N+ = 1.01033E-06  RECOMB COEFF = 1.01452E-13 CM+3 SEC-1  IONIZ COEFF = 1.00415E-07 CM+3 SEC-1
```

I	N	F1	F2	F3	B(CHECK)	B(ACTUAL)	NN/(BN*N+)
1	1	0.00000E+00	4.22257E+05	1.07427E+15	1.07472E+09	1.07472E+09	9.40109E-16
2	2	9.03269E+09	3.77642E+00	1.90419E+09	1.10339E+04	1.10339E+04	3.75276E-15
3	3	3.27110E+09	2.50566E+00	3.72697E+08	3.68009E+03	3.68009E+03	8.44053E-15
4	4	1.38276E+09	1.72873E+00	8.89060E+07	1.48767E+03	1.48767E+03	1.50034E-14
5	5	4.65572E+08	1.25911E+00	1.96737E+07	4.91313E+02	4.91313E+02	2.34414E-14
6	6	1.55704E+08	1.08781E+00	4.77562E+06	1.63175E+02	1.63175E+02	3.37545E-14
7	7	5.87510E+07	1.03338E+00	1.41410E+06	6.18052E+01	6.18052E+01	4.59426E-14
8	8	2.50081E+07	1.01425E+00	4.92186E+05	2.67728E+01	2.67728E+01	6.00059E-14
9	9	1.20056E+07	1.00684E+00	1.98482E+05	1.33349E+01	1.33349E+01	7.59443E-14
10	10	6.55794E+06	1.00373E+00	9.26893E+04	7.72209E+00	7.72209E+00	9.37578E-14
11	11	4.29257E+06	1.00244E+00	5.28243E+04	5.39216E+00	5.39216E+00	1.13446E-13
12	12	2.66749E+06	1.00151E+00	2.88629E+04	3.72541E+00	3.72541E+00	1.35010E-13
13	15	6.45607E+05	1.00036E+00	4.69556E+03	1.65733E+00	1.65733E+00	2.10952E-13
14	20	9.49494E+04	1.00005E+00	5.01251E+02	1.09648E+00	1.09648E+00	3.75024E-13
15	30	1.10830E+04	1.00001E+00	5.29440E+01	1.01126E+00	1.01126E+00	8.43800E-13
16	40	2.32656E+03	1.00000E+00	1.07290E+01	1.00236E+00	1.00236E+00	1.50009E-12
17	50	6.76789E+02	1.00000E+00	3.06759E+00	1.00069E+00	1.00069E+00	2.34388E-12
18	60	2.38809E+02	1.00000E+00	1.07145E+00	1.00024E+00	1.00024E+00	3.37519E-12
19	70	9.29529E+01	1.00000E+00	4.13889E-01	1.00009E+00	1.00009E+00	4.59401E-12
20	80	3.58867E+01	1.00000E+00	1.58384E-01	1.00004E+00	1.00004E+00	6.00034E-12
21	90	1.07020E+01	1.00000E+00	4.61460E-02	1.00001E+00	1.00001E+00	7.59418E-12
22	100	-1.50137E+00	1.00000E+00	-8.06097E-03	9.99998E-01	9.99998E-01	9.37553E-12

BN = F1*(N1/N+) + F2 + F3*(NH/NE)
N1 = POPULATION OF GROUND STATE OF ION
N+ = POPULATION OF GROUND STATE OF NEXT IONISATION STAGE
NN = POPULATION OF PRINCIPAL QUANTUM SHELL N OF ION
BN = SAHA-BOLTZMANN FACTOR FOR PRINCIPAL QUANTUM SHELL N
EH = NEUTRAL HYDROGEN BEAM ENERGY
W = RADIATION DILUTION FACTOR
Z0 = NUCLEAR CHARGE
Z1 = ION CHARGE+1

NIP = 0 INTD = 3 IPRS = 1 ILOW = 1 IONIP = 1 NIONIP= 2 ILPRS = 1 IVDISP= 1
ZEFF = 4.0 TS = 1.00D+08 W = 0.00D+00 CION =1.0 CPY =1.0 W1 = 1.00D+08 ZIMP = 4.0

Table 3.10b.

```
    0 /SVREF=4.826E+00 /SPEC=   /DATE=08/07/96 /CODE=ADAS310
-------------------------------------------------------------------------------
    8   10 /TREF=5.000E+07
-------------------------------------------------------------------------------
 2.000E+04 3.000E+04 4.000E+04 5.000E+04 6.000E+04 7.000E+04 8.000E+04 1.000E+05
 1.000E+12 2.000E+12 5.000E+12 1.000E+13 2.000E+13 5.000E+13 1.000E+14 2.000E+14
 5.000E+14 1.000E+15
-------------------------------------------------------------------------------
 4.435E+00 4.435E+00 4.435E+00 4.435E+00 4.435E+00 4.435E+00 4.435E+00 4.435E+00
 4.454E+00 4.454E+00 4.454E+00 4.454E+00 4.454E+00 4.454E+00 4.454E+00 4.454E+00
 4.504E+00 4.504E+00 4.504E+00 4.504E+00 4.504E+00 4.504E+00 4.504E+00 4.504E+00
 4.566E+00 4.566E+00 4.566E+00 4.566E+00 4.566E+00 4.566E+00 4.566E+00 4.566E+00
 4.654E+00 4.654E+00 4.654E+00 4.654E+00 4.654E+00 4.654E+00 4.654E+00 4.654E+00
 4.826E+00 4.826E+00 4.826E+00 4.826E+00 4.826E+00 4.826E+00 4.826E+00 4.826E+00
 5.013E+00 5.013E+00 5.013E+00 5.013E+00 5.013E+00 5.013E+00 5.013E+00 5.013E+00
 5.271E+00 5.271E+00 5.271E+00 5.271E+00 5.271E+00 5.271E+00 5.271E+00 5.271E+00
 5.756E+00 5.756E+00 5.756E+00 5.756E+00 5.756E+00 5.756E+00 5.756E+00 5.756E+00
 6.282E+00 6.282E+00 6.282E+00 6.282E+00 6.282E+00 6.282E+00 6.282E+00 6.282E+00
-------------------------------------------------------------------------------
    9 /EREF=5.000E+04 /NREF=5.000E+13
-------------------------------------------------------------------------------
 1.000E+07 2.000E+07 3.000E+07 4.000E+07 5.000E+07 6.000E+07 7.000E+07 8.000E+07
 1.000E+08
-------------------------------------------------------------------------------
 1.116E+00 7.764E+00 6.286E+00 5.416E+00 4.826E+00 4.393E+00 4.058E+00 3.789E+00
 3.379E+00
-------------------------------------------------------------------------------
```

Notes:

ADAS312: Post-process population data for beam stopping and emission

In the generation of beam stopping coefficients and Balmer alpha beam emission coefficients using the code ADAS310, very complete calculations of the excited population structure of hydrogen are in fact performed. From these only the one piece of information, the stopping coefficient or Balmer alpha beam emission coefficient, is extracted and tabulated into the data formats *adf21* or *adf22*. The whole collection of information is actually available in formatted pages as a passing file *adas310.pass1* sent to the pass directory. ADAS312 is a new code, written by Harvey Anderson, which accesses data collections of the above passing file organisation and allows extraction of any hydrogen line spectral emissivity rather than just Balmer alpha. The extracted data is again returned as output in the *adf21/adf22* format. Such data consists of two dimensional arrays of coefficients in density and beam energy and then one dimensional scans in temperature and Zeff away from a set of reference conditions. We thought is would be helpful to display the surface plot of the extracted coefficient as function of density and beam energy as part of the routine. IDL of course handles such things easily, so Harvey has created a new pattern of graphical output widget for ADAS which does this. We hope to include more of this type of display in appropriate ADAS codes in the. Because of this development we have started to save the *adas310.pass1* files in a new data format, *adf26*. Also we use the mnemonic '*bdn*', standing for the 'bundle-n' population model, for such data.

Background theory:

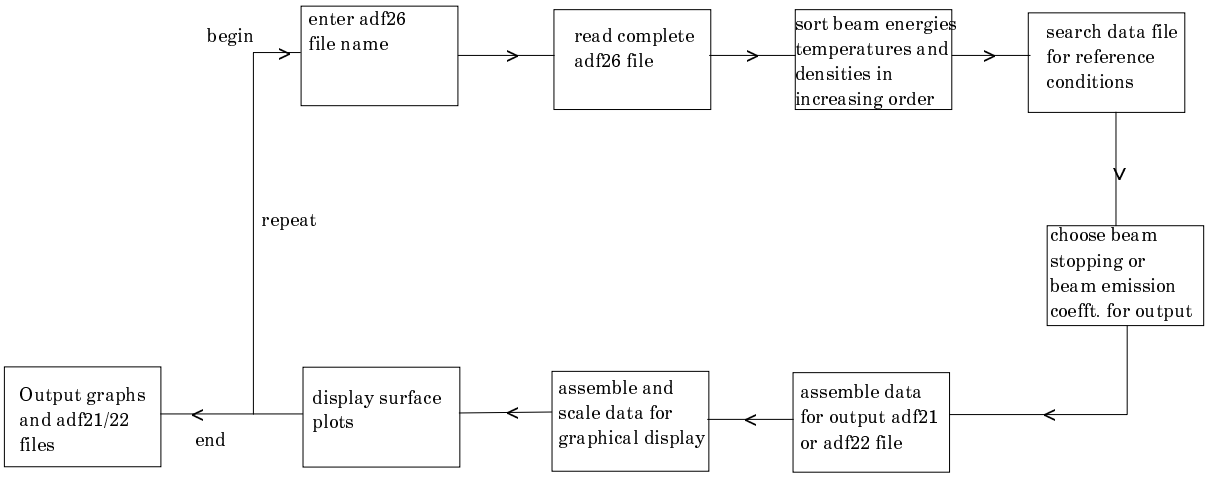
For hydrogen or hydrogenic ions in a plasma, the largest collision cross-sections are those for which n=n' and l=l'±1. For these cases the transition energy is nearly zero and the cross-

determines the effective charge for the single impurity and its number density.

Program steps:

These are summarised in the figure below.

Figure 3.12



Interactive parameter comments:

The program which makes use of data from archived ADAS data-sets initiates an interactive dialogue with the user in three parts, namely, input data file selection, entry of user data and disposition of output. The primary calculations may be conducted in foreground or background.

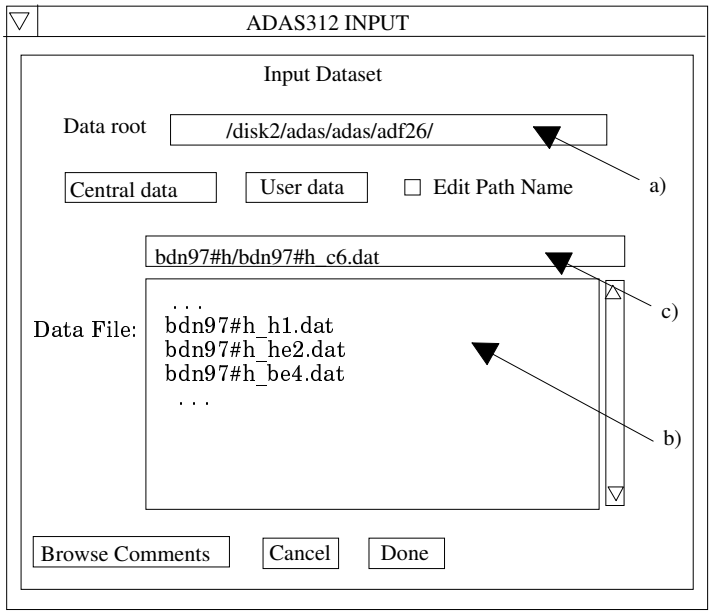
Move to the directory in which you wish the ADAS created files to appear. These include the output text file produced after executing any ADAS program (*paper.txt* is the default), and up

to four further output data files. There is no graphical output from this program Initiate ADAS312 from the program selection menus in the usual manner.

The **file selection window** has the appearance shown below

1. Data root a) shows the full pathway to the appropriate data sub directories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas,* to use this facility.

2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.



3. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.

4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual data-files are presented for selection. Data-files all have the termination *.dat*.

5. Once a data file is selected, the set of buttons at the bottom of the main window become active.

6. Clicking on the *Browse Comments* button displays any information stored with the selected data-file. It is important to use this facility to find out what is broadly available in the data-set. The possibility of browsing the comments appears in the subsequent main window also.

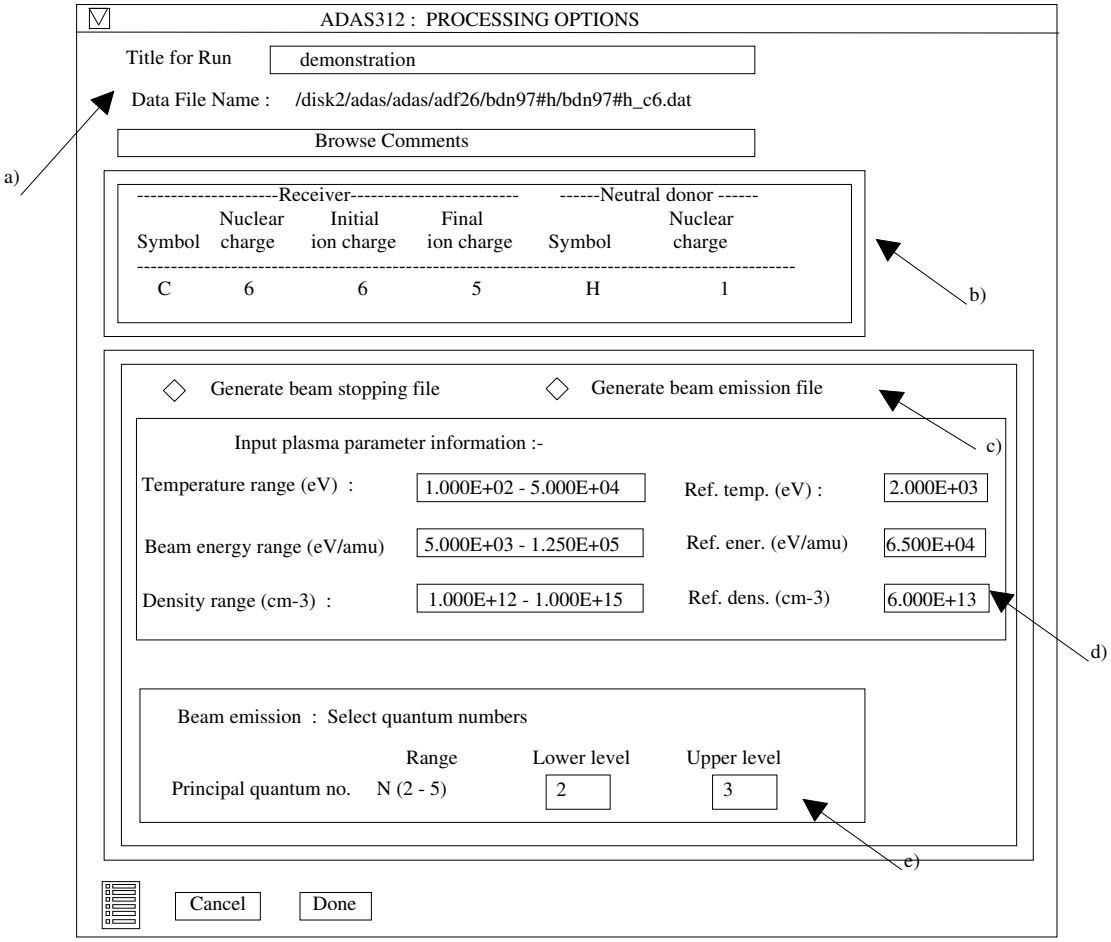
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window.

The **processing options window** has the appearance shown below.

8. An arbitrary title may be given for the case being processed. For information the full pathway to the data-set being analysed is also shown at a). The button *Browse comments* again allows display of the information field section at the foot of the selected data-set, if it exists.

9. At b) some additional information on the beam donor species and the impurity in the plasma which is the receiver in charge exchange reactions. These data are extracted

from the data set name. Note that a bundle-n population data set of type *adf26* being analysed is for a single plasma impurity.



10. The code scans the very extensive tabulations in the data set and extracts selected data from them according to the type of output file required by the user. The choices available at this time are beam stopping coefficients and beam emission coefficients. Select the output you wish to be generated at c). The *adf26* data sets in fact contain a large variety of other population information which may be provided at a later stage. With *Generate beam emission file* selected, additional information must be entered at e).

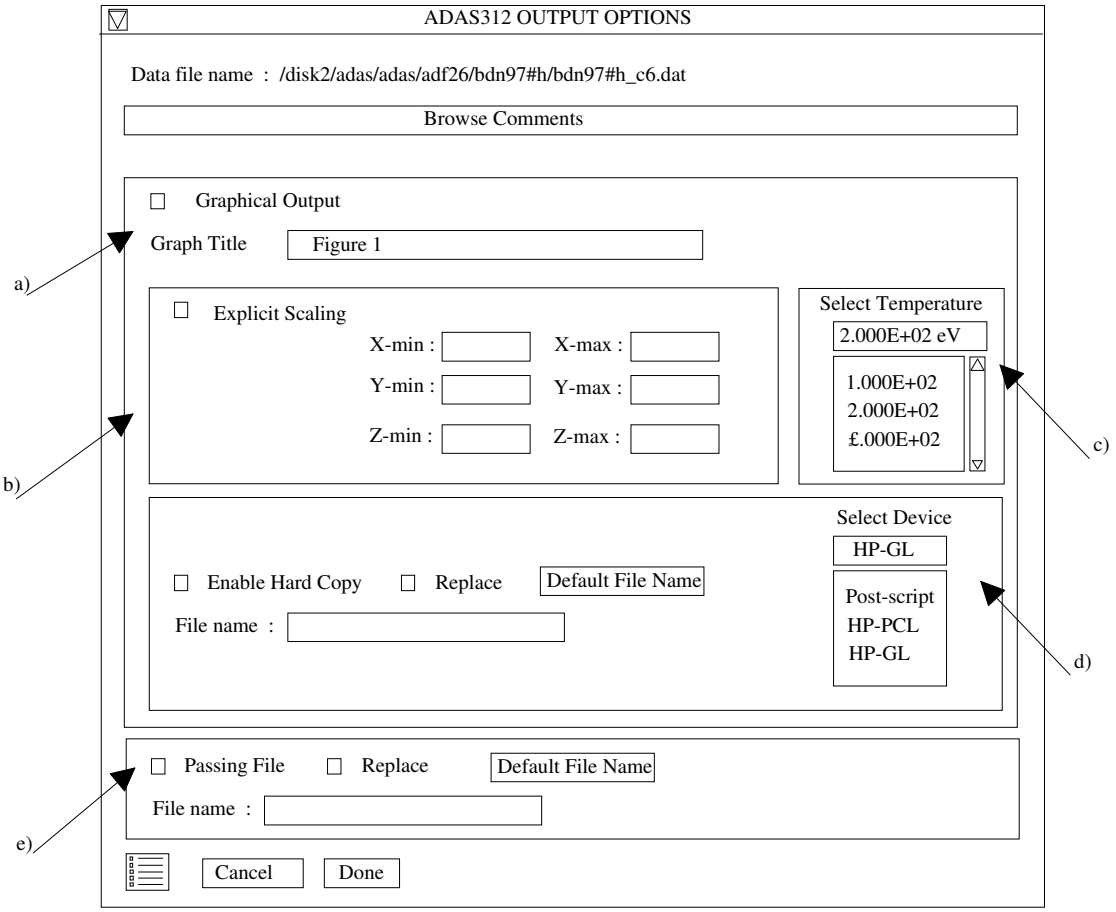
11. Additional information on the plasma temperature, beam energy and plasma density ranges used in the creation of the adf26 data set is given at d) together with the reference conditions used. Note that the adf26 data set contains two-dimensional arrays of beam energy and ion density data and a one dimensional array in ion temperature from a reference condition.

12. The sub-window at e) becomes active if generation of beam emission data is requested. The choices available are the upper and lower principal quantum numbers of the radiative transition of the hydrogen beam species. The range of choice has been restricted to principal quantum numbers less than or equal to five. The adf26 data set contains results for much higher quantum shells also, so we can extended the available range in the future is desired.

13. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 3 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

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

14. As in the previous window, the full pathway to the file being analysed is shown for information at a). Also the *Browse comments* button is available.



15. Graphical display is activated by the *Graphical Output* button a). This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.

16. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button at b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable. In this case, a three-dimensional surface plot is presented with x-axis: beam energy, y-axis: density, z-axis: selected coefficient.

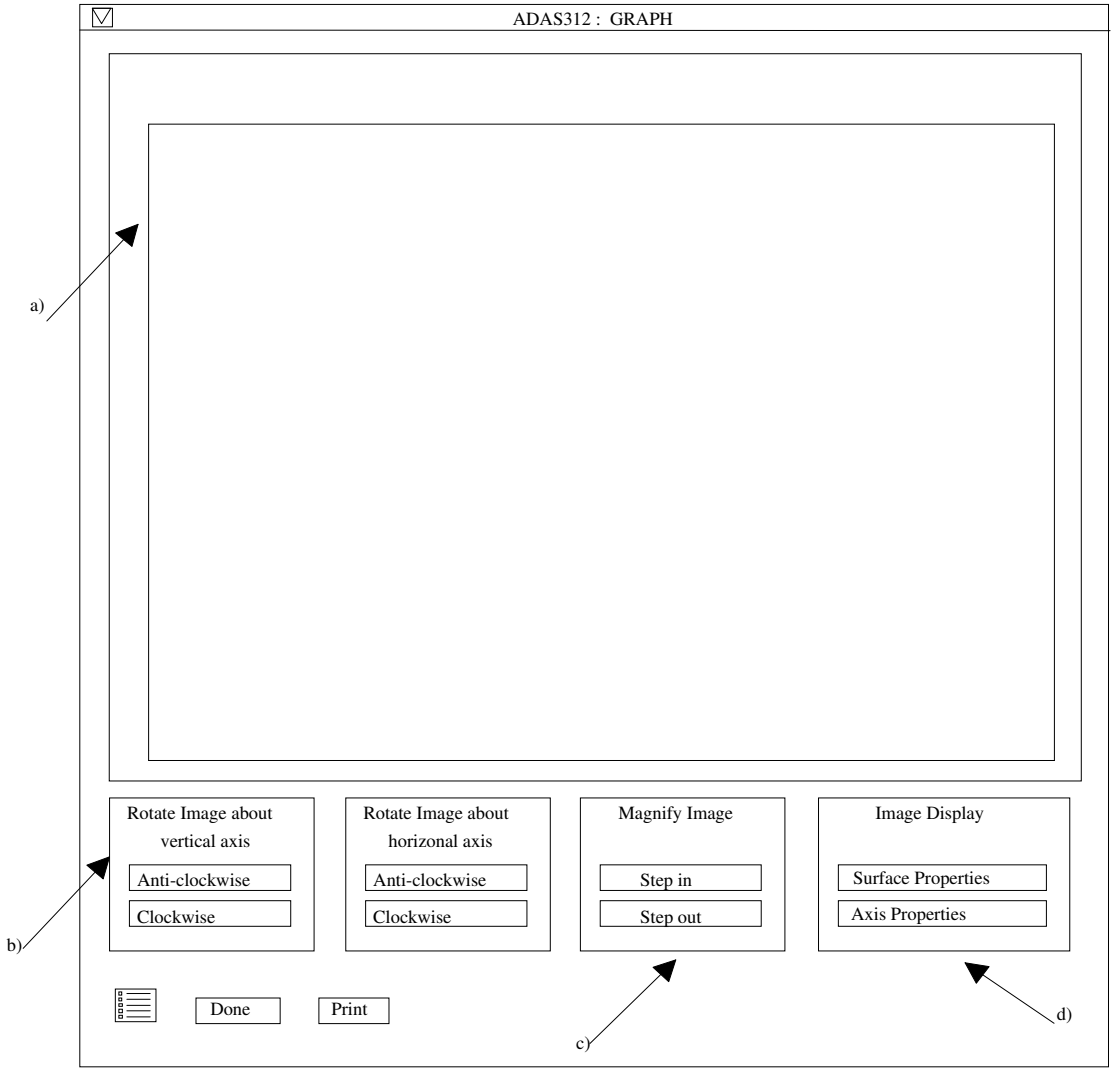
17. The surface plot is produced at a selected plasma ion temperature. Make this choice at c).

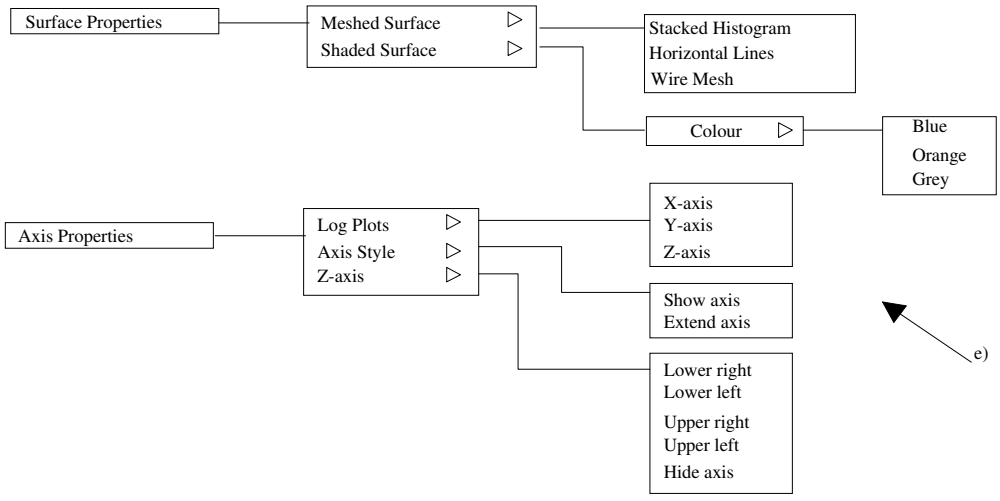
18. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exists and the *Replace* button has not been activated, a 'pop-up' window issues a warning.

19. A choice of output graph plotting devices is given in the Device list window at d). Clicking on the required device selects it. It appears in the selection window above the Device list window.

20. At e) output of the *Passing File* of results is enabled. This is of *adf21* or *adf22* format according to earlier choices.. The *passing* is written on exiting ADAS312 and is placed by default in your */pass* directory as *adas312.pass*. It is fully structured for reassignment into your personal ADAS data base of the appropriate data format.

The **graphical output window** appearance is shown below





21. This is a new style of graphical output widget to ADAS. A three-dimensional surface plot is given at a). There is much more control over it than in our usual graph displays.

22. At b), there are the controls for the orientation of the figure. By clicking repeatedly on a button, the figure may be rotated clockwise or anti-clockwise is small steps. You may rotate about a vertical or horizontal axis.

23. At c), there are two buttons to zoom in or out on the figure.

24. At d), the controls on the appearance of the figure are available. Note the nesting of menu buttons in more than one layer. The choices are laid out at e) below the main figure. Thus one may choose a meshed surface or shaded surface, the colour of the shaded surface may be selected and so on. You may feel we have gone to overkill here.

25. Then there are choices on the axes, whether they are linear or logarithmic, whether they are to be displayed or not etc. There is an additional point. At b) when the figure is rotated the position of the axis of rotation matters. For rotations about a vertical axis, the figure Z-axis is used and it may be moved to any corner of the projected area on the X/Z plane.

26. Finally note that when the figure is printed, it is the figure as displayed in the graphic output window which you get.

27. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 3 menu. Remember that *Done* takes you back to the previous screen. The *Print* button appears if graphical hard-copy is selected on the output options window.

Illustration:

Table 3.12a.

EFFECTIVE CONTRIBUTION TABLE FOR ION PRINCIPAL QUANTUM SHELL POPULATIONS IN THERMAL PLASMA

HYDROGEN Z0 = 1.00E+00 Z1 = 1.00E+00

TRAD = 1.00E+08 K TE = 5.80E+07 K TP = 5.80E+07 K
W = 0.00E+00 NE = 1.00E+12 CM-3 NP = 0.00E+00 CM-3

EH = 5.00E+03 EV/AMU NH = 1.00E+06 CM-3 NH/NE = 1.00E-06 FLUX = 9.78E+13 CM-2 SEC-1

CHARGE EXCHANGE OFF: N1/N+ = 3.96967E-10 RECOMB COEFF = 3.98614E-17 CM+3 SEC-1 IONIZ COEFF = 1.00415E-07 CM+3 SEC-1

CHARGE EXCHANGE ON : N1/N+ = 1.01033E-06 RECOMB COEFF = 1.01452E-13 CM+3 SEC-1 IONIZ COEFF = 1.00415E-07 CM+3 SEC-1

I	N	F1	F2	F3	B(CHECK)	B(ACTUAL)	NN/(BN*N+)
1	1	0.00000E+00	4.22257E+05	1.07427E+15	1.07472E+09	1.07472E+09	9.40109E-16
2	2	9.03269E+09	3.77642E+00	1.90419E+09	1.10339E+04	1.10339E+04	3.75276E-15
3	3	3.27110E+09	2.50566E+00	3.72697E+08	3.68009E+03	3.68009E+03	8.44053E-15
4	4	1.38276E+09	1.72873E+00	8.89060E+07	1.48767E+03	1.48767E+03	1.50034E-14
5	5	4.65572E+08	1.25911E+00	1.96737E+07	4.91313E+02	4.91313E+02	2.34414E-14
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15	30	1.10830E+04	1.00001E+00	5.29440E+01	1.01126E+00	1.01126E+00	8.43800E-13
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18	60	2.38809E+02	1.00000E+00	1.07145E+00	1.00024E+00	1.00024E+00	3.37519E-12
19	70	9.29529E+01	1.00000E+00	4.13889E-01	1.00009E+00	1.00009E+00	4.59401E-12
20	80	3.58867E+01	1.00000E+00	1.58384E-01	1.00004E+00	1.00004E+00	6.00034E-12
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NIP = 0 INTD = 3 IPRS = 1 ILOW = 1 IONIP = 1 NIONIP= 2 ILPRS = 1 IVDISP= 1
ZEFF = 4.0 TS = 1.00D+08 W = 0.00D+00 CION =1.0 CPY =1.0 W1 = 1.00D+08 ZIMP = 4.0

Table 3.10b.

```
    0 /SVREF=4.826E+00 /SPEC=   /DATE=08/07/96 /CODE=ADAS310
-------------------------------------------------------------------------------
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-------------------------------------------------------------------------------
 2.000E+04 3.000E+04 4.000E+04 5.000E+04 6.000E+04 7.000E+04 8.000E+04 1.000E+05
 1.000E+12 2.000E+12 5.000E+12 1.000E+13 2.000E+13 5.000E+13 1.000E+14 2.000E+14
 5.000E+14 1.000E+15
-------------------------------------------------------------------------------
 4.435E+00 4.435E+00 4.435E+00 4.435E+00 4.435E+00 4.435E+00 4.435E+00 4.435E+00
 4.454E+00 4.454E+00 4.454E+00 4.454E+00 4.454E+00 4.454E+00 4.454E+00 4.454E+00
 4.504E+00 4.504E+00 4.504E+00 4.504E+00 4.504E+00 4.504E+00 4.504E+00 4.504E+00
 4.566E+00 4.566E+00 4.566E+00 4.566E+00 4.566E+00 4.566E+00 4.566E+00 4.566E+00
 4.654E+00 4.654E+00 4.654E+00 4.654E+00 4.654E+00 4.654E+00 4.654E+00 4.654E+00
 4.826E+00 4.826E+00 4.826E+00 4.826E+00 4.826E+00 4.826E+00 4.826E+00 4.826E+00
 5.013E+00 5.013E+00 5.013E+00 5.013E+00 5.013E+00 5.013E+00 5.013E+00 5.013E+00
 5.271E+00 5.271E+00 5.271E+00 5.271E+00 5.271E+00 5.271E+00 5.271E+00 5.271E+00
 5.756E+00 5.756E+00 5.756E+00 5.756E+00 5.756E+00 5.756E+00 5.756E+00 5.756E+00
 6.282E+00 6.282E+00 6.282E+00 6.282E+00 6.282E+00 6.282E+00 6.282E+00 6.282E+00
-------------------------------------------------------------------------------
    9 /EREF=5.000E+04 /NREF=5.000E+13
-------------------------------------------------------------------------------
 1.000E+07 2.000E+07 3.000E+07 4.000E+07 5.000E+07 6.000E+07 7.000E+07 8.000E+07
 1.000E+08
-------------------------------------------------------------------------------
 1.116E+00 7.764E+00 6.286E+00 5.416E+00 4.826E+00 4.393E+00 4.058E+00 3.789E+00
 3.379E+00
-------------------------------------------------------------------------------
```

Notes: