## ADAS211: Radiative recombination - process for specific ion file

The program calculates state-selective radiative recombination coefficients to LS-coupled terms in a one-electron Slater type model potential adjusted to observed energies. A template file must be supplied which lists the energy levels and their energies and supplies the electron temperatures at which the coefficients are to be calculated. The template files are built from the energy level lists at the head of adf04 files. The purpose of ADAS211 is to supplement these 'target' adf04 files with radiative recombination data. The code provides two outputs. The first is a set of ' R -lines' containing the radiative recombination coefficients as a function of electron temperature ready for manually editing into the target adf04 file. Secondly, it writes a file of ADAS data format $a d f 08$ with the tabulated results, suitable for archiving. adf08 files, without the computed results, that is just including the energy level lists and requested temperature lines in fact form the input template files. Thus ADAS211 takes an incomplete adf08 file without the coefficients and returns the complete file.

## Background theory:

The basic spontaneous recombination reaction in the vicinity of a $z+1$ times ionised ion $\mathscr{A}^{+z+1}$ in the state $\gamma$ is

$$
\mathscr{A}^{+z+1}(\gamma)+e(E l) \rightarrow \mathscr{A}^{+z}\left(\gamma, n^{\prime} l^{\prime}\right)+h v
$$

The reverse reaction is photo-ionisation and the reaction set is completed by stimulated recombination. $E$ is the initial energy and $E^{\prime}$ the final energy of the jumping electron. The energy of the emitted photon is $h v=E-E^{\prime}$ with $v$ the frequency and $l$ and $l^{\prime}$ are the corresponding orbital angular momenta. An overall constraint of single configuration initial state $\gamma$ and one electron jumps is adopted in this work. Resonances are therefore excluded and the initial parent ion remains unchanged in the process.
The problem is conveniently expressed in terms of Gaunt factors with the bound-free Gaunt factor denoted by $g^{I I}$. The basic formulation given here is in pure configuration RussellSaunders coupling. For many purposes resolution to $L S J$ levels is over precise, term and shell averages being sufficient. Averaging here is considered over whole principal quantum shell $n$, spin system $n S$, shell $n l S$, term $n l S L$ and level $n l S L J$. Whole principal quantum shell resolution is sometimes called the bundle-n picture and shell resolution the resolved-nl picture. In the following paragraphs, the theory is presented for arbitrary resolution. At this time the operation of the code ADAS211 is restricted to term resolution although this constraint will be lifted in the future.

Gaunt factors: It is convenient to introduce some notation. Let $z_{0}$ be the nuclear charge of the ions $\mathscr{A}^{+z}$ and put $z_{1}=z+1$. Introduce $\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{\prime}, \quad \kappa$ and $\boldsymbol{v}^{\prime}$ defined by $\varepsilon=\kappa^{2}=E / z_{1}^{2} I_{H}$ and $\varepsilon^{\prime}=-1 / v^{\prime 2}=E^{\prime} / z_{1}^{2} I_{H} . \quad v^{\prime}$ is the effective principal quantum number for the quantum shell $n^{\prime}$. Denote the spin and orbital quantum numbers of the state $\gamma$ (that is the parent state corresponding to the $z+1$ times ionised ion ) by $S_{p} L_{p}$. At the fine structure resolution level the Gaunt factor is

$$
g^{I I}\left(\left(S_{p} L_{p}\right) \kappa l S L J,\left(S_{p} L_{p}\right) v^{\prime} l^{\prime} S l^{\prime} J^{\prime}\right)
$$

The Gaunt factors at other resolution levels are related by simple sums so that

$$
\begin{align*}
g^{I I}\left(\left(S_{p} L_{p}\right) \kappa,\left(S_{p} L_{p}\right) v^{\prime}\right) & =\sum_{S} g^{I I}\left(\left(S_{p} L_{p}\right) \kappa S,\left(S_{p} L_{p}\right) v^{\prime} S\right) \\
& =\sum_{l, l^{\prime}, S} g^{I I}\left(\left(S_{p} L_{p}\right) \kappa l S,\left(S_{p} L_{p}\right) v^{\prime} l^{\prime} S\right) \\
& =\sum_{l, l, L, L, L^{\prime}, S} g^{I I}\left(\left(S_{p} L_{p}\right) \kappa l S L,\left(S_{p} L_{p}\right) v^{\prime} l^{\prime} S L^{\prime}\right) \\
& =\sum_{l, l^{\prime}, L, L, S, S, J, J^{\prime}} g^{I I}\left(\left(S_{p} L_{p}\right) \kappa l S L J,\left(S_{p} L_{p}\right) v^{\prime} l^{\prime} S L^{\prime} J^{\prime}\right)
\end{align*}
$$

These can be expressed as one-electron integrals as

$$
g^{I I}=\frac{\sqrt{3}}{\pi 2^{4}}\left(\frac{E-E^{\prime}}{z_{1}^{2}}\right)^{4} \frac{1}{\omega_{\gamma}} Q_{i, i^{\prime}} R_{i, i^{\prime}}^{I I}\left(k, v^{\prime}\right)
$$

The $Q_{i, i^{\prime}}$ and $R_{i, i^{\prime}}^{I I}$ are given in the table below for the various resolutions. The $Q_{i, i^{\prime}}$ are shown above the dashed line separator and the $R_{i, i^{\prime}}^{I I}$ below.

| $i \quad \ \quad i^{\prime}$ | $\left(S_{p} L_{p}\right) n^{\prime} l^{\prime} S L^{\prime} J^{\prime}$ | $\left(S_{p} L_{p}\right) n^{\prime} l^{\prime} S L^{\prime}$ | $\left(S_{p} L_{p}\right) n^{\prime} l^{\prime} S$ | $\left(S_{p} L_{p}\right) n^{\prime} S$ |
| :---: | :---: | :---: | :---: | :---: |
| $\left(S_{p} L_{p}\right) n l S L J$ | $\begin{aligned} & (2 J+1)(2 L+1)\left(2 J^{\prime}+1\right)\left(2 L^{\prime}+1\right) . \\ & \left\{\begin{array}{lll} L^{1} & 1 & L \\ J & S & J \end{array}\right\}^{2}\left\{\begin{array}{lll} L^{\prime} & 1 & L \\ l & L_{p} & l \end{array}\right\}^{2} \end{aligned}$ $\left.\frac{\pi v^{\prime 3}}{2} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2}$ | $\begin{aligned} & (2 J+1)\left(2 L^{\prime}+1\right) . \\ & \left\{\begin{array}{lll} L^{\prime} & 1 & L \\ l & L_{p} & l \end{array}\right\}^{2} \end{aligned}$ $\left.\frac{\pi v^{\prime 3}}{2} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2}$ | $\frac{(2 J+1)}{(2 l+1)}$ $\left.\frac{\pi v^{\prime 3}}{2} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2}$ | $\begin{gathered} \frac{(2 J+1)}{(2 l+1)} \\ \left.\frac{\pi v^{\prime 3}}{2} \sum_{l^{\prime}} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2} \end{gathered}$ |
| $\left(S_{p} L_{p}\right) n l S L$ | $\begin{aligned} & (2 L+1)\left(2 J^{\prime}+1\right) . \\ & \left\{\begin{array}{lll} L & 1 & L \\ l & L_{p} & l \end{array}\right\}^{2} \end{aligned}$ $\left.\frac{\pi v^{\prime 3}}{2} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2}$ | $\begin{aligned} & (2 S+1)(2 L+1)\left(2 L^{\prime}+1\right) . \\ & \left\{\begin{array}{lll} L & 1 & L \\ l & L_{p} & l \end{array}\right\}^{2} \end{aligned}$ $\left.\frac{\pi v^{\prime 3}}{2} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2}$ | $\frac{(2 S+1)(2 L+1)}{(2 l+1)}$ $\left.\frac{\pi v^{\prime 3}}{2} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2}$ | $\begin{gathered} \frac{(2 S+1)(2 L+1)}{(2 l+1)} \\ \left.\frac{\pi v^{\prime 3}}{2} \sum_{l^{\prime}} l_{>} \right\rvert\,\langle\kappa l\|---------------- \end{gathered}$ |
| $\left(S_{p} L_{p}\right) n l S$ | $\frac{\left(2 J^{\prime}+1\right)}{\left(2 l^{\prime}+1\right)}$ $\left.\frac{\pi v^{\prime 3}}{2} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2}$ | $\frac{(2 S+1)\left(2 L^{\prime}+1\right)}{\left(2 l^{\prime}+1\right)}$ $\left.\frac{\pi v^{\prime 3}}{2} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2}$ | $(2 S+1)\left(2 L_{p}+1\right)$ $\left.\frac{\pi v^{\prime 3}}{2} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2}$ | $(2 S+1)\left(2 L_{p}+1\right)$ $\left.\frac{\pi v^{\prime 3}}{2} \sum_{l^{\prime}} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2}$ |
| $\left(S_{p} L_{p}\right) n S$ | $\begin{gathered} \frac{\left(2 J^{\prime}+1\right)}{\left(2 l^{\prime}+1\right)} \\ \left.\frac{\pi v^{\prime 3}}{2} \sum_{l} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2} \end{gathered}$ | $\frac{(2 S+1)\left(2 L^{\prime}+1\right)}{\left(2 l^{\prime}+1\right)}$ $\left.\frac{\pi v^{\prime 3}}{2} \sum_{l} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle \mid$ | $(2 S+1)\left(2 L_{p}+1\right)$ $\left.\frac{\pi v^{\prime 3}}{2} \sum_{l} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2}$ | $(2 S+1)\left(2 L_{p}+1\right)$ $\left.\frac{\pi v^{\prime 3}}{2} \sum_{l, l^{\prime}} l_{>}\|\langle\kappa l\| \rho\| v^{\prime} l^{\prime}\right\rangle\left.\right\|^{2}$ |

Derived quantities: The two groups of atomic coefficients relevant for plasma modelling are the photon emission coefficients and the energy emission coefficients. The former enter the statistical balance equations (that is number conservation) and the latter the energy balance
equations. Maxwell averages of the free-bound coefficients are required for thermalised electron plasmas.
The photon emission coefficients $\left(\mathrm{cm}^{3} \mathrm{~s}^{-1}\right)$ is

$$
\frac{16 \pi \alpha^{4} c a_{0}^{2}}{3 \sqrt{3} I_{H}}\left(\frac{2 z_{1}^{2}}{v^{\prime 3}}\right) \frac{z_{1}}{\kappa}\left(\frac{I_{H}}{h v}\right) g_{i, i^{\prime}}^{I I}\left(\kappa, v^{\prime}\right)
$$

The energy emission coefficients ( $\mathrm{erg} \mathrm{cm}^{3} \mathrm{~s}^{-1}$ ) is

$$
\frac{16 \pi \alpha^{4} c a_{0}^{2}}{3 \sqrt{3}}\left(\frac{2 z_{1}^{2}}{v^{\prime 3}}\right) \frac{z_{1}}{\kappa} g_{i, i^{\prime}}^{I I}\left(\kappa, v^{\prime}\right)
$$

The Maxwell averaged photon emission coefficient $\left(\mathrm{cm}^{3} \mathrm{~s}^{-1}\right)$ is

$$
\begin{gather*}
8\left(\frac{\pi a_{0}^{2} I_{H}}{k T_{e}}\right)^{3 / 2} \frac{4 \pi \alpha^{4} c a_{0}^{2}}{3 \sqrt{3} I_{H}} z_{1}^{4}\left(\frac{2}{v^{\prime 3}}\right) \exp \left(z_{1}^{2} I_{H} / v^{\prime 2} k T_{e}\right) \\
\\
\int_{z_{1}^{2} I_{H} / v^{\prime 2} k T_{e}}^{\infty} g_{i, i^{\prime}}^{I I}\left(\kappa, v^{\prime}\right) \frac{e^{-x}}{x} d x
\end{gather*}
$$

that is the familiar radiative recombination coefficient.
The Maxwell averaged energy emission coefficient ( $\mathrm{erg} \mathrm{cm}^{3} \mathrm{~s}^{-1}$ ) is

$$
\begin{gather*}
8\left(\frac{\pi a_{0}^{2} I_{H}}{k T_{e}}\right)^{3 / 2} \frac{4 \alpha^{4} c}{3 \sqrt{3} \pi a_{0}}\left(k T_{e}\right) z_{1}^{4}\left(\frac{2}{v^{\prime 3}}\right) \exp \left(z_{1}^{2} I_{H} / v^{\prime 2} k T_{e}\right) \\
\int_{z_{1}^{2} I_{H} / v^{\prime 2} k T_{e}}^{\infty} g_{i, i^{\prime}}^{I I}\left(\kappa, v^{\prime}\right) e^{-x} d x
\end{gather*}
$$

The interactive ADAS211 program delivers only the Maxwell averaged photon emissivity coefficient at this time.

Calculation of Gaunt factors and radial dipole integrals: Bound-free radial integrals are required for hydrogenic and non-hydrogenic ions. Procedures for their evaluation are according to the following points:

1. For large $l$ the radial integrals are effectively hydrogenic.
2. For small $l$, quantum defects may be large and non-hydrogenic approximations become necessary.
3. Partial $l$ sum rules are available which enable non-hydrogenic radial integrals for low $l$ 's to be combined with hydrogenic sums for high $l$ 's.
4. Calculation time is short for hydrogenic radial integrals but increases sharply with increasing refinement in the non-hydrogenic radial integrals.
5. More elaborate specification of the ion state is required for non-hydrogenic radial integrals, which may not be readily available.

Hydrogenic radial integrals: Recurrence relations in $l$ are convenient for generation of the dipole radial integrals $\left\langle\kappa\left\|\| \rho v^{\prime} l^{\prime}\right\rangle\right.$. The recurrence relations take their simplest form in terms of $\mathscr{G}\left(\varepsilon l, \varepsilon^{\prime} l^{\prime}\right)$ defined by

$$
<\kappa l|\rho| v^{\prime} l^{\prime}>=\sqrt{\prod_{s=1}^{l}\left(1+s^{2} \varepsilon\right) \prod_{s^{\prime}=1}^{l^{\prime}}\left(1+s^{\prime 2} \varepsilon^{\prime}\right)} \mathscr{G}\left(\varepsilon l, \varepsilon^{\prime} l^{\prime}\right)
$$

The 'mixed' recurrence relation is then

$$
\begin{gather*}
(2 l+2) \mathscr{G}\left(\varepsilon l-1, \varepsilon^{\prime} l\right)=(2 l+1)\left[1+(l+1)^{2} \varepsilon^{\prime}\right] \mathscr{G}\left(\varepsilon l, \varepsilon^{\prime} l+1\right)+ \\
{\left[1+(l+1)^{2} \varepsilon\right] \mathscr{G}\left(\varepsilon l+1, \varepsilon^{\prime} l\right)}
\end{gather*}
$$

This form is less widely known than the 'monotonic' forms (that is relating $\mathscr{G}\left(\varepsilon l-2, \varepsilon^{\prime} l-1\right), \mathscr{G}\left(\varepsilon l-1, \varepsilon^{\prime} l\right)$ and $\left.\mathscr{G}\left(\varepsilon l, \varepsilon^{\prime} l+1\right)\right)$ It is very fast and stable for downward recurrence and demonstrates the positive definiteness of the radial integrals. The starting values are

$$
\begin{aligned}
\mathscr{G}\left(\varepsilon n^{\prime}, \varepsilon^{\prime} n^{\prime}-1\right)= & \sqrt{\frac{\pi}{2\left(1-e^{-2 \pi / \kappa}\right.}} \frac{1}{2 n^{\prime 3 / 2}}\left(\frac{4 n^{\prime 2} \kappa^{2}}{1+n^{\prime 2} \kappa^{2}}\right)^{n^{\prime}+2} . \\
& \frac{1}{\left(2 n^{\prime}\right)!} \exp \left[-2 \kappa^{-1} \tan \left(n^{\prime} \kappa\right)\right]
\end{aligned}
$$

and

$$
\mathscr{G}\left(\varepsilon l, \varepsilon^{\prime} l^{\prime}\right)=0
$$

where $n^{\prime}$ is the principal quantum number associated with the effective principal quantum number $v^{\prime}$.

Numerical method for non-hydrogenic radial integrals: We adopt a parametrised effective central potential as a basis for calculating numerical wave functions. The central potential is established by defining a screening configuration,

$$
n_{1} l_{1}^{q_{1}} n_{2} l_{2}^{q_{2}} \ldots . . n_{s} l_{s}^{q_{s}}
$$

such that

$$
q_{1}+q_{2}+\ldots \ldots+q_{s}=z_{0}-z_{1}
$$

The electron in shell $i$ is supposed to be screened from the nucleus by the other electrons in shells $<i$ and partially screened by the other electrons in the shell $i$ itself. So the effective charge for the $i$ th shell electrons is

$$
z_{i}=z_{0}-\sum_{j=1}^{i-1} q_{j}-\frac{1}{2} q_{i}
$$

The adopted (Slater type) potential is then

$$
V(r)=\frac{z_{0}}{r}-\sum_{i=1}^{s} \frac{q_{i}}{r} e^{-\alpha_{i} z_{i} r / n_{i}} r^{n_{i}}\left(\sum_{k=0}^{n_{i}} a_{i k} r^{-k}\right)
$$

The $\alpha_{i}$ are adjustable parameters chosen so that the one electron wave function satisfies the one electron Schrodinger equation with the potential $V(r)$ and the specified eigenenergy $\varepsilon$ and quantum defect $\mu$. In practice, we set $\alpha_{i}=\overline{\alpha_{i}} \alpha$ with the $\overline{\alpha_{i}}$ fixed so that only the overall scaling parameter $\alpha$ is varied to match the observed quantum defect. In the most precise work, the potential is adjusted separately for the bound and free waves using the quantum defect of the bound state and the continuum phase (extrapolated from bound state quantum defect data for the series). This is not possible with the available data from the adf04 file. Thus the potential parameter $\alpha$ is determined from the bound state and then fixed at that value for the free wave.
l-sums and combination of hydrogenic and non-hydrogenic Gaunt factors: Closed analytic expressions are available for the $l$ - summed Gaunt factor $g^{I I}\left(\kappa, n^{\prime}\right)$ in the hydrogenic case, denoted by $g_{H}^{I I}\left(\kappa, n^{\prime}\right)$. A simple fitting to $g_{H}^{I I}\left(\kappa, n^{\prime}\right)$ is

$$
\begin{gather*}
g_{H}^{I I}\left(\kappa, n^{\prime}\right)=1 /\left\{1-\frac{4}{3} \frac{0.1728(u-1)}{n^{\prime 2 / 3}(u+1)^{2 / 3}}+\left(\frac{28}{13}\left[\frac{0.1728(u-1)}{n^{\prime 2 / 3}(u+1)^{2 / 3}}\right]^{2}+\right.\right. \\
\left.\left.\frac{4}{3}\left[\frac{0.0496\left(u^{2}+\frac{4}{3} u+1\right)}{n^{\prime 4 / 3}(u+1)^{4 / 3}}\right]^{2}\right)\right\}^{3 / 4}
\end{gather*}
$$

where $u=n^{\prime 2} \kappa^{2}$. The expression is accurate to $\sim 0.5 \%$ up to the peak of the $g^{I I}$ function and gives approximately the correct asymptotic behaviour at large $\kappa$. The combination of non-hydrogenic Gaunt factors for low $l$ and hydrogenic Gaunt factors for large $l$ to form improved $l$ summed Gaunt factors is simplified by using the $l$ sum rule

$$
\begin{array}{r}
\sum_{l, l^{\prime} \geq l_{0}} g_{H}^{I I}\left(\kappa l, n^{\prime} l^{\prime}\right)=-\left[\frac{n^{\prime 2}\left(l_{0}+1\right)^{-2}+1}{n^{\prime 2} \kappa^{2}-1}\right] g_{H}^{I I}\left(\kappa l_{0}, n^{\prime} l_{0}+1\right)+ \\
{\left[\frac{n^{\prime 2}\left(l_{0}+1\right)^{-2}+1}{n^{\prime 2} \kappa^{2}-1}\right] g_{H}^{I I}\left(\kappa l_{0}+1, n^{\prime} l_{0}\right)}
\end{array}
$$

Then the non-hydrogenic Gaunt factor is given by

$$
g^{I I}\left(\kappa l, v^{\prime} l^{\prime}\right)=\sum_{l, l^{\prime}<l_{0}} g^{I I}\left(\kappa l, v^{\prime} l^{\prime}\right)+\sum_{l, l^{\prime} \geq l_{0}} g_{H}^{I I}\left(\kappa l, n^{\prime} l^{\prime}\right)
$$

Integrals of Gaunt factors: The integral $\int_{x_{0}} \frac{g^{I I} e^{-x}}{x} d x$ is evaluated numerically by Gaussian techniques. Accuracy is improved by treating separately the range $\int_{x_{0}}^{1}$ for $x_{0}$ small and by subtracting the analytic integrals obtained by setting $g^{I I}$ constant at the threshold value prior to numerical integration.

## Program steps:

These are summarised in figure 2-11
Figure 2-11


## Interactive parameter comments:

Move to the directory in which you wish the output text file produced after executing any ADAS program (paper.txt is the default) to appear. There is no graphic output from this program. Initiate ADAS211 from the program selection menus in the usual manner.
The file selection the appearance shown below:


1. adf08 in template form is the appropriate format for use by the program ADAS211. Your template data should be held in such a file, in the same directory structure as central ADAS, but with your identifier replacing the first adas. You should finally, if the code operates correctly replace you adf08 template file with the adf08 type output file.
2. Available sub-directories are shown in the large file display window at b). Scroll bars appear if the number of entries exceed the file display window size. There are a large number of these. They are usually stored in sub-directories by isoelectronic sequence of the recombining ion. It is useful to use a naming convention for the final part of the file name which includes the ion and 'LS' (eg. blike/blike_c1ls.dat) to indicate that the data is for terms.
3. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then the individual datafiles are presented for selection. Datafiles all have the termination .dat.
4. Once a data file is selected, the set of buttons at the bottom of the main window become active.
5. 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 has gone into the dataset and the attribution of the dataset. The possibility of browsing the comments appears in the subsequent main window also.
6. Clicking the Done button moves you forward to the next window. Clicking the Cancel button takes you back to the previous window
7. There is no processing options window for ADAS211.
8. The output options window is shown below. There is no graphical output possibility but in addition to the usual text file, two output data files may be produced.
9. The data output file called the Specific Ion Output is activated by the button at a). The default file name is data04.pass and it is sent to your pass directory. It is prepared preformatted according to 'R-lines' for adf04 files and can be patched directly into the adf04 file, which was used as reference for the template input adf08 file, at the foot of the transition list before the terminator. See central ADAS for examples.
10. The second output file at b), called the Resolved Recombination Output is sent by default as data08.pass to your pass directory. Assuming the code has worked correctly, it is a direct replacement for the template adf08 file. It simply includes all the state selective recombination coefficient results requested below the temperature lines in the template.
11. As the calculations may take some time, the option is given of executing in the background. There are therefore two ways in which output can be generated:
12. By pressing Run Now at d), you can wait for the output to be generated before continuing. When this option is taken a small information box opens showing the progress the program has made. This is shown below. Once this has been done the calculations cannot be halted, but an execution time of less than 30 seconds can usually be expected.

13. By pressing Run in Batch the actual calculations required to produce the output are run at a later time, but it is necessary for a batch file containing all relevant data to be created or updated. Again a small information box opens showing the progress made in doing this. The process will normally be considerably quicker than when pressing Run Now. A larger batch job can be built up by returning to the Processing Options Window and making new selections before returning to the Output Options Window and again clicking on Run in Batch. When you exit the Processing Options Window of ADAS211 by clicking on Cancel to return to the Input Options Window, the program takes this as a signal that the batch job is completed and submits it for execution. A small information box opens giving the name of the job and information on when execution will begin. Calculations run in this way will normally run more quickly than those run using the Run Now button. When the batch job is complete, the output files are generated and a mail message sent from the operating system to say that it is finished. This will normally contain a simple message which says 'Your batch job has completed successfully'. It is possible to build a queue of batch jobs by submitting one as described above, constructing another and submitting that in the same way, but due to the relatively short time taken by the calculations it is not anticipated that this will happen very often.


## Illustration:

Table 3.11a shows the template data set for calculation of state selective radiative recombination coefficients for $C^{+3}+e \rightarrow C^{+2}+h v$. There is only a single (nprnti=l) recombining parent term $2 s{ }^{2} S$. which appears under the Parent Term Indexing. The target terms (ntrm=0) of the recombined ion then follow under the LS Resolved Term Indexing. Finally the electron temperature list is given $(T e=\ldots)$. For this last line use the precise
positioning of the 'key' $T E=$, and the position and format of the electron temperatures (maximum of 14).

Table 3.11a


Table 3.11b shows the final adf08 output file. Note that the recombination coefficients now appear as a function of term index and electron temperature. If their are more than one parent, then dashed half lines separate the capture from each of them into blocks. The parent index (Prti), parent term assignment (Trmprt) ansd parent spin (Spnprt) of the relevant parent immediately follows the dashed half line.

Table 3.11 c shows the ' $R$-lines' which should be edited into the target adf04 file. Usually, these areplaced after the electron impact excitation lines. The descriptive comments should be pasted at the end of the comments in the target adf04 file and you should add your name as a matter of course in case the updated adf04 file is used by others.

Table 3.11 d shows the paper.txt standard text output file from the program. This is essentially diagnostic check data monitoring the course of the calculation. Note the entries under Alfa Estimated and Calculated. In its search for the potential scaling parameter, the program initially sets it to 1 . The final calculated values is usually a bit less than 1 . Values down to $\sim .5$ are not a cause for alarm, but very large values are. If this occurs check the ionisation energies of the levels and hence their quantum defects. If the quantum defect is negative the program cannot find the scaling parameter. In these circumstances, the program puts in hydrogenic values for the recombination coefficient. Such cases may warrant more detailed study.

Table 3.11b


Table 3.11c


Table 3.11d


Notes

