## ADAS409: Equilibrium ionisation - prepare G(Te,Ne) function tables

The program is an extension of ADAS405 which works two-dimensionally with independent electron temperatures and densities. Recall that ADAS405 used a model, that is with temperature/density pairs, so that it was a one-dimensional calculation. ADAS409 computes an equilibrium ionisation balance for an element or a range of ions of an element by drawing on relevant iso-nuclear master file data (format $a d f 11$ ). These data consist of (generalised) collisional-radiative coefficients for the ions of the element and may be of the stage-to-stage (standard) form or of the metastable distinguishing form (partial). The program calculates also the equilibrium radiated power by the element. A main objective of the code is to generate ionisation equilibrium emissivity functions for specific spectrum lines. These quantities, also known as (generalised) contribution functions, combine emissivity coefficient data with ionisation balance fractional abundances. They are the most relevant quantities for analysis of spectral observations of ionisation equilibrium plasmas (cf. differential emission measure analysis). ADAS409 achieves this by drawing on photon emissivity coefficient data collections in the ADAS database ('pec' files of format adf15).

## Background theory:

## The unresolved case:

Consider the evolution of populations of ions of an element in a plasma. For an element $X$ of nuclear charge $z_{0}$, the populations of the ionisation stages are denoted by

$$
N^{(z)}: z=0, \ldots, z_{0}
$$

The time dependence of the ionisation stage populations is given by the equations

$$
\begin{align*}
& d / d t N^{(z)}=N_{e} S_{C D}^{(z-1 \rightarrow z)} N^{(z-1)} \\
& -\left(N_{e} S_{C D}^{(z \rightarrow z+1)}+N_{e} \alpha_{C D}^{(z \rightarrow z-1)}+N_{H} C_{C D, \rho \rightarrow \rho^{\prime}}^{(z \rightarrow z-1)}\right) N^{(z)} \\
& +N_{e} \alpha_{C D}^{(z+1 \rightarrow z)} N^{(z+1)}+N_{H} C_{C D}^{(z+1 \rightarrow z)} N^{(z+1)}
\end{align*}
$$

This is called an unresolved or stage to stage picture. The coefficients are the (ordinary) collisional radiative coefficients. In equilibrium ionisation balance, the time derivatives are set to zero and the stage populations are the solutions of the matrix equation

$$
N_{e}\left[\begin{array}{cccc}
-S_{C D}^{(0 \rightarrow 1)} & \alpha_{C D}^{(1 \rightarrow 0)}+\left(N_{H} / N_{e}\right) C_{C D}^{(1 \rightarrow 0)} & 0 & 0 \\
S_{C D}^{(0 \rightarrow 1)} & -\left(S_{C D}^{(1 \rightarrow 2)}+\alpha_{C D}^{(1 \rightarrow 0)}+\left(N_{H} / N_{e}\right) C_{C D}^{(1 \rightarrow 0)}\right) & \alpha_{C D}^{(1 \rightarrow 0)} & 0 \\
0 & S_{C D}^{(1 \rightarrow 2)} & \cdot & \cdot \\
0 & 0 & \cdot & \cdot
\end{array}\right]\left[\begin{array}{c}
N^{(0)} \\
N^{(1)} \\
N^{(2)} \\
\cdot
\end{array}\right]=0
$$

subject to the normalisation

$$
N_{\text {tot }}=\sum_{z=0}^{z_{0}} N^{(z)}
$$

where $N_{\text {tot }}$ is the number density of ions of element $X$ in any ionisation stage. The equilibrium fractional abundances $N^{(z)} / N_{\text {tot }}$ at a set of temperatures and densities are sought. The code accesses standard iso-nuclear master file data of type ADF11 to obtain the coefficients of equations 5.9.3. In practical solution of the equations, note must be taken of the very small fractions which can obtain for ionisation stages distant from the dominant ionisation stage at a given temperature and density. Therefore the progressive elimination algorithm for the tri-diagonal matrix equations is performed towards the dominant ionisation
stage from both the neutral and fully ionised stages to avoid overflows rather than the usual 'single pass'.

From the equilibrium stage population solution, the total radiated power function $P_{\text {tot }}$, is calculated as

$$
\begin{align*}
P_{\text {tot }} & =\sum_{z=0}^{z_{0}} P^{(z)}\left(N^{(z)} / N_{\text {tot }}\right) \\
& =\sum_{z=0}^{z_{0}}\left[P_{L T}^{(z)}+P_{R B}^{(z)}+\left(N_{H} / N_{e}\right) P_{R C}^{(z)}\right]\left(N^{(z)} / N_{t o t}\right)
\end{align*}
$$

with separate radiated power coefficient $\left(P^{(z)}\right)$ contributions arising from low level line power, recombination-bremsstrahlung-cascade power and charge exchange recombination power. Also contribution functions to line emission known as $G\left(T_{e}\right)$ functions may be evaluated for arbitrary lines as

$$
G_{i \rightarrow j}^{(z)}=\left[\varepsilon_{i \rightarrow j}^{e x c} N^{(z)}+\varepsilon_{i \rightarrow j}^{r e c} N^{(z+1)}+\left(N_{H} / N_{e}\right) \varepsilon_{i \rightarrow j}^{C X} N^{(z+1)}\right] / N_{t o t}
$$

The $\varepsilon_{i \rightarrow j}$ are called photon emissivity coefficients (c.f. PE( coefficients in the metastable resolved case - see the descriptions of ADAS503 and ADAS208 in the last chapter) They occur in independent parts $\varepsilon_{i \rightarrow j}^{e x c}, \varepsilon_{i \rightarrow j}^{\text {rec }}$ and $\varepsilon_{i \rightarrow j}^{C X}$, distinguished by the driving process.

## The resolved case:

Properly, although the populations of excited states may be neglected compared with those of metastable and ground states of ions, it is not correct to combine the ground and metastable populations into a single stage population in the time dependent equations. This is because ground and metastable populations may have comparable populations and evolve on similar time-scales. The ground and metastable populations

$$
N_{\rho}^{(z)}: z=0, \ldots, z_{0} ; \rho=1, \ldots, M_{z}
$$

where $M_{z}$ is the number of metastable states (including the ground state) of ionisation stage $z$, should be treated separately The time dependence of the metastable populations is then given by the equations

$$
\begin{aligned}
d / d t N_{\rho}^{(z)} & =N_{e} \sum_{\rho^{\prime}=1}^{M_{z-1}} S_{C D, \rho^{\prime} \rightarrow \rho}^{(z-1 \rightarrow z)} N_{\rho^{\prime}}^{(z-1)} \\
& -\left(N_{e} \sum_{\rho^{\prime \prime}=1}^{M_{z+1}} S_{C D, \rho \rightarrow \rho^{\prime \prime}}^{(z \rightarrow z+1)}+N_{e} \sum_{\rho^{\prime}=1}^{M_{z-1}} \alpha_{C D, \rho \rightarrow \rho^{\prime}}^{(z \rightarrow z-1)}+N_{H} \sum_{\rho^{\prime}=1}^{M_{z-1}} C_{C D, \rho \rightarrow \rho^{\prime}}^{(z \rightarrow z-1)}\right. \\
& \left.+N_{e} \sum_{\sigma=1}^{M} Q_{C D, \rho \rightarrow \sigma}^{(z \rightarrow z)}+N_{e} \sum_{\rho^{\prime}=1}^{M_{z}} X_{C D, \rho \rightarrow \sigma}^{(z \rightarrow z)}\right) N_{\rho}^{(z)} \\
& +N_{e} \sum_{\rho^{\prime \prime}=1}^{M_{z+1}} \alpha_{C D, \rho^{\prime \prime} \rightarrow \rho}^{(z+1 \rightarrow z)} N_{\rho^{\prime}}^{(z+1)}+N_{H} \sum_{\rho^{\prime \prime}=1}^{M_{z+1}} C_{C D, \rho^{\prime \prime} \rightarrow \rho}^{(z+1 \rightarrow z)} N_{\rho^{\prime \prime}}^{(z+1)} \\
& +N_{e} \sum_{\sigma=1}^{M_{z}} Q_{C D, \sigma \rightarrow \rho}^{(z \rightarrow z)} N_{\sigma}^{(z)}+N_{e} \sum_{\sigma=1}^{M_{z}} X_{C D, \sigma \rightarrow \rho}^{(z \rightarrow z)} N_{\sigma}^{(z)}
\end{aligned}
$$

where there is such an equation for each $z$ and $\rho$. This is called a resolved or generalised picture. The coefficients are the generalised collisional radiative coefficients. In equilibrium ionisation balance, the time derivatives are set to zero and the metastable populations are the solutions of the partitioned matrix equations
$N_{e}\left[\begin{array}{cccc}-\mathbf{S}_{C D}^{(0)} & \mathbf{a}_{C D}^{(1 \rightarrow 0)}+\left(N_{H} / N_{e}\right) \mathbf{C}_{C D}^{(1 \rightarrow 0)} & 0 & 0 \\ \mathbf{S}_{C D}^{(0 \rightarrow 1)} & -\left(\mathbf{S}_{C D}^{(1)}+\mathbf{Q}_{C D}^{(1 \rightarrow 1)}+\mathbf{X}_{C D}^{(1 \rightarrow 1)}+\mathbf{a}_{C D}^{(1)}+\left(N_{H} / N_{e}\right) \mathbf{C}_{C D}^{(1)}\right) & \mathbf{a}_{C D}^{(2 \rightarrow 1)}+\left(N_{H} / N_{e}\right) \mathbf{C}_{C D}^{(2 \rightarrow 1)} & 0 \\ 0 & \mathbf{S}_{C D}^{(1 \rightarrow 2)} & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot\end{array}\right]\left[\begin{array}{l}\mathbf{N}^{(0)} \\ \mathbf{N}^{(1)} \\ \mathbf{N}^{(2)} \\ \cdot\end{array}\right]=0$
which must be interpreted for the metastable resolved case. Each element of the matrix in eqns. 5.9.9 is now itself a matrix extending over the metastable sets of the ionisation stage involved. Thus

$$
\mathbf{S}_{C D}^{(0 \rightarrow 1)}=\left[\begin{array}{cccc}
\cdot & \cdot & \cdot & \cdot \\
\cdot & S_{C D, \rho-1 \rightarrow \sigma-1}^{(0 \rightarrow 1)} & S_{C D, \rho-1 \rightarrow \sigma}^{(0 \rightarrow 1)} & \cdot \\
\cdot & S_{C D, \rho \rightarrow \sigma-1}^{(0 \rightarrow 1)} & S_{C D, \rho \rightarrow \sigma}^{(0 \rightarrow 1)} & \cdot \\
\cdot & \cdot & \cdot & \cdot
\end{array}\right]
$$

and

$$
\mathbf{S}_{C D}^{(0)}=\left[\begin{array}{cccc}
\cdot & . & \cdot & \cdot \\
. & \sum_{\sigma=1}^{M_{1}} S_{C D, \rho-1 \rightarrow \sigma}^{(0 \rightarrow \rightarrow 1)} & 0 & \cdot \\
\cdot & 0 & \sum_{\sigma=1}^{M_{1}} S_{C D, \rho \rightarrow \sigma}^{(0 \rightarrow 1)} & \cdot \\
. & \cdot & . & .
\end{array}\right]
$$

where the index $\rho: 1, \ldots, M_{0}$ spans the metastables of stage 0 and $\sigma: 1, \ldots, M_{1}$ spans the metastables of stage 1 . Also

$$
\mathbf{Q}_{C D}^{(1 \rightarrow 1)}=\left[\begin{array}{cccc}
. & \cdot & \cdot & \cdot \\
\cdot & -\sum_{\rho^{\prime}=1 ; \rho^{\prime} \neq \rho-1}^{M_{1}} Q_{C D, \rho^{\prime} \rightarrow \sigma-1}^{(1 \rightarrow 1)} & Q_{C D, \rho-1 \rightarrow \sigma}^{(1 \rightarrow 1)} & \cdot \\
\cdot & Q_{C D, \rho \rightarrow \sigma-1}^{(1 \rightarrow 1)} & -\sum_{\rho^{\prime}=1 ; \rho^{\prime} \neq \rho}^{M_{1}} Q_{C D, \rho^{\prime} \rightarrow \sigma}^{(1 \rightarrow 1)} & \cdot \\
. & \cdot & \cdot &
\end{array}\right]
$$

Similar definitions apply for the $\mathbf{a}_{C D}^{(1 \rightarrow 0)}, \mathbf{X}_{C D}^{(1 \rightarrow 1)}$ etc. Also the population vector is

$$
\mathbf{N}^{(0)}=\left[\begin{array}{c}
N_{1}^{(0)} \\
\cdot \\
\cdot \\
N_{M_{0}}^{(0)}
\end{array}\right]
$$

and the normalisation

$$
N_{\text {tot }}=\sum_{z=0}^{z_{0}} \sum_{\rho=1}^{M_{z}} N_{\rho}^{(z)}
$$

The equilibrium fractional abundances $N_{\rho}^{(z)} / N_{t o t}$ at a set of temperatures and densities are sought. The code accesses partial iso-nuclear master file data of type ADF11 to obtain the coefficients of the equations 5.9.9. Practical solution in the resolved case is achieved by an equivalent method to the unresolved case but with matrix operations replacing the scalar operations.

From the population solution, the total radiated power function is calculated as

$$
P_{t o t}=\sum_{z=0}^{z_{0}} \sum_{\rho=1}^{M_{z}}\left[P_{L T, \rho}^{(z)}+P_{R B, \rho}^{(z)}+\left(N_{H} / N_{e}\right) P_{R C, \rho}^{(z)}\right]\left(N_{\rho}^{(z)} / N_{t o t}\right)
$$

with contributions arising from low level line power, recombination-bremsstrahlung-cascade power and charge exchange recombination power. Also contribution functions to line emission known as $G\left(T_{e}\right)$ functions may be evaluated for arbitrary lines as

$$
\begin{align*}
G_{i \rightarrow j}^{(z)} & =\left[\sum_{\rho=1}^{M_{7}} \mathscr{P} \mathscr{E} \mathscr{C}_{\rho, i \rightarrow j}^{(e x c)} N_{\rho}^{(z)}+\sum_{v^{\prime}=1}^{M_{z+1}} \mathscr{P} \mathscr{C} \mathscr{C}_{v^{\prime}, i \rightarrow j}^{(r e c)} N_{\rho^{\prime}}^{(z+1)}\right. \\
& \left.+\left(N_{H} / N_{e}\right) \sum_{v^{\prime}=1}^{M_{z+1}} \mathscr{P} \mathscr{E} \mathscr{C}_{v^{\prime}, i \rightarrow j}^{(C X)} N_{\rho^{\prime}}^{(z+1)}\right] / N_{\text {tot }}
\end{align*}
$$

In practice, there may be very many choices of $G\left(T_{e}\right)$ functions of interest.

## Program steps:

These are summarised in figure 5.9.
Figure 5.9


## Interactive parameter comments:

Move to the directory in which you wish any ADAS created files to appear. These include the output text file produced after executing any ADAS program (paper.txt is the default), the graphical output file and the generalised $G\left(T_{e}, N_{e}\right)$ contribution function file. The latter is formatted to a tentative specification which will probably be assigned as adf32. Initiate ADAS409 from the program selection menus in the usual manner.
The file selection window appears first as illustrated above.

1. Two types of data file are identified in the file selection, namely, the iso-nuclear master files required for the ionisation balance and power calculations and the script file. The top part of the file selection window is concerned with identifying the master file data required and the lower part with identifying the script file.
2. adf11 is the appropriate data format for use by the program ADAS405. Your personal data of this type should be held in a similar file structure to central ADAS, but with your identifier replacing the first adas. The central ADAS database has extensive data of this form and the collection is steadily being extended. It is also subject to periodic revision as the influences of improved fundamental data are computed.
3. Click on the Select button at (a) to drop down a selection list of master file data classes. Activate the buttons at the data classes required for your analysis. It is obligatory to select the 'acd' and 'scd' electron impact effective recombination and ionisation data classes since otherwise an ionisation balance cannot proceed. However the other data classes selected are at the user's choice. This enables investigative studies of the importance of different contributions for example to radiated power.

4. At JET Joint Undertaking, effective radiated power coefficients ('prb', 'plt' and 'prc') are often made available both as the whole emitted power and as the power which would pass through certain filters (such as $\mathrm{Be} / \mathrm{Si}$ windows). The filter is specified either simply as an energy cut-off (eg. ev2000) or as filter specification (eg. ft1235). These codes appear as an extension in the relevant master file names. Specify the filter choice at (b). Note the present IDL-ADAS database contains very little filtered power data but it can be added if there is an interest amongst users.
5. The remainder of the file identification (c) follows the general pattern described for ADAS401 above. Note that a default year must be specified. Often the complete set of data classes for a particular year and type are not available and the capability of filling in from a default (perhaps less accurate but more complete) year is allowed.
6. In general the two digit year number is used to provide the main groupings of data. Thus ' 89 ' is the standard, unresolved, JET base line data of low precision but fairly complete. ' 93 ' is metastable resolved data, but available only for light elements of primary importance to fusion. Some flexibility for subdivision within a year is provided by allowing a two character 'member prefix' (eg. ' $p j$ ') which may be present in the final part of a file name (eg. '/../acd93r/acd93r_pj\#c.dat').
7. The distinctions between standard and partial master file types and resolved and unresolved types must be clarified. Standard data is stage -to stage and has a specific layout. Partial data distinguishes metastables and has a different layout. Within the partial data layout it is possible simply to have each stage represented only by its ground state and therefore to be similar to standard data However the layout is the partial one. We call such data partial but unresolved. The usual partial data with
metastables present is called resolved. This distinction and added flexibility are helpful in iso-nuclear master file preparation and archiving.
8. Clicking the Display data set availability button at (d) causes display of a file availability summary window as illustrated below. It is important to use this facility since it shows which master files classes sought by the user were not available, where default data files were substituted etc.
9. Script file selection is made in the conventional manner at (e). We have found it convenient to group script files in a personal ADAS database under a subdirectory classification /scripts 409 . Also, it is possible to bypass contribution function calculation and display by selecting the ' $N U L L$ ' script. You may find it helpful to copy the ' $N U L L$ ' script from the central ADAS database to your own space. Note that scripts apply to particular cases. Thus the references to emissivity coefficient data in a script applying to metastable resolved will not in general work for unresolved data, indeed will probably crash. We have not built much protection against faulty references into script files at the moment. More protection may be added if this proves a stumbling point for users. You may find it helpful to fetch the test_c script from central ADAS for first trials.


The processing options window has the appearance shown below

1. The script file selected by the user is identified at (a). The Browse Comments button displays the comments field at the foot of the script file.
2. Information is presented at (b) of the element and master files classes selected in the previous file selection option step.
3. Enter isotope mass numbers for the selected element and background neutral hydrogen in the plasma at (c). This information is only used if charge exchange recombination master file data has been selected.
4. The spectrum lines set up in the script file are shown in the display window at (d). This operates in the same manner as line display and selection windows in interrogation codes such as ADAS503 (see bulletin nov19-94). Click on a line to select it. The selected line is shown in the selection window above the display window. Only one line is treated at a time for graphical display. However all lines and line ratios in the script file are computed and tabulated in the output text file.
5. The selection of temperature and density values for data output are made at (e). Note the difference from ADAS405 in that the temperatures and densities are independent sets.
6. 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.
7. It follows the usual pattern except that there is a choice of graphs to display. Thus the fractional abundances, power functions and contribution functions are all of potential interest. Click on the appropriate button at (a). Generally, we find that on the first one or two occasions we wish to see the fractional abundances and powers but then have a more sustained interested in the contribution function shapes and their location in temperature. All the graphs are provided as a function of electron temperature.
8. The window presented at (b) depends on the graph choice above. The default scaling may be over-ridden and explicit values for the graph limits entered.
9. Graphical output is enabled in the window at (c) together with hard copy device and output file name. This follows the pattern of other ADAS programs. Likewise text output selection at (d) is standard.
10. The 'Goft Passing File' is the name used for the output data of calculated contribution functions. It is organised according to a tentative ADAS data format $a d f 32$. The output file name is specified at (e). The expected practice is that ADAS409 will be used either recursively or in distinct runs to examine contribution functions and then decide which to put into the Goft file. Thus an Append button has been provided to allow an existing output Goft file to be extended. The Replace and Default file name buttons have their usual meanings.


The graphical output window is shown below.
11. There is a new facility here. The calculated data are functions of temperature and density but are plotted here as a function of temperature. The slider at c) allows you to scan through the density values. The displayed graphs continually update making the display like a movie. We should be interested in your opinion of this addition.
12. Other options such as the Print button remain the same. Note that the current density frame is the one printed.


## Illustration:

The output from the program is illustrated for carbon in the resolved case. Figure 5.9a shows the equilibrium metastable fractional abundances for the first seven metastables as a function of temperature at a fixed density. The balance is at the electron density shown in the figure as selected by the density slider on the interactive graphical display. Figure 5.9 b shows similarly the total equilibrium radiated power function (TOT) for carbon, the separation into recombination + bremsstrahlung power function (PRB) and total line power function (PLT) and the line power function contributions from the last seven metastables states evaluated using the generalised collisional radiative coefficients. Seven curves only are displayed on each graph Figure 5.9c shows the equilibrium generalised contribution function for the CI 1561A resonance line. As can be seen from the script file, contributions from each of the four $\mathrm{C}^{+0}$ metastables are included.

Figure 5.9a


Figure 5.9b


Figure 5.9c

CONTRIBUTION FUNCTION VS. ELECTRON TEMPERATURE:
ADAS
FILE
KEY ADAS RELEASE: ADAS98 V2. 1 PROGRAM: ADAS409 V1.3 DATE: $20 / 04 / 99$ TIME: $10: 31$
KPCkOges/ados/ados/Scripts409/strathclyde_testcc-r SPECIES:CARBON YEAR: 93
DEFAULT YEAR: 93


Table 5.9a shows the tabular output from the carbon equilibrium ionisation balance. This is presented in a similar manner to that from ADAS405. Note however that the tabulation is for a particular electron density. Table 5.9 b gives the $G\left(T_{e}, N_{e}\right)$ functions. These are presented as simple indexed lists analogous to data format adfl6, however it is the two-dimensional function which is tabulated. Note that the tabular from ADAS409 has not been finalised. It is planned to use ADAS409 as a mass producer of two-dimensional $G\left(T_{e}, N_{e}\right)$ functions as ADAS412 is used for one-dimensional $G\left(T_{e}\right)$. The output tabulations will be assigned to a new ADAS data format $a d f 32$. The corresponding interrogation code on adf32, which will provide a 'collection file', will be ADAS508 and will be suited to advanced differential emission measure analysis (differential in temperature and density).

Table 5.9a


| 1 /disk2/adas/adas/adf15/pec93\#c/pec93\#c_pjr\#c0.dat <br> 2 /disk2/adas/adas/adf15/pec93\#c/pec93\#c_pjr\#c1.dat <br> 3 /disk2/adas/adas/adf15/ionelec/ionelec_pec\#c2.dat <br> 4 /disk2/adas/adas/adf15/ionelec/ionelec_pec\#c3.dat |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| IONISATION STAGE/METASTABLE SUMMARY: |  |  |  |  |  |  |  |  |
| NUCLEAR CHARGE |  |  |  |  |  |  |  |  |
| LOWEST CHARGE STATE |  |  |  |  |  |  |  |  |
| HIGHEST CHARGE STATE = 6 |  |  |  |  |  |  |  |  |
| NUMBER OF STAGES $=7$ |  |  |  |  |  |  |  |  |
| NUMBER OF METASTABLE STATES = 13 |  |  |  |  |  |  |  |  |
| OUTPUT PLASMA TEMPERATURE AND DENSITY SETS: |  |  |  |  |  |  |  |  |
| ELECTRON TEMPERATURE$($ kelvin $)$$(e V)$ |  |  | $\begin{aligned} & \text { ELECTRON } \\ & \text { DENSITY (cm-3) } \end{aligned}$ |  |  |  |  |  |
| $1.16 \mathrm{D}+04$ | $1.00 \mathrm{D}+00$ |  | $1.00 \mathrm{D}+01$ |  | $8.00 \mathrm{D}+00$ |  |  |  |
| $1.51 \mathrm{D}+04$ | $1.30 \mathrm{D}+00$ |  | $1.00 \mathrm{D}+05$ |  | $8.00 \mathrm{D}+04$ |  |  |  |
| $1.74 \mathrm{D}+04$ | $1.50 \mathrm{D}+00$ |  | $1.00 \mathrm{D}+06$ |  | $8.00 \mathrm{D}+05$ |  |  |  |
| 2.32D+04 | 2.00D+00 |  | $1.00 \mathrm{D}+07$ |  | $8.00 \mathrm{D}+06$ |  |  |  |
| $3.48 \mathrm{D}+04$ | $3.00 \mathrm{D}+00$ |  | $3.00 \mathrm{D}+07$ |  | $2.40 \mathrm{D}+07$ |  |  |  |
| $5.80 \mathrm{D}+04$ | $5.00 \mathrm{D}+00$ |  | $1.00 \mathrm{D}+08$ |  | $8.00 \mathrm{D}+07$ |  |  |  |
| 8.12D+04 | $7.00 \mathrm{D}+00$ |  | $3.00 \mathrm{D}+08$ |  | $2.40 \mathrm{D}+08$ |  |  |  |
| $1.16 \mathrm{D}+05$ | $1.00 \mathrm{D}+01$ |  | $1.00 \mathrm{D}+09$ |  | $8.00 \mathrm{D}+08$ |  |  |  |
| $1.51 \mathrm{D}+05$ | $1.30 \mathrm{D}+01$ |  | $3.00 \mathrm{D}+09$ |  | $2.40 \mathrm{D}+09$ |  |  |  |
| $10 \quad 1.74 \mathrm{D}+05$ | $1.50 \mathrm{D}+01$ |  | 1.00D+10 |  | $8.00 \mathrm{D}+09$ |  |  |  |
| 11 2.32D+05 | $2.00 \mathrm{D}+01$ |  | $3.00 \mathrm{D}+10$ |  | $2.40 \mathrm{D}+10$ |  |  |  |
| 12 3.48D+05 | $3.00 \mathrm{D}+01$ |  | 1.00D+11 |  | $8.00 \mathrm{D}+10$ |  |  |  |
| 13 5.80D+05 | $5.00 \mathrm{D}+01$ |  | $3.00 \mathrm{D}+11$ |  | $2.40 \mathrm{D}+11$ |  |  |  |
| 14 8.12D+05 | $7.00 \mathrm{D}+01$ |  | $1.00 \mathrm{D}+12$ |  | $8.00 \mathrm{D}+11$ |  |  |  |
| 15 1.16D+06 | $1.00 \mathrm{D}+02$ |  | $3.00 \mathrm{D}+12$ |  | $2.40 \mathrm{D}+12$ |  |  |  |
| 16 1.51D+06 | $1.30 \mathrm{D}+02$ |  | 1.00D+13 |  | $8.00 \mathrm{D}+12$ |  |  |  |
| 17 1.74D+06 | $1.50 \mathrm{D}+02$ |  | $3.00 \mathrm{D}+13$ |  | $2.40 \mathrm{D}+13$ |  |  |  |
| 18 2.32D+06 | 2.00D+02 |  | $1.00 \mathrm{D}+14$ |  | $8.00 \mathrm{D}+13$ |  |  |  |
| 19 3.48D+06 | $3.00 \mathrm{D}+02$ |  | $1.00 \mathrm{D}+15$ |  | $8.00 \mathrm{D}+14$ |  |  |  |
| 20 5.80D+06 | $5.00 \mathrm{D}+02$ |  | $1.00 \mathrm{D}+20$ |  | $8.00 \mathrm{D}+19$ |  |  |  |
| ELECTRON DENSITY SELECTED FOR OUTPUT |  |  |  |  |  |  |  |  |
| $18 \quad 1.00 \mathrm{D}+14 \mathrm{~cm}-3$ |  |  |  |  |  |  |  |  |
| EQUILIBRIUM FRACTIONAL ABUNDANCES, GCF FUNCTIONS AND LINE RATIOS: |  |  |  |  |  |  |  |  |
| TE (eV) | $1.00 \mathrm{D}+00$ | $1.30 \mathrm{D}+00$ | $1.50 \mathrm{D}+00$ | $2.00 \mathrm{D}+00$ | $3.00 \mathrm{D}+00$ | 5.00D+00 | 7.00D+00 | $1.00 \mathrm{D}+01$ |
| NE (cm-3) | $1.00 \mathrm{D}+01$ | $1.00 \mathrm{D}+05$ | $1.00 \mathrm{D}+06$ | $1.00 \mathrm{D}+07$ | $3.00 \mathrm{D}+07$ | $1.00 \mathrm{D}+08$ | $3.00 \mathrm{D}+08$ | $1.00 \mathrm{D}+09$ |
| NH ( $\mathrm{cm}-3$ ) | $8.00 \mathrm{D}+00$ | 8.00D+04 | 8.00D+05 | 8.00D+06 | $2.40 \mathrm{D}+07$ | 8.00D+07 | $2.40 \mathrm{D}+08$ | 8.00D+08 |
| IND ION MET |  |  |  |  |  |  |  |  |
| $1 \mathrm{c}+0$ ( 1) | $1.31 \mathrm{D}-01$ | $1.05 \mathrm{D}-02$ | $3.21 \mathrm{D}-03$ | 4.35D-04 | 1.15D-05 | 4.58D-08 | 5.51D-10 | 1.99D-12 |
| $2 \mathrm{c}+0$ ( 2) | $2.11 \mathrm{D}-02$ | 2.21D-03 | $7.47 \mathrm{D}-04$ | 1.18D-04 | 3.80D-06 | 1.97D-08 | 2.84D-10 | 1.22D-12 |
| $3 \mathrm{c}+0$ ( 3) | $1.02 \mathrm{D}-03$ | 1.46D-04 | 5.60D-05 | 1.08D-05 | 4.33D-07 | 2.61D-09 | 3.94D-11 |  |
| $4 \mathrm{c}+0$ ( 4) | $1.12 \mathrm{D}-03$ | 2.12D-04 | 8.90D-05 | 1.94D-05 | 8.17D-07 | 4.25D-09 | 5.23D-11 |  |
| $5 \mathrm{c}+1$ ( 1) | $8.42 \mathrm{D}-01$ | $9.73 \mathrm{D}-01$ | $9.74 \mathrm{D}-01$ | 9.01D-01 | 1.67D-01 | 3.57D-03 | 1.02D-04 | 8.34D-07 |
| $6 \mathrm{c}+1$ ( 2) | $3.85 \mathrm{D}-03$ | 1.42D-02 | 2.13D-02 | 4.10D-02 | 2.18D-02 | 1.03D-03 | 3.60D-05 | 3.27D-07 |
| $7 \mathrm{c}+2$ ( 1) | $3.92 \mathrm{D}-07$ | 8.60D-05 | 9.34D-04 | 4.27D-02 | 4.57D-01 | 3.28D-01 | 4.51D-02 | 1.33D-03 |
| $8 \mathrm{c}+2$ ( 2) | $1.23 \mathrm{D}-09$ | $2.06 \mathrm{D}-06$ | 6.88D-05 | 1.46D-02 | 3.53D-01 | 3.45D-01 | 5.89D-02 | 1.97D-03 |
| $9 \mathrm{c}+3$ ( 1) |  |  |  | $3.91 \mathrm{D}-08$ | 9.55D-04 | 3.22D-01 | 7.68D-01 | 2.15D-01 |
| $10 \mathrm{c}+4 \mathrm{l}$ ( ) |  |  |  |  | 3.53D-10 | 1.00D-03 | 1.28D-01 | 7.82D-01 |
| $11 \mathrm{c}+4$ ( 2) |  |  |  |  |  |  |  |  |
| $12 \mathrm{c}+5$ ( 1) |  |  |  |  |  |  |  |  |
| $13 \mathrm{c}+6$ ( 1) |  |  |  |  |  |  |  |  |
| PRB (W cm3) | 1.88D-30 | 2.37D-30 | 2.86D-30 | 5.40D-30 | 1.63D-29 | 3.83D-29 | 4.78D-29 | 2.59D-29 |
| PLT (W cm3) | $5.40 \mathrm{D}-29$ | 2.33D-28 | 3.91D-28 | $1.17 \mathrm{D}-27$ | $1.01 \mathrm{D}-26$ | 3.26D-26 | 4.51D-26 | 1.43D-26 |
| PRAD (W cm3) | 5.59D-29 | 2.35D-28 | $3.94 \mathrm{D}-28$ | $1.17 \mathrm{D}-27$ | $1.02 \mathrm{D}-26$ | $3.26 \mathrm{D}-26$ | 4.51D-26 | $1.43 \mathrm{D}-26$ |
| SPECTRAL LINE GCF FUNCTIONS ( $\mathrm{cm} 3 \mathrm{~s}-1$ ) : |  |  |  |  |  |  |  |  |
| TE (eV) | $1.00 \mathrm{D}+00$ | $1.30 \mathrm{D}+00$ | $1.50 \mathrm{D}+00$ | $2.00 \mathrm{D}+00$ | $3.00 \mathrm{D}+00$ | 5.00D+00 | 7.00D+00 | $1.00 \mathrm{D}+01$ |
| NE (cm-3) | $1.00 \mathrm{D}+01$ | 1.00D+05 | 1.00D+06 | 1.00D+07 | $3.00 \mathrm{D}+07$ | 1.00D+08 | $3.00 \mathrm{D}+08$ | $1.00 \mathrm{D}+09$ |
| NH ( $\mathrm{cm}-3$ ) | $8.00 \mathrm{D}+00$ | 8.00D+04 | 8.00D+05 | 8.00D+06 | $2.40 \mathrm{D}+07$ | 8.00D+07 | 2.40D+08 | 8.00D+08 |
| $\begin{array}{r} \text { IND ION WVLEN.(A) } \\ (I C, I Z, I M, I P, I F) \end{array}$ |  |  |  |  |  |  |  |  |
| 1 CI 1561A | 4.41D-12 | 1.85D-12 | 1.12D-12 | 4.49D-13 | 3.58D-14 | 3.45D-16 | 6.03D-18 | 2.87D-20 |
| $\left(\begin{array}{llllll}1 & 0 & 1 & 1 \mathrm{E} & 1\end{array}\right)$ | $1.49 \mathrm{D}-12$ | $6.68 \mathrm{D}-13$ | 4.31D-13 | 1.97D-13 | 1.87D-14 | 2.13D-16 | 4.06D-18 | 2.06D-20 |
| $\left(\begin{array}{lllll}2 & 0 & 2 & 54 \mathrm{E} & 1\end{array}\right)$ | $1.70 \mathrm{D}-12$ | 7.09D-13 | 4.26D-13 | 1.63D-13 | 1.16D-14 | 9.57D-17 | 1.52D-18 | 6.43D-21 |
| $\left(\begin{array}{lllll}3 & 0 & 3 & 107 \mathrm{E} & 1\end{array}\right)$ | 5.39D-14 | 2.16D-14 | 1.25D-14 | 4.45D-15 | 2.90D-16 | 2.11D-18 | 3.08D-20 | 1.20D-22 |
| $\left(\begin{array}{lllll}4 & 0 & 160 \mathrm{E} & 1\end{array}\right)$ | 1.17D-12 | 4.49D-13 | 2.51D-13 | 8.44D-14 | 5.20D-15 | 3.35D-17 | 4.26D-19 | 1.45D-21 |
| 2 CII 904A | 8.04D-14 | 1.87D-12 | 7.71D-12 | 6.39D-11 | $1.07 \mathrm{D}-10$ | 1.31D-11 | 7.86D-13 | 1.12D-14 |
| $\left(\begin{array}{llllll}1 & 1 & 1 & 3 \mathrm{E} & 2\end{array}\right)$ | $7.22 \mathrm{D}-14$ | 1.69D-12 | 7.11D-12 | 5.99D-11 | 1.00D-10 | 1.24D-11 | 7.49D-13 | 1.08D-14 |
| $\left(\begin{array}{lllll}2 & 1 & 2 & 25 \mathrm{E} & 2\end{array}\right)$ | $8.19 \mathrm{D}-15$ | 1.75D-13 | $6.00 \mathrm{D}-13$ | 4.02D-12 | $6.98 \mathrm{D}-12$ | 7.73D-13 | 3.67D-14 | 3.95D-16 |
| SPECTRAL LINE RATIOS: |  |  |  |  |  |  |  |  |
| IR JL KL |  |  |  |  |  |  |  |  |
| $1 \begin{array}{lll}1 & 1\end{array}$ | $5.48 \mathrm{D}+01$ | 9.90D-01 | 1.45D-01 | 7.02D-03 | 3.34D-04 | 2.62D-05 | 7.68D-06 | 2.57D-06 |
| EQUILIBRIUM FRACTIONAL ABUNDANCES, GCF FUNCTIONS AND LINE RATIOS: |  |  |  |  |  |  |  |  |
| TE (eV) | $2.00 \mathrm{D}+01$ | $3.00 \mathrm{D}+01$ | $5.00 \mathrm{D}+01$ | 7.00D+01 | $1.00 \mathrm{D}+02$ | 1.30D+02 | 1.50D+02 | $2.00 \mathrm{D}+02$ |



Table 5.9b

```
            2 /c GENERALISED CONTRIBUTION FUNCTIONS/
            1561 A 20/c + 0/CODE= ADAS409/SCRIPT= /TYPE= LINE/ISEL =
    1.00D+01 1.00D+05 1.00D+06 1.00D+07 3.00D+07 1.00D+08 3.00D+08 1.00D+09
    3.00D+09 1.00D+10 3.00D+10 1.00D+11 
    3.00D+13 1.00D+14 1.00D+15 1.00D+20
    1.00D+00 1.57D-11 1.43D-11 1.40D-11 1.37D-11 1.36D-11 1.34D-11 1.32D-11
    1.29D-11 1.26D-11 1.24D-11 1.22D-11 1.18D-11 1.11D-11 1.01D-11 8.97D-12
    7.41D-12 5.91D-12 4.41D-12 2.28D-12 1.36D-15
    1.30D+00 3.36D-11 2.10D-11 1.83D-11 1.60D-11 1.50D-11 1.39D-11 1.29D-11
    1.18D-11 1.08D-11 9.88D-12 9.07D-12 7.99D-12 6.86D-12 5.57D-12 4.45D-12
    3.37D-12 2.55D-12 1.85D-12 9.63D-13 5.28D-15
    5.00D+02 1.58D-30 7.92D-32 3.75D-32 1.77D-32 1.22D-32 7.98D-33 5.22D-33
    3.07D-33 1.77D-33 9.29D-34 5.26D-34 2.98D-34 1.84D-34 1.07D-34 6.30D-35
    3.20D-35 1.49D-35 5.12D-36 2.61D-37 7.86D-47
            904 A 20/c + 1/CODE= ADAS409/SCRIPT= /TYPE= LINE/ISEL =
    1.00D+01 1.00D+05 1.00D+06 1.00D+07 3.00D+07 1.00D+08 3.00D+08 1.00D+09
    3.00D+09 1.00D+10 3.00D+10 1.00D+11 3.00D+11 1.00D+12 3.00D+12 1.00D+13
    3.00D+13 1.00D+14 1.00D+15 1.00D+20
    1.00D+00 1.15D-14 1.73D-14 1.98D-14 1.2.28D-14 2.46D-14 2.68D-14 2.92D-14
    3.24D-14 3.60D-14 4.10D-14 4.67D-14 5.42D-14 6.15D-14 6.89D-14 7.42D-14
    7.75D-14 7.93D-14 8.04D-14 8.17D-14 4.99D-15
    1.30D+00 1.12D-12 1.35D-12 1.41D-12 1.47D-12 1.50D-12 1.54D-12 1.59D-12
    1.64D-12 1.71D-12 1.80D-12 1.90D-12 2.00D-12 2.06D-12 2.08D-12 2.04D-12
    1.97D-12 1.91D-12 1.87D-12 1.88D-12 6.56D-13
    5.00D+02 8.55D-25 2.20D-25 1.57D-25 1.10D-25 9.25D-26 7.48D-26 5.95D-26
    4.36D-26 3.07D-26 2.01D-26 1.41D-26 1.05D-26 8.74D-27 7.56D-27 6.75D-27
    5.82D-27 4.67D-27 3.10D-27 6.60D-28 5.14D-32
C-
GENERALISED CONTRIBUTION FUNCTIONS
C SOURCE SPECIFIC ION FILE:/packages/adas/adas/scripts409/strathclyde_test_c_r
```



Notes:

