

ADAS208: Specific z excitation - advanced population processing

The program allows calculation of excited state populations of ions in a plasma of specified temperatures and densities by drawing on fundamental energy level and rate coefficient data from a specific ion file. It extends ADAS205 by inclusion of metastable parents, the condensed influence of very highly excited level populations and inner shell ionisation forming excited states. It allows consistent inclusion of three-body recombination and selective improvement of metastable ionisation rates. Datafiles of derived generalised collisional-radiative coefficients may be generated.

Background theory:

Consider ions X^{+z} of the element X . The adjacent ionisation stages are X^{+z+1} and X^{+z-1} . Let the levels of the ion X^{+z} be separated into the *metastable levels* X_ρ^{+z} , indexed by Greek indices, and *excited levels* X_i^{+z} , indexed by Roman indices. The collective name metastable states as used here includes the ground state. The 'initiating' driving mechanisms considered for populating the excited levels X_i^{+z} are excitation from the metastable levels X_ρ^{+z} , recombination from the metastable levels of the adjacent ion X_τ^{+z+1} , and ionisation from the metastable levels of the adjacent ion X_μ^{+z-1} . Collisional and radiative processes between all levels then redistribute populations. The dominant population densities of the ions in the plasma are those of the levels X_ρ^{+z} , X_τ^{+z+1} and X_μ^{+z-1} , denoted by N_ρ , N_τ^+ and N_μ^- respectively. They, or at least their ratios to N_1 are assumed known from a dynamical ionisation balance. The other dominant population densities in the plasma are the electron density N_e , the proton density N_p and the neutral hydrogen density N_H . The excited populations, denoted by N_i , are assumed to be in a *quasi-static equilibrium* with respect to the dominant populations. The program evaluates the dependence of the excited populations on the dominant populations with this assumption.

Let M denote the number of metastable levels, and O denote the number of excited levels, hereafter called *ordinary* levels of the ion X^{+z} . The ordinary levels are those identified explicitly in the specific ion file. Collectively, the metastable levels and ordinary levels of X^{+z} constitute the *low level group*. The low level group is assumed to comprise all those levels belonging to a set of principal quantum shells n : $n_0 \leq n \leq n_1$. In addition, there are the *high levels*, extending up to the metastable continua of X^{+z+1} , that is with \bar{n} : $n_1 < \bar{n} < \infty$ which must be included in a complete treatment. The latter may to a reasonable approximation be grouped into n-shell populations and associated with a particular parent (metastable of the X^{+z+1}) and spin system. The grouped populations are called *bundle-nS* populations. The statistical balance equations for a specified parent, τ , and spin system, S , take the form.

$$\begin{bmatrix} -C_{mS, m'S} & -C_{mS, \bar{m}'S} & N_e r_{mS, v'} \\ -C_{\bar{m}S, m'S} & -C_{\bar{m}S, \bar{m}'S} & N_e r_{\bar{m}S, v'} \\ N_e S_{v, m'S} & N_e S_{v, \bar{m}'S} & -C_{v, v'} \end{bmatrix} \begin{bmatrix} N_{m'S} \\ N_{\bar{m}'S} \\ N_{v'}^+ \end{bmatrix} = \begin{bmatrix} \frac{d}{dt} N_{mS} \\ 0 \\ \frac{d}{dt} N_v^+ \end{bmatrix} \quad 3.8.1$$

For conciseness, charge exchange recombination parts have been omitted. They add to the free electron recombination parts but are driven by N_H rather than N_e . The indices v, v' denote metastable levels of X^{+z+1} to which the specific parent τ also belongs. The high n-shell populations \bar{n} are assumed in quasi-static equilibrium with the low n-shell populations n and the adjacent stage metastables (parents). The high n-shell populations may be *condensed* onto the low n-shell populations n to give

$$\begin{bmatrix} -\overline{C}_{nS, n'S} & N_e \overline{r}_{nS, v'} \\ N_e \overline{S}_{v, n'S} & -\overline{C}_{v, v'} \end{bmatrix} \begin{bmatrix} N_{n'S} \\ N_{v'}^+ \end{bmatrix} = \begin{bmatrix} \frac{d}{dt} N_{nS} \\ \frac{d}{dt} N_{v'}^+ \end{bmatrix} \quad 3.8.2$$

On the other hand the population equations of the low level partition take the form

$$\begin{bmatrix} \cdot & \cdot & 0 & 0 \\ N_e S_{\rho, \mu'} & -C_{\rho, \sigma} & -C_{\rho, j} & N_e r_{\rho, v'} \\ N_e S_{i, \mu'} & -C_{i, \sigma} & -C_{i, j} & N_e r_{i, v'} \\ 0 & N_e S_{v, \sigma} & N_e S_{v, j} & -C_{v, v'} \end{bmatrix} \begin{bmatrix} N_{\mu'}^- \\ N_{\sigma} \\ N_j \\ N_{v'}^+ \end{bmatrix} = \begin{bmatrix} \frac{d}{dt} N_{\mu}^- \\ \frac{d}{dt} N_{\rho} \\ 0 \\ \frac{d}{dt} N_{v'}^+ \end{bmatrix} \quad 3.8.3$$

where the contributions from inner shell ionisation have been included. These two sets of equations are complementary. The first set includes all the population influences occurring via high levels but in the simplified bundle-nS picture. The second includes all the direct influences of low level populations on each other in detail but excludes those via the very high levels. The direct couplings between the n shells in equation. 3.8.2 may be subtracted to leave only the indirect couplings, denoted by

$$\begin{bmatrix} \overline{\overline{C}}_{nS, n'S} & \overline{\overline{N_e r}}_{nS, v'} \\ \overline{\overline{N_e S}}_{v, n'S} & \overline{\overline{C}}_{v, v'} \end{bmatrix} \quad 3.8.4$$

The barred indirect matrices may be expanded over the low level manifold using level weighting factors as

$$\begin{aligned} \overline{\overline{C}}_{nS, n'S} &\rightarrow \begin{bmatrix} C_{\rho, \sigma}^{indir} & C_{\rho, j}^{indir} \\ C_{i, \sigma}^{indir} & C_{i, j}^{indir} \end{bmatrix} \\ \overline{\overline{S}}_{v, n'S} &\rightarrow \begin{bmatrix} S_{v, \sigma}^{indir} & S_{v, j}^{indir} \end{bmatrix} \\ \overline{\overline{r}}_{nS, v'} &\rightarrow \begin{bmatrix} r_{\rho, v'}^{indir} \\ r_{i, v}^{indir} \end{bmatrix} \end{aligned} \quad 3.8.5$$

and then added to equations. 3.8.3 to give

$$\begin{bmatrix} \cdot & \cdot & 0 & 0 \\ N_e \mathcal{S}_{\rho, \mu'} & -\mathcal{C}_{\rho, \sigma} & -\mathcal{C}_{\rho, j} & N_e \mathcal{R}_{\rho, v'} \\ N_e \mathcal{S}_{i, \mu'} & -\mathcal{C}_{i, \sigma} & -\mathcal{C}_{i, j} & N_e \mathcal{R}_{i, v'} \\ 0 & N_e \mathcal{S}_{v, \sigma} & N_e \mathcal{S}_{v, j} & -\mathcal{C}_{v, v'} \end{bmatrix} \begin{bmatrix} N_{\mu'}^- \\ N_{\sigma} \\ N_j \\ N_{v'}^+ \end{bmatrix} = \begin{bmatrix} \frac{d}{dt} N_{\mu}^- \\ \frac{d}{dt} N_{\rho} \\ 0 \\ \frac{d}{dt} N_{v'}^+ \end{bmatrix} \quad 3.8.6$$

where $\mathcal{C} \equiv C + C^{indir}$, $\mathcal{R} \equiv r + r^{indir}$, $\mathcal{S} \equiv S + S^{indir}$ and $\mathcal{C}_{vv'} \equiv C_{vv'} + \overline{\overline{C}}_{vv'}$. These equations constitute the extension to the simpler low level population equations. The solution for the ordinary populations is then

$$\begin{aligned} N_j &= -\sum_{i=1}^O \mathcal{C}_{ji}^{-1} \sum_{\sigma=1}^M \mathcal{C}_{i\sigma} N_{\sigma} + \sum_{v'} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{R}_{iv'} N_e N_{v'}^+ \\ &\quad + \sum_{v'} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{Q}_{iv'}^{(CX)} N_H N_{v'}^+ + \sum_{v'} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{P}_{i\mu'}^{(ion)} N_e N_{\mu'}^- \\ &\equiv \sum_{\sigma=1}^M \mathcal{F}_{j\sigma}^{(exc)} N_e N_{\sigma} + \sum_{v'} \mathcal{F}_{jv'}^{(rec)} N_e N_{v'}^+ + \sum_{v'} \mathcal{F}_{jv'}^{(CX)} N_H N_{v'}^+ \\ &\quad + \sum_{v'} \mathcal{F}_{j\mu'}^{(ion)} N_e N_{\mu'}^- \end{aligned} \quad 3.8.7$$

where an additional term has been added arising from charge exchange recombination. The $\mathcal{F}_{j\sigma}^{(exc)}$, $\mathcal{F}_{jv'}^{(rec)}$, $\mathcal{F}_{jv'}^{(CX)}$ and $\mathcal{F}_{j\mu'}^{(ion)}$ are the effective contributions to the excited populations from excitation from the metastables, from free electron capture by parent metastables, from charge exchange recombination from neutral hydrogen by parent metastables and from ionisation respectively. All these coefficients depend on density as well as temperature. The actual population density of an ordinary level may be obtained from them when the dominant population densities are known.

The full statistical equilibrium of the metastable level populations of the ion X^{+z} may also be obtained by setting $\frac{d}{dt} N_\rho = 0$ in equation 3.8.6

$$\begin{aligned} \sum_{\sigma=1}^M \mathcal{C}_{\rho\sigma} N_\sigma = & - \sum_{j=1}^O \mathcal{C}_{\rho j} N_j + \sum_{v'} \mathcal{R}_{\rho v'} N_e N_{v'}^+ \\ & + \sum_{v'} \mathcal{Q}_{\rho v'}^{(CX)} N_H N_{v'}^+ + \sum_{\mu'} \mathcal{S}_{\rho\mu'}^{(ion)} N_e N_{\mu'}^- \end{aligned} \quad 3.8.8$$

Eliminating the ordinary level populations from the quasi-equilibrium solution of equation 3.8.7 in the matrix equations 3.8.6 gives

$$\begin{bmatrix} \frac{d}{dt} N_\mu^- \\ \frac{d}{dt} N_\rho \\ \frac{d}{dt} N_v^+ \end{bmatrix} = \begin{bmatrix} -\mathcal{C}_{\mu\mu'} & \dots & 0 \\ N_e (\mathcal{S}_{\rho\mu'} - \sum_{j=1}^O \mathcal{C}_{\rho j} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{S}_{i\mu'}) & -(\mathcal{C}_{\rho\sigma} - \sum_{j=1}^O \mathcal{C}_{\rho j} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{C}_{i\sigma}) & N_e (\mathcal{R}_{\rho v'} + \sum_{j=1}^O \mathcal{C}_{\rho j} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{R}_{iv'}) \\ 0 & N_e (\mathcal{S}_{v\sigma} - \sum_{j=1}^O \mathcal{S}_{vj} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{C}_{i\sigma}) & + N_H (\mathcal{Q}_{\rho v'} + \sum_{j=1}^O \mathcal{C}_{\rho j} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{Q}_{iv'}) \end{bmatrix} \begin{bmatrix} N_{\mu'}^- \\ N_\sigma \\ N_{v'}^+ \end{bmatrix} \quad 3.8.9$$

The partitioned matrix elements are the generalised collisional radiative coefficients. These are the ionisation coefficients

$$S_{CD,\sigma \rightarrow v} = (\mathcal{S}_{v\sigma} - \sum_{j=1}^O \mathcal{S}_{vj} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{C}_{i\sigma}) \quad 3.8.10$$

the free electron recombination coefficients

$$\alpha_{CD,v' \rightarrow \rho} = (\mathcal{R}_{\rho v'} + \sum_{j=1}^O \mathcal{C}_{\rho j} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{R}_{iv'}) \quad 3.8.11$$

the charge exchange recombination coefficients

$$C_{CD,v' \rightarrow \rho} = (\mathcal{Q}_{\rho v'} + \sum_{j=1}^O \mathcal{C}_{\rho j} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{Q}_{iv'}) \quad 3.8.12$$

the metastable cross-coupling coefficients

$$X_{CD,\sigma \rightarrow \rho} = (\mathcal{C}_{\rho\sigma} - \sum_{j=1}^O \mathcal{C}_{\rho j} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{C}_{i\sigma}) / N_e \quad 3.8.13$$

and the parent metastable cross-coupling coefficients

$$Q_{CD,v' \rightarrow v} = \sum_{j=1}^O \mathcal{I}_{vj} \sum_{i=1}^O \mathcal{C}_{ji}^{-1} \mathcal{R}_{iv'} \quad 3.8.14$$

Note the latter coefficients distinguish the parts occurring via recombination from conventional metastable cross-coupling as they are determined in the course of the population structure calculation for the z-times ionised ion. The radiated power loss coefficients are obtained by summing over the population structure. ADAS208 provides an improved estimate of the total excitation line power coefficient as

$$P_{LT,\sigma} = \sum_{k,j} \Delta E_{kj} A_{j \rightarrow k} \mathcal{F}_{j\sigma}^{(exc)} \quad 3.8.15$$

The free electron recombination cascade bremsstrahlung power coefficients $P_{RB,\vartheta}$, and the charge exchange power coefficients $P_{RC,\vartheta}$, are not improved by ADAS208 over those generated by ADAS204.

There are two kinds of derived coefficients associated with individual spectrum line emission in common use in fusion plasma diagnosis. These are *photon emissivity coefficients* (\mathcal{PEC}) and S / XB ratios (\mathcal{SXB}). The reciprocals of the latter are also known as *photon efficiencies*. From equations 3.8.7, the emissivity in the spectrum line $j \rightarrow k$ is

$$\begin{aligned} \varepsilon_{j \rightarrow k} = A_{j \rightarrow k} & \left(\sum_{\sigma=1}^M \mathcal{F}_{j\sigma}^{(exc)} N_e N_{\sigma} + \sum_{v'=1}^{M_{z+1}} \mathcal{F}_{jv'}^{(rec)} N_e N_{v'}^+ + \right. \\ & \left. \sum_{v'=1}^{M_{z+1}} \mathcal{F}_{jv'}^{(CX)} N_H N_{v'}^+ + \sum_{\mu'=1}^{M_{z-1}} \mathcal{F}_{j\mu'}^{(ion)} N_e N_{\mu'}^- \right) \end{aligned} \quad 3.8.16$$

This allows specification of the *excitation* photon emissivity coefficient

$$\mathcal{PEC}_{\sigma,j \rightarrow k}^{(exc)} = A_{j \rightarrow k} \mathcal{F}_{j\sigma}^{(exc)} \quad 3.8.17$$

the *recombination* photon emissivity coefficient

$$\mathcal{PEC}_{v',j \rightarrow k}^{(rec)} = A_{j \rightarrow k} \mathcal{F}_{jv'}^{(rec)} \quad 3.8.18$$

the *charge exchange* photon emissivity coefficient

$$\mathcal{PEC}_{v',j \rightarrow k}^{(CX)} = A_{j \rightarrow k} \mathcal{F}_{jv'}^{(CX)} \quad 3.8.19$$

and the *ionisation* photon emissivity coefficient

$$\mathcal{PEC}_{\mu',j \rightarrow k}^{(ion)} = A_{j \rightarrow k} \mathcal{F}_{j\mu'}^{(ion)} \quad 3.8.20$$

The S / XB are only meaningful for the excitation part of the emissivity and are

$$\mathcal{SXB}_{\sigma,j \rightarrow k} = \sum_{v=1}^{M_{z+1}} S_{CD,\sigma \rightarrow v} / (A_{j \rightarrow k} \mathcal{F}_{j\sigma}^{(exc)}) \quad 3.8.21$$

Each of these coefficients is associated with a particular metastable σ , v' or μ' of the X^{+z} , X^{+z+1} or X^{+z-1} ions respectively.

Source data :

The program operates on collections of fundamental rate coefficient data called specific ion files. The allowed content, organisation and formatting of these files is specified in ADAS data format ADF04. The scope of operation of ADAS208 is determined by the content of the specific ion file processed. The minimum content is the ion identification, ion, effective ion and nuclear charges, ionisation potential, an indexed energy level and level assignment list, a set of temperatures and a set of level to level spontaneous transition probabilities and electron impact Maxwell averaged rate parameters at the specified temperatures. Data for upper to lower level only is required. Electron impact rate coefficients for both excitation and deexcitation are evaluated by interpolation at user selected values from the tabulated rate

parameters in the specific ion file. Transition rate data is not required for all possible upper/lower level pairs, but the code checks that there are no 'untied' levels, that is without populating or depopulating processes. Strict energy ordering is not required in the specific ion file, the code reorders as necessary. More complex data including proton induced rates and metastable resolved free electron recombination rates, charge exchange recombination rates and inner shell ionisation rates may be present in the specific ion file. These may only be activated in the code if such data is present in the specific ion file. Transition data of these types are identified by a single letter code in the transition data line in the specific ion file. ADAS208 is specifically designed to exploit the more complex data. The code sorts the transition lines in the specific ion file into the allowed categories.

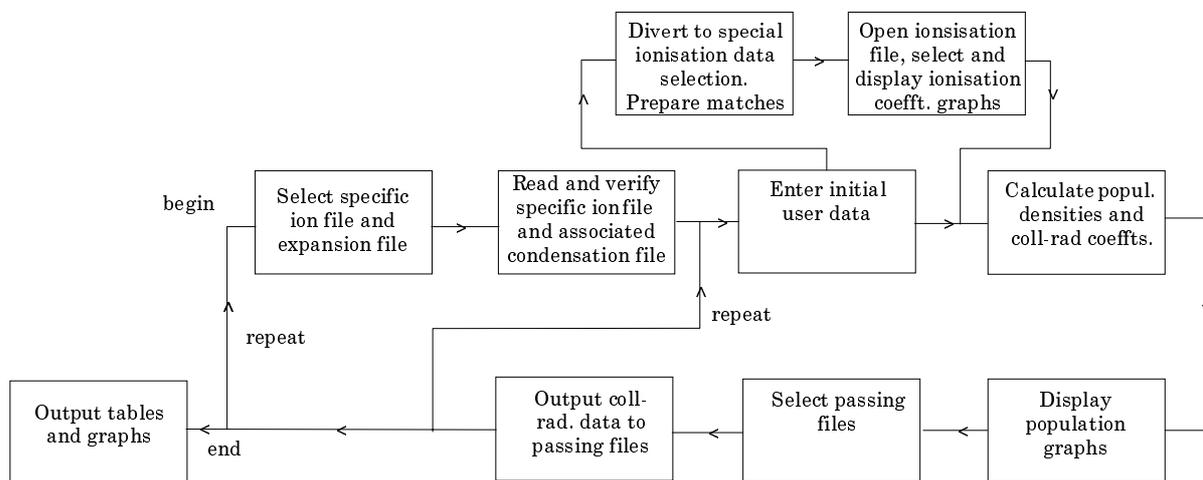
Condensation matrices from the bundle-nS calculations of ADAS204 may be used by ADAS208. These data are organised according to ADAS data format ADF17. Access to these data sets is by an *expansion definition file* of type ADF18. Such files are specific to an ion and associated with a particular specific ion file for that ion.

Zero density metastable resolved ionisation rate coefficient data may also be accessed by ADAS208. These data are organised by element according to ADAS data format ADF07.

Program steps:

These are summarised in figure 3.8.

Figure 3.8



Interactive parameter comments:

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

1. Data root a) shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. The appropriate ADAS data format for input to this program is ADF04 ('specific ion files'). 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 datafiles are presented for selection. Datafiles 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 datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. A second file selection is given. This is the choice of expansion file of type ADF18 (subdirectory */a17_p208*) which cross-references projection matrices (ADF17) into the specific ion file under examination. The expansion file must be consistent with the specific ion file with which it is linked and in fact contains the specific ion file name.
8. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

ADAS208 INPUT

Input COPASE Dataset

Data root a)

Edit Path Name

Data File:

- ...
- hps94cr.dat
- hps95cr.dat
- ...

b)

Input EXPANSION File

Data root d)

Edit Path Name

e)

Data File:

- DUMMY
- a09_a04
- a09_p204
- a17_p208 . . .
- bndlen_exp#h0.dat

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

9. There are three 'pop-up' windows for setting temperatures, densities and for designating metastable levels. For the temperature window a), click on the *Edit Table* button to open up the table editor. The editing operations are as described in the introductory chapter. Note that there is a set of input electron temperatures from the selected file. These indicate the safe range of temperatures if extrapolation is to be avoided. Note that altering units (which must be done with the table edit window activated) converts the input values and interprets the output values in the selected units. It **does not convert** output values already typed in. *Default Temperatures* are inserted in the selected units on clicking the appropriate button. Note that the ion and neutral hydrogen temperatures are **only used if** such collisional data is present in the input ADF04 file.
10. There are three choices of densities tables. Click the choice to enter the table in the display window. Thereafter it is handled in like manner to the temperature table. Note that in this case there are no input density values. Thus unit changing only affects the interpretation of the output values created by the user. The N_H/N_e , etc.) **are only used if** the corresponding data are present in input ADF04 file. These vectors are specified at each electron density so the vectors and electron density vector are of the same

length. That is a model is specified. By contrast the output electron temperatures are independent so that final calculated populations are obtained at points of a two-dimensional electron temperature/electron density grid.

11. The Metastable State *Selections* button c) pops up a window indexing all the energy levels. Activate the buttons opposite levels which you wish treated as metastables.
12. Various processes, supplementary to the primary electron excitation collisions and bound-bound radiative transitions, are activated as desired by clicking on the appropriate buttons e). Note again these only have an effect if such data is present in the ADF04 file except for *Ionisation rates*. This activates ionisation out of excited states and is obtained by an internal calculation of these rates in the ECIP approximation. **Warning**-ionisation should **not** be switched on if you have included autoionising levels in your ADF04 dataset but have omitted the details of alternative thresholds etc present in advanced ADF04 files.

ADAS208 PROCESSING OPTIONS

Title for Run: Nuclear Charge: 24 Ion Charge: 0

Data File Name: /disk2/adas/adas/adf04/crlike/hps95cr.dat b)

a) **Temperatures**

Index	Electron	Ion	Neutral Hydrogen	Input Value
1	1.000E+00	1.000E+00	1.000E+00	9.995E-01
2
3
4

Temperature Units: eV

b) **Densities**

Input densities: NE & NH N(z-1) N(z+1)

Index	Electron Densities	Ion Densities	NH/NE Ratio
1	1.000E+11	0.0	0.0
2
3
4

Density Units: cm-3

Metastable States

a6S)4s(a7S) (7)S(3.0)

a6S)4s(a5S) (5)S(2.0)

c)

Reaction Selection

Proton Impact Collisions d)

Scale Proton Impact for Zeff

Enter Z-effective for Collisions:

Ionisation Rates

Neutral H Charge Exchange e)

Free Electron Recombination

Inner shell ionisation

Include projection data

Single metastable: normalise power and PEC to total stage pop. Ionisation Coefficient Search

Limits for PEC and SXB files: Lower limit of A-values (sec-1): f)

Short wavelength limit (A): Long wavelength limit (A):

Edit the processing options data and press Done to proceed h)

14. Proton collisions may be present in the ADF04 file. If so, these rate coefficients may be scaled to represent a mixture of other charged projectiles with a mean Z-effective d).

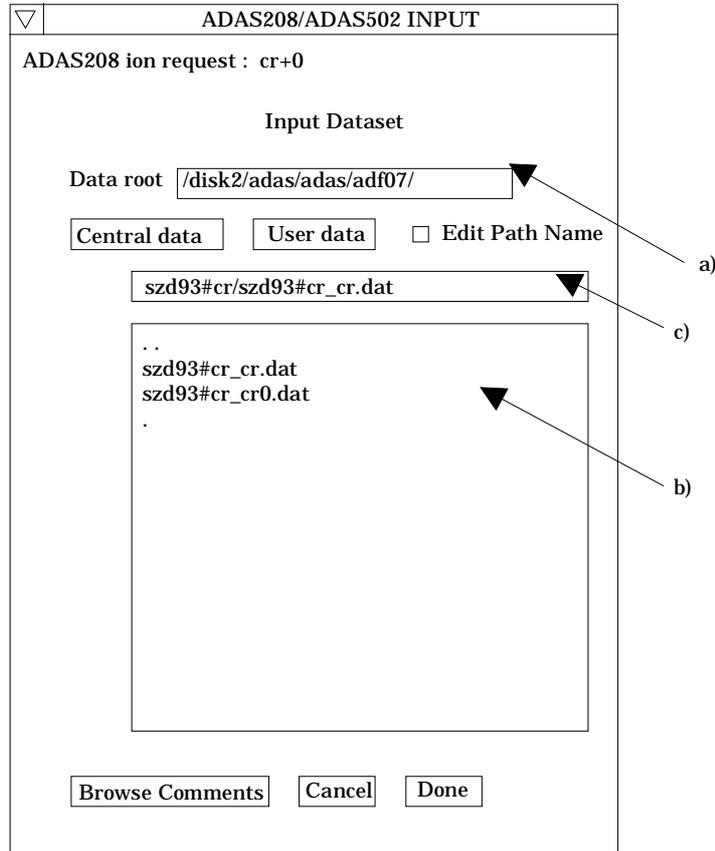
15. The *Ionisation coefficient search* button activates a new process equivalent to ADAS502 and is described further below.

16. The code prepares photon emissivity and radiative power data and for these an issue of normalisation must be decided. When there is more than one metastable, the partial emissivity coefficients are defined relative to their driving metastable population. When there is only one metastable specified (in normal circumstances the ground state), a confusion can arise in applications as to whether the emissivities and powers are specified relative to the metastable population or the whole ionisation stage population. At g), either choice can be made. Note that this matters in practice when highly populated metastables are present but these are not identified as metastables at c) in the population calculation. Generalised collisional-radiative modelling treats such issues consistently.

17. The unrestricted production of emissivity and ionisation per photon coefficients can be very large. At h), the number can be restricted. The choices are related to what one choose for a particular spectrometer. It is envisaged that the user would prepare and archive personal selections here.

The **Ionisation rate coefficient acquisition windows** are as follow:

18. The usual file selection window is presented, in this case for an ADF07 file containing ionisation rate coefficients. The ion for which data is required is given for information.



19. The processing options window is similar to the usual ADAS502 one but with an extra sub-window a) for matching the selected coefficients to the initial state/ final state metastable pairs in the ADAS208 program. The ADAS208 code notifies the initial state/final state metastable pairs it needs and these appear in the lower transition list window b). If a requested transition from ADAS208 is not satisfied then a default ionisation rate coefficient is used for that transition.
20. Note that the output temperatures c) are not editable but transmitted from ADAS208. The 'Exit to menu' icon at d) in this case in fact restores the spawning ADAS208 window.
21. Press the *Done* button to progress to the output options window as for ADAS502. The ionisation coefficient graph may be displayed in the usual manner.
22. It is possible to fill the ionisation coefficient requirements by opening other ADF07 files. Simply move back to the file selection window for ADAS208/ADAS502 above.
23. Return to the spawning ADAS208 window by clicking the *Cancel* button on the ADAS208/ADAS502 file selection window above or the 'Exit to menu' icon.

ADAS502 (208) PROCESSING OPTIONS

Title for run

Data file name : /disk2/adas/adas/adf07/szd93#crszd93#cr.dat

Polynomial fitting

Fit Polynomial value % :

Select data block

Index	Initial ion	Metastable index	Final ion	Metastable index
2	CR+ 0	1	CR+ 1	1
1	CR+ 0	1	CR+ 1	0
2	CR+ 0	1	CR+ 1	1
3	CR+ 0	1	CR+ 1	2
4	CR+ 0	2	CR+ 1	0
5	CR+ 0	2	CR+ 1	1

Initial ion: 0 + 4 Final ion : 0 + 5
Select matching states

INDEX	Initial metastable	Final metastable
1	1(7)S(3.0)	1(6S)
1	1(7)S(3.0)	1(6S)
2	1(7)P(3.0)	2(6D)
3	1(7)P(3.0)	3(4D)
4	2(5)P(2.0)	1(6S)
5	2(5)P(2.0)	2(6D)

Output Electron Temperature

Index	Output	Input
1	1.000E+00	1.000E+00
2	2.000E+00	2.000E+00
3	5.000E+00	5.000E+00
4	1.000E+01	1.000E+01
5	2.000E+01	2.000E+01
6	5.000E+01	5.000E+01
7	1.000E+02	1.000E+02
8	2.000E+02	2.000E+02

Temperature units : eV

Edit the processing options data and press Done to proceed

a) Graphical display button

b) Explicit Scaling button

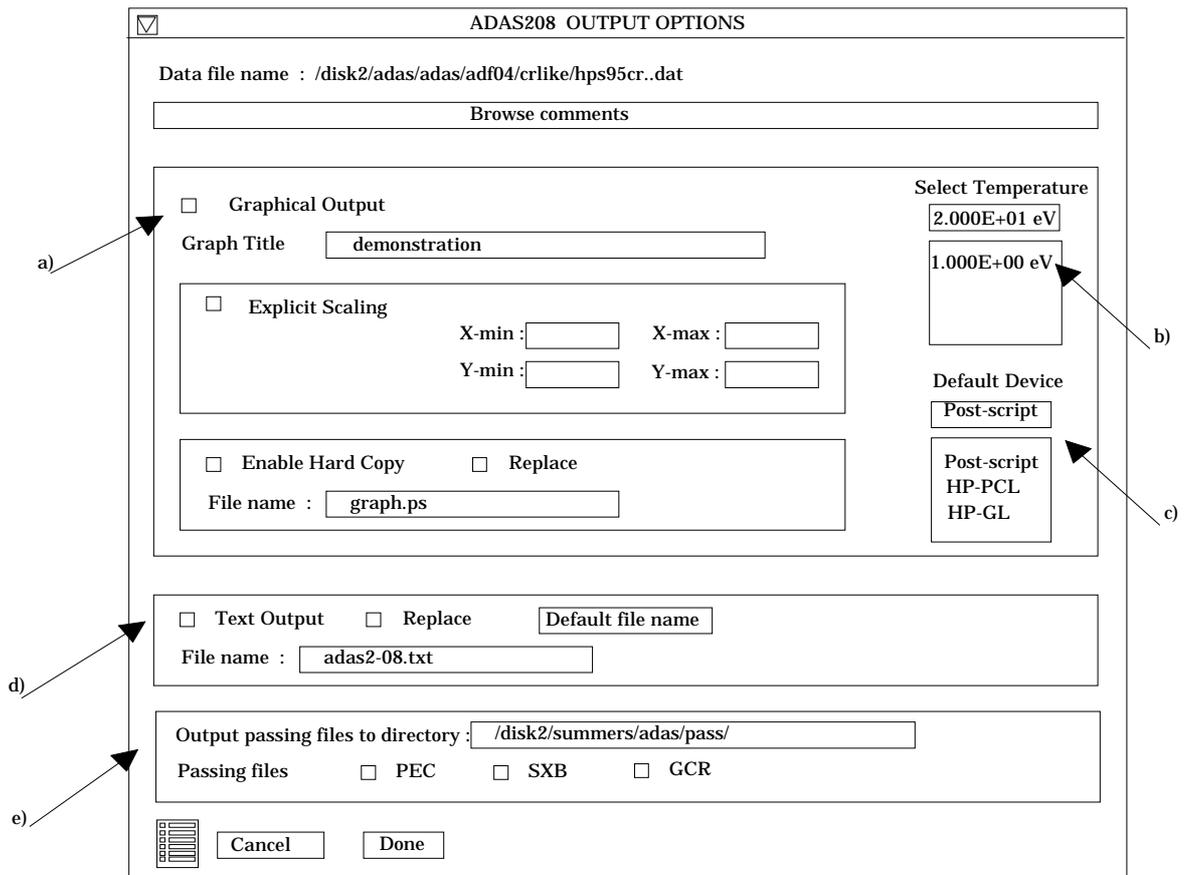
c) Device list window

d) Text Output button

The ADAS208 **output options window** has the appearance shown below

25. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
26. 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. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.
27. 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.
28. A choice of output graph plotting devices is given in the Device list window c). Clicking on the required device selects it. It appears in the selection window above the Device list window.
29. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. 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 *Replace* button has not been activated.



31. Several output files are created by ADAS208 if requested. These are the PEC, photon emissivity file, the SXB, ionisation per photon file and the GCR, generalised collisional-radiative files. These are of ADF15, ADF13 and ADF10 structure respectively. The GCR files in fact refer to a group of files (ACD, SCD etc). The various files go by defaults into

/..../<uid>/adas/pass/pec.pass
 /..../<uid>/adas/pass/sxb.pass
 /..../<uid>/adas/pass/<..>.pass

respectively.

- 32. The graph is displayed in a following **Graphical Output** when the *Done* button is pressed.
- 33. The graph has at its foot a *Done* button, and possibly *Next* and *Previous* buttons if there is a sequence of graphs to be displayed. A *Print* button is also present if the *Enable Hard Copy* button on the previous window was activated.
- 34. Press the *Next* button to show the next graph in a sequence and the *Previous* button to show the previous graph.
- 35. Press the *Print* button to make a hard copy of the currently displayed picture.
- 36. Pressing the *Done* button restores the previous Output Options window.

Illustration:

Figure 3.8a

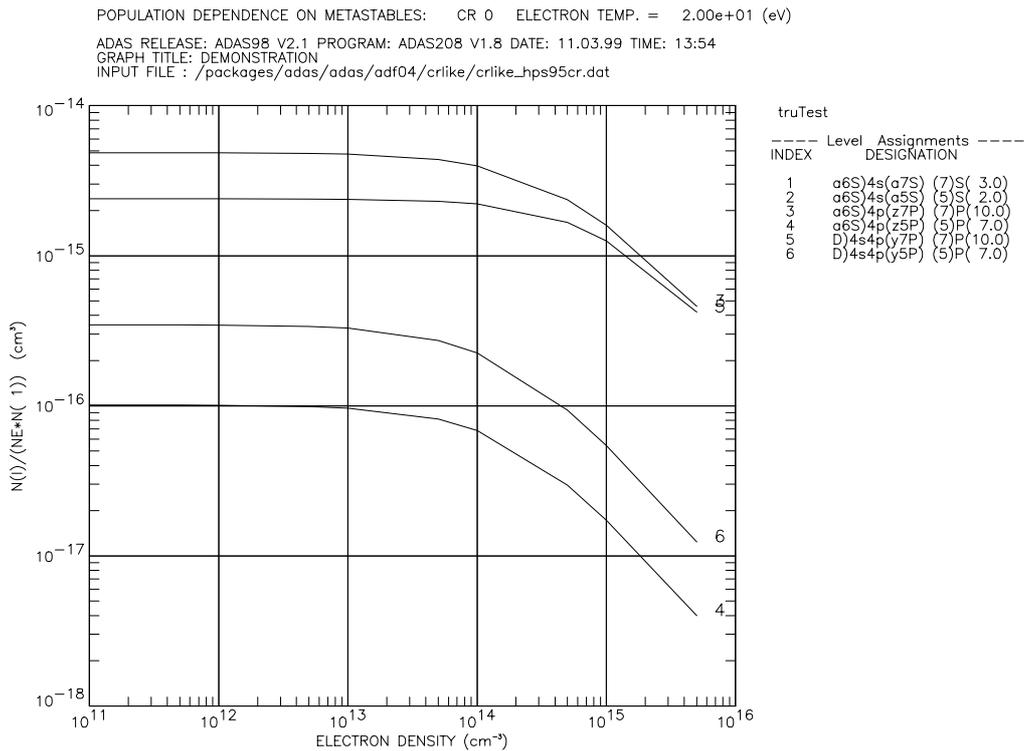


Table 3.8.

```

ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS208 V1.8 DATE: 11.03.99 TIME: 13:54
***** TABULAR OUTPUT FROM METASTABLE POPULATION PROGRAM: ADAS208 - DATE: 11.03.99 *****
INPUT COPASE FILE NAME: /packages/adas/adas/adf04/crlike/crlike_hps95cr.dat
INPUT EXPANSION FILE NAME: /packages/adas/adas/adf18/a17_p208/exp93#o/exp93#o_o01s.dat

ION      NUCLEAR      RECOMBINING      ----- IONIZATION POTENTIALS-----
CHARGE (Z0)      ION CHARGE (Z1)      (wave number <cm-1>)      (rydbergs)
-----
CR+ 0      24      1      54576.      0.4973342

      66853.      0.6092107
      92890.      0.8464778

----- ENERGY LEVELS -----
INDEX CONFIGURATION (2S+1)L(J) PRT - ENERGY RELATIVE TO LEVEL 1 - ENERGY RELATIVE TO PARENT IONIS. POTEN.
      (wave number <cm-1>) (rydbergs) (wave number <cm-1>) (rydbergs)
-----
1 (a6S)4s(a7S) (7)0( 3.0) {1} 0. 0.0000000 54576. 0.4973342
2 (a6S)4s(a5S) (5)0( 2.0) {1} 7593. 0.0691945 46983. 0.4281397
3 (a6S)4p(z7P) (7)1(10.0) {1} 23415. 0.2133755 31161. 0.2839587
4 (a6S)4p(z5P) (5)1( 7.0) {1} 26793. 0.2441590 27783. 0.2531751
5 (5D)4s4p(y7P) (7)1(10.0) {1} 27848. 0.2537684 26728. 0.2435658
6 (5D)4s4p(y5P) (5)1( 7.0) {1} 29664. 0.2703179 24912. 0.2270162

-- INPUT COPASE FILE TEMPERATURES: (TE=TP=TH) --
INDEX (kelvin) (eV) (reduced)
-----
1 1.16D+04 1.00D+00 1.16D+04
2 2.32D+04 2.00D+00 2.32D+04
3 5.80D+04 5.00D+00 5.80D+04
4 1.16D+05 1.00D+01 1.16D+05
5 2.32D+05 2.00D+01 2.32D+05
6 5.80D+05 5.00D+01 5.80D+05
7 1.16D+06 1.00D+02 1.16D+06
8 2.32D+06 2.00D+02 2.32D+06

INPUT COPASE FILE INFORMATION:
-----
NUMBER OF ELECTRON IMPACT TRANSITIONS = 9
NUMBER OF PROTON IMPACT TRANSITIONS = 0
NUMBER OF STATE SELECTIVE CAPTURES BY (Z+1) = 0
  
```

NUMBER OF STATE SELECTIVE IONIS. FROM (Z-1) = 0
 NUMBER OF ACTIVE METASTABLE STATES OF (Z+1) = 3
 NUMBER OF ACTIVE METASTABLE STATES OF (Z-1) = 0
 NUMBER OF STATE SELECTIVE RECOMBS. BY (Z+1) = 9

METASTABLE INFORMATION:

NUMBER OF ORDINARY LEVELS = 4
 NUMBER OF METASTABLES = 2

----- METASTABLE DETAILS -----

METASTABLE INDEX	ENERGY LEVEL INDEX	DESIGNATION
1	1	a6S)4s(a7S) (7)S(3.0)
2	2	a6S)4s(a5S) (5)S(2.0)

OUTPUT PLASMA PARAMETERS:

NUMBER OF TEMPERATURES = 8
 NUMBER OF DENSITIES/RATIOS = 10

INDEX	TEMPERATURES (UNITS: eV)			INDEX	DENSITIES (UNITS: CM-3)	
	ELECTRON <TE>	PROTON <TP>	NEUTRAL HYDROGEN <TH>		ELECTRON <NE>	PROTON <NP>
1	9.995D-01 *	9.995D-01 #	9.995D-01 #	1	1.000D+11	1.000D+11 #
2	1.999D+00	1.999D+00 #	1.999D+00 #	2	5.000D+11	5.000D+11 #
3	4.998D+00	4.998D+00 #	4.998D+00 #	3	1.000D+12	1.000D+12 #
4	9.995D+00	9.995D+00 #	9.995D+00 #	4	5.000D+12	5.000D+12 #
5	2.000D+01	2.000D+01 #	2.000D+01 #	5	1.000D+13	1.000D+13 #
6	4.998D+01	4.998D+01 #	4.998D+01 #	6	5.000D+13	5.000D+13 #
7	9.995D+01	9.995D+01 #	9.995D+01 #	7	1.000D+14	1.000D+14 #
8	1.999D+02	1.999D+02 #	1.999D+02 #	8	5.000D+14	5.000D+14 #
				9	1.000D+15	1.000D+15 #
				10	5.000D+15	5.000D+15 #

KEY: * = WARNING - TEMPERATURE OUT OF RANGE
 - EXTRAPOLATION REQUIRED
 # = PARAMETER NOT USED IN CALCULATIONS

OUTPUT PLASMA PARAMETERS FOR EQUILIBRIUM POPULATIONS:

INDEX	RATIOS N(Z+1,M)/N(Z,1)			NH/NE	RATIOS N(Z-1,M)/N(Z,1)		
	M=1	M=2	M=3		M=1	M=2	M=3
1	1.000D+00 #	0.000D+00 #	0.000D+00 #	0.000D+00 #			
2	1.000D+00 #	0.000D+00 #	0.000D+00 #	0.000D+00 #			
3	1.000D+00 #	0.000D+00 #	0.000D+00 #	0.000D+00 #			
4	1.000D+00 #	0.000D+00 #	0.000D+00 #	0.000D+00 #			
5	1.000D+00 #	0.000D+00 #	0.000D+00 #	0.000D+00 #			
6	1.000D+00 #	0.000D+00 #	0.000D+00 #	0.000D+00 #			
7	1.000D+00 #	0.000D+00 #	0.000D+00 #	0.000D+00 #			
8	1.000D+00 #	0.000D+00 #	0.000D+00 #	0.000D+00 #			
9	0.000D+00 #	0.000D+00 #	0.000D+00 #	0.000D+00 #			
10	0.000D+00 #	0.000D+00 #	0.000D+00 #	0.000D+00 #			

NOTE: NH/NE = NEUTRAL HYDROGEN DENSITY / ELECTRON DENSITY
 N(Z+1,M)/N(Z,1) = ABUNDANCES OF (Z+1) METASTABLES
 N(Z-1,M)/N(Z,1) = ABUNDANCES OF (Z-1) METASTABLES

PROTON IMPACT COLLISIONS - NOT INCLUDED
 EXCITED STATE IONIZATION RATES - NOT INCLUDED
 STATE SELECTIVE CX BY (Z+1) - NOT INCLUDED
 STATE SELECTIVE RECOM. BY (Z+1) - NOT INCLUDED
 STATE SELECTIVE IONIS. OF (Z-1) - NOT INCLUDED
 COEFF. NORMAL. TO STAGE TOTALS - NOT INCLUDED

TABLE KEY:

NE = ELECTRON DENSITY

TE = ELECTRON TEMPERATURE

I = ENERGY LEVEL INDEX

IOR = ORDINARY LEVEL INDEX

IMET = METASTABLE INDEX
NUMBER OF PROTON IMPACT COLLISIONS INCLUDED = 0
NUMBER OF STATE SELECTIVE RECOM. BY (Z+1) INCLUDED = 0
NUMBER OF STATE SELECTIVE IONIS. BY (Z-1) INCLUDED = 0
NUMBER OF STATE SELECTIVE CX BY (Z+1) INCLUDED = 0

NE(CM-3)= 1.0000E+11 5.0000E+11 1.0000E+12 5.0000E+12 1.0000E+13 5.0000E+13 1.0000E+14 5.0000E+14

EQUILIBRIUM METASTABLE POPULATION DEPENDENCE ON DENSITY AT TE = 1.00E+00 EV = 1.16E+04 KELVIN

IMET I
1 1 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00
2 2 3.0415E-01 3.0412E-01 3.0408E-01 3.0380E-01 3.0345E-01 3.0104E-01 2.9865E-01 2.8944E-01

POPULATION DEPENDENCE ON DENSITY AND METASTABLE 1

IOR I
1 3 3.3551E-05 1.6755E-04 3.3460E-04 1.6531E-03 3.2581E-03 1.4614E-02 2.5986E-02 7.2118E-02
2 4 3.8963E-06 1.9468E-05 3.8904E-05 1.9318E-04 3.8297E-04 1.7767E-03 3.2362E-03 9.2116E-03
3 5 4.3803E-06 2.1911E-05 4.3845E-05 2.2013E-04 4.4240E-04 2.2757E-03 4.6315E-03 2.1468E-02
4 6 8.9136E-06 4.4393E-05 8.8355E-05 4.2537E-04 8.1359E-04 3.0689E-03 4.8077E-03 9.8040E-03

POPULATION DEPENDENCE ON DENSITY AND METASTABLE 2

IOR I
1 3 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
2 4 5.2349E-05 2.6151E-04 5.2244E-04 2.5889E-03 5.1201E-03 2.3468E-02 4.2429E-02 1.1920E-01
3 5 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
4 6 5.3949E-05 2.6900E-04 5.3616E-04 2.6104E-03 5.0594E-03 2.0727E-02 3.4710E-02 8.3700E-02

...

NE(CM-3)= 1.0000E+11 5.0000E+11 1.0000E+12 5.0000E+12 1.0000E+13 5.0000E+13 1.0000E+14 5.0000E+14

EQUILIBRIUM METASTABLE POPULATION DEPENDENCE ON DENSITY AT TE = 2.00E+02 EV = 2.32E+06 KELVIN

IMET I
1 1 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00
2 2 1.6017E+00 1.5986E+00 1.5950E+00 1.5671E+00 1.5346E+00 1.3426E+00 1.2000E+00 8.8515E-01

POPULATION DEPENDENCE ON DENSITY AND METASTABLE 1

IOR I
1 3 4.1666E-04 2.0820E-03 4.1608E-03 2.0676E-02 4.1038E-02 1.9345E-01 3.6124E-01 1.1895E+00
2 4 5.3465E-07 2.6694E-06 5.3292E-06 2.6267E-05 5.1615E-05 2.2640E-04 3.9253E-04 9.4986E-04
3 5 2.1664E-04 1.0829E-03 2.1651E-03 1.0796E-02 2.1519E-02 1.0474E-01 2.0270E-01 8.0062E-01
4 6 2.1598E-06 1.0783E-05 2.1525E-05 1.0603E-04 2.0822E-04 9.0910E-04 1.5697E-03 3.7515E-03

POPULATION DEPENDENCE ON DENSITY AND METASTABLE 2

IOR I
1 3 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
2 4 1.1654E-03 5.8176E-03 1.1612E-02 5.7156E-02 1.1213E-01 4.8641E-01 8.3493E-01 1.9600E+00
3 5 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
4 6 7.1183E-04 3.5573E-03 7.1101E-03 3.5364E-02 7.0245E-02 3.3007E-01 6.0628E-01 1.7118E+00

***** EQUILIBRIUM POPULATIONS *****

LEVEL = 1 - EQUILIBRIUM POPULATION

NE (CM-3) 1.00D+11 5.00D+11 1.00D+12 5.00D+12 1.00D+13 5.00D+13 1.00D+14 5.00D+14 1.00D+15

TE (EV)
1.00D+00 | 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00
2.00D+00 | 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00
5.00D+00 | 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00
9.99D+00 | 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00
2.00D+01 | 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00
5.00D+01 | 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00
1.00D+02 | 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00
2.00D+02 | 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00

...

LEVEL = 6 - EQUILIBRIUM POPULATION

NE (CM-3) 1.00D+11 5.00D+11 1.00D+12 5.00D+12 1.00D+13 5.00D+13 1.00D+14 5.00D+14 1.00D+15

TE (EV)
1.00D+00 | 2.53D-05 1.26D-04 2.51D-04 1.22D-03 2.35D-03 9.31D-03 1.52D-02 3.40D-02 4.14D-02

5.00D+00	7.16D-04	3.57D-03	7.11D-03	3.46D-02	6.70D-02	2.67D-01	4.24D-01	8.00D-01	9.00D-01
9.99D+00	1.15D-03	5.72D-03	1.14D-02	5.53D-02	1.07D-01	4.15D-01	6.48D-01	1.18D+00	1.31D+00
2.00D+01	1.42D-03	7.10D-03	1.41D-02	6.84D-02	1.31D-01	5.03D-01	7.82D-01	1.41D+00	1.58D+00
5.00D+00	1.47D=04	3.80D=04	1.46D=02	3.05D=02	1.76D=02	5.25D=02	8.24D=01	3.54D+00	3.33D+00
1.00D+02	1.33D-03	6.63D-03	1.32D-02	6.43D-02	1.24D-01	4.95D-01	7.92D-01	1.55D+00	1.77D+00
2.00D+02	1.14D-03	5.70D-03	1.14D-02	5.55D-02	1.08D-01	4.44D-01	7.29D-01	1.52D+00	1.76D+00

Notes: