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# Atomic Data and Analysis Structure User Manual, Special Edition for Solar Astrophysical Applications 

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# Atomic Data and Analysis Structure 

User manual
Special edition for solar astrophysical appilcations

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## Introduction

The Atomic Data and Analysis Structure (ADAS) is an interconnected set of computer codes and data collections for modelling the radiating properties of ions and atoms in plasmas and for assisting in the analysis and interpretation of spectral measurements. The strucuure has both interactive and non-interactive capabilities. The interactive part provides immediate display of important fundamental and derived quantities used in analysis together with a substantial capability for exploring parameter dependences and diagnostic predictions of atomic population and plasma models. The second part is non-interactive but provides a set of subroutines which can be accessed from the user's own codes to draw in necessary data from the derived ADAS database.

## Solar analysis objectives

This manual focusses on a subset of ADAS relevant to basic atomic modelling tasks required in spectroscopic studies of the solar upper atmosphere. These include examining emission spectrum lines and the relative intensities of such lines. Ratios of intensities are frequently used for diagnosis of temperature and density in the solar atmosphere. Theoretical input for this is provided by ADAS in a series of codes concerned with excited populations of ions, called series 2. Two ADAS2 series codes, ADAS205 and ADAS207, of special relevance, are described here. The ionisation state of ions in the solar atmosphere is another key piece of information for absolute intensity studies. ADAS4 series codes concentrate on this area with ADAS405, which evaluates equilibrium ionisation balance, described here. Theoretical line emission functions are a necessary ingredient of most analyses. Two codes from ADASS series, which provide such an analysis path are described here. ADAS506 allows interrogation of large collections of theoretical emission functions and their organisation for what has become a standard 'inverse' approach - differential emission measure analysis (DEM). ADAS509 is such a DEM code.

It is all too easy to be overwhelmed with atomic data, especially since modern atomic structure and collisional codes can mass produce such data. Two special codes, ADAS209 and ADAS210 from ADAS2 series are provided to render some assistance in some situations which commonly arise. ADAS itself however is organised in a manner to cope with large flows of numerical data.

Many spectral analyses of the solar atmosphere have ultimately been left in doubt because of real or imagined inaccuracy in the theoretical atomic inputs such as the emission functions. ADAS has a deep capability for investigating and validating such data. Some of this advanced capability is described in the last chapter of this manual. Relevant are ADAS502, ADAS503 and ADAS208. ADAS405, referred to earlier contributes also to this deeper analysis.

## General organisation

The various ADAS routines are essentially of two types, namely those which are interrogative on the ADAS database (both fundamental and derived parts) and those which execute atomic modelling calculations. The latter may relay substantial quantities of data for further processing or for addition to the derived database.
In the interrogative codes, the principle objective has been to allow graphical display of any part of the database. All codes satisfy this quick look and check facility. In ADAS interrogation codes, cubic spline interpolation is performed on the source data from the database. These interpolated values are given as convenient printer tabulations. Atomic modelling codes generally create output data sets as well as normal tabular output. These files are structured according to the requirement of the ADAS data base or for futher ADAS programs. It is anticipated that the user will edit these files into standard ADAS named files when establishing a personal database after being satisfied of their correctness.
ADAS as a whole is organised into the five code series shown below. In technical terms there objectives are as follow: ADAS1 is concerned with fundamental, that is essentially individual reaction data. This is to be distinguished from the composite effects of many processes which are the subject of the rest of ADAS. ADAS2 is concerned with evaluating excited populations of specific ions in a plasma environment and then their radiation emission. It relies on availability of a reaction rate data collection for the ion in the ADAS database although ADAS has some provision for generating an approximate collection of such data when this is not so. ADAS3 is of special interest to fusion applications. ADAS4 is concerned with the ground and metastable populations of ions in a plasma and particularly their preparation and calculation for dynamical plasma models. It therefore operates with generalised collisional dielectronic recombination and ionisation coefficients, associated power loss coefficients and metastable fractions. It also mediates a transfer from an isoelectronic sequence storage of data which is the preferred choice for atomic data preparation and manipulation to an isonuclear sequence storage preferred for applied studies in dynamical plasma models. ADAS5 provides a set of supplementary programs interrogating data collections in the derived database. The data classes addressed are those which have been found of particular importance for reduction of calibrated observed data. ADAS6 series has data analysis codes.

| Series | Content |
| :--- | :--- |
| ADAS1 | Entry and validation of fundamental atomic data |
| ADAS2 | Excited state populations of ions in a plasma |
| ADAS3 | Charge exchange related emission |
| ADAS4 | Recombination, ionisation and radiated power |
| ADAS5 | Supplementary programs |
| ADAS6 | Data analysis programs |

There are 24 distinct data types in the ADAS databases. Each data set type has its layout and content precisely described. These prescriptions are called ADAS data formats or ADFs and must be rigidly adhered to in preparation of personal data for use by the ADAS package. A full description of all the ADAS data formats is given in appendix B of the main manual. These formats apply both to fundamental and derived data. The most important here are

| ADF04 | resolved specific ion data collections |
| :--- | :--- |
| ADF07 | direct resolved electron impact ionisation coefficients |
| ADF11 | isonuclear master files |
| ADF15 | photon emissivity coefficients |
| ADF20 | G(Te) functions |

## ADAS on a Unix workstation

The interactive ADAS is intended for use by the non-specialist but informed user. It is implemented as a shell command on the Unix workstations. Some preliminaries are necessary. It is assumed that the user has basic knowledge of Unix command structure and experience of a typical 'desktop'.

## Initial checks

$$
\begin{array}{ll}
c d / \text { /isk2/<user identifier> } & \text { Change to your home directory } \\
\text { is } & \text { Check file and directories present }
\end{array}
$$

If the directory/adas is not present create it.
mkdir adas
cd adas
mkdir defaults
mkdir pass
mkdir scripts405
mkdir arch 101

Make you personal adas database top directory
Move into the directory adas
Make a defaults directory if it does not exist
Make a passing file directory if it does not exist
Make a script file directory for ADAS405 if it does not exist

Make an archive file directory for ADAS101 if it does not exist

Sub-directories for various ADAS data formats may be created here if you wish to make up a personal adas database and they are not already present. For example
mkdir adf04
Create an ADF04 subdirectory
Central ADAS data has the directory path /disk2/adas/adas on the SOLG DEC ALPHA workstations. You can look at them.

| $c d /$ disk2/adas/adas/adf04/belike | move to a Be-like specific ion file sub-directory |
| :--- | :--- |
| ls | list data files available |
| cat belike jll990o.dat | list a particular file for $\mathrm{O}^{+4}$ prepared by J. Lang |

## Starting ADAS

| $c d /$ disk2/<user identifier> | return to your home directory |
| :--- | :--- |
| adas | start ADAS |

The top level ADAS selection menu should be displayed as below


## Central ADAS documentation

## Documentation is placed in the/disk2/adas/docs directory under three headings

1. Bulletins: files named as /disk2/adas/docs/bulletin/<date>.ps where <date> is of the form <month><day>-<year> [eg. mov18-94 (this bulletin)].
2. Usernotes: files named as /disk2/adas/docs/usernotes/<library code>/<code name>.ps
where <library code> is the associated Fortran library name [eg. adaslib, adas2xx, etc.]
and <code name> is the Fortran subroutine name [eg. ssxb, xissxb etc.]
3. Manual: files named as /disk2/adas/docs/manual/chap<i>-<nn>.ps where $<\mathrm{i}>$ denotes chapter number from the ADAS User Manual and <nn> denotes the sub-chapter. The manual has been split into these sub-chapters for easy of interrogation.

All these files are 'postscript' files.


To look at the files, activate a CDA viewer tool:
axvdoc
bring up CDA viewer window
Button select FILE FORMAT choice PS
Double click on directory names to move to required sub-directory
Click on required file to select it
Button select $O K$
To terminate CDA viewer
Button select FILE at top left of window
Button select EXIT on drop down menu.

## Table Editor

A necessary operation in interactive ADAS is catry of user values into a table. Since this is common to many ADAS programs, a special widget has been doveloped to assist in this tank. To avoid repetition in the description of each code, a summary of how to use Table Editer is given here. A typical appearance is shown below

| Tempersture \& Donity Vatues |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| Index | Ortput | Input | Outpux | Input |
| 1 | $1.0003+00$ | $1.0008+00$ | $1.0000+18$ | $1.0000+11$ |
| 2 | $20008+\infty$ | $20000+00$ | 1.000 $0+18$ | $20000+11$ |
| 3 | $500085+00$ | 60008+00 | 1.0003+18 | 50000 +11 |
| 4 | $1.0005+01$ | $10006+01$ | $1.00003+18$ | $1.0000 \cdot 12$ |
| 5 | $20006+01$ | $20006+01$ | $1.0000+18$ | $20006+12$ |
| 6 | $500015+01$ | S.000E+01 | 1.0000718 | 40000 +12 |
| 7 | $1.0008+02$ | $10008+00$ | 1.000 ${ }^{1}+18$ | $1.00000^{2} 13$ |
| 8 | 2000E+02: | $2000 \mathrm{E}+02$ | 1.0000+18 | $20008+13$ |
| 9 | $50008+02$ | $1.000 \mathrm{E}+00$ | 1.000E+18 | $500008+13$ |
| 10 | $1.0006+03$ | 1000E 003 | 1.0003618 | 1.0000 +14 |
| $\triangle$ Delet | $\triangle$ Pemow | $\triangle$ Inmert | $\triangle$ Copy | $\triangle$ Prase |
| - Row |  | nstip | Scroll up | Scroll down |
| Tempersture Units |  |  |  |  |
| Kelvin eV Hectucad |  |  |  |  |
| Cancel Done |  |  |  |  |

1. The values in italic font are your input data. Click in any of these boxes to edit the number within it. The workstation cut, paste and copy keys operate. Press the return key on the keyboard to record any change.
2. The set of triangular and square buttons below the table are designed to help in some editing tasks. You must be careful to remember the sequence of operations since it is different from that on personal computers. Activate the appropriate button, position the mouse text cursor or drag over required digits, press the return key on the keyboard to complete the sequence. Triangular buttons operate for the next immediate action. Square buttons have a continuing effect until an alternative is pressed. The Delete button allows deletion of the value in a box, leaving an empty box; the Remove button allows deletion of a value with the column then being pushed up; the Insert button creates a new empty box, pushing the column down. The Row skip button causes a jump to the next editable box in a row when the return key on the keyboard is pressed; Column_skip causes jumping to next box in a column. Scroll up moves the whole window down. Note that the window only shows ten values in a column, but the whole table may be longer that this. Preferred Temperature units for working with may be chosen. Changing units causes the Inputs from the file to change to the new units. It does
net change any Output values already typed in. It merely interprets Output values in the selected units.
3. Press the Done button to record the changes and return to the screen from which Table Editor was initiated. The Cancel button prevents the new values being substituted on return.

## Graph Editor

In the fundamental data entry and verification sections of interactive ADAS, flexibility in adjustment, deletion and insertion of points on a displayed comparative graph is useful. Since this is common to a number of ADAS programs, a special widget has been developed to assist in this task. To avoid repetition in the description of each code, a summary of how to use Graph Editor is given here. A typical appearance is shown below


1. A Typical Graph Editor window as shown below. Input values are displayed as circles. In this particular illustration, a least squares spline fit is made to these tabular points. The spline passes through five special knot points which are distinguished. The points can be modified by using the buttons a) beneath the graph in association with the mouse. The knot points may only be moved vertically and a special button is present for this case.
2. To move a point, click the move a point button. Then use the left mouse button to pick and drag a point to a new position. Note that the $x$-ordering of points
should be maintained although not forcod by the editor. Each point has a small active zone around it for picking by the mouse. Terminute point moving operations by pressing the right mouse button. To delete a point, click the delete a point button. Then click the left mouse button with the pointer over the point to be deleted. Terminate point deletion operations by prossing the right mouse button. To add a new point in the x-ordered position between two existing points, click the add $X$-point button. Then click the leff mouse button with the pointer at the position where the new point is to be inserted. Terminate point insertion operations by pressing the right mouse button. For completeness, the capability for adding a point anywhere is given although physically unreasonable. The operation is slightly different. Click the add amywhere button. With the left mouse button pick a point after which you wish the new point added. Press the left mouse button with the pointer at the insertion point. Multiple insertions may be made by continuing to click the left mouse button. Click the right mouse button to terminate this particular insertion. Press the right mouse button a second time to terminate insertion operations.
3. To insert a point by value use sub-window $b$ ).
4. The buttons at c) provide the usual cancel, print and done options. In addition the help button displays some information on using the graph editing facilities. The original data and graph can be restored by clicking the refresh button. Note that after leaving the graph editor window with the done button, the modified and or additional points replace the original user input data. Note that with the ADAS analysis option, if any points are modified, the program cycles back to the Output Options window for reanalysis. With the Burgess analysis option, movement only of the spline knots does not force reanalysis.

## Populations and line ratio studies

Two programs from ADAS2 series are presented in this section. They are designed to allow detailed study of theoretical emissivities of spectrum lines from a selected ion in a thermal plasma. The two programs are linked. The starting point is a collection of 'complete' reaction data for an identified group of levels of an individual ion, called a specific ion file (type ADF04). Such a dataset can include state selective recombination, charge exchange recombination, electron impact ionisation and ion impact excitation coefficient data, but the primary content is electron impact excitation data. The electron impact excitation data in such files are individually prepared for the highest precision but can also be produced semiautomatically by direct calculation or, for members of prepared isoelectronic sequences, by another ADAS2 series program. The excited level populations are calculated at an array of temperatures and densities in the quasi-equilibrium approximation with respect to identified metastables of the ion. The basic program for this is ADAS205 and it produces plots and tables of populations and prepares two output files. The first of these is a file of metastable fractions (MET) which is not of special interest at this stage. Secondly it produces a temporary 'passing' file of the complete population set for use by the program ADAS207. ADAS207 is a program which supports diagnostic line studies by plotting line emissivities and emissivity ratios as functions of temperature, density or as contours in the temperature/density plane. It is particularly useful for evaluating line ratios as potential density or temperature indicators. The organisation, data sets and linkages between the programs are shown in figure 2.0.
It should be mentioned that ADAS2 series has a second stream of advanced population modelling concerned with the prediction of effective recombination and ionisation coefficients in finite density thermal plasma. Details are given in the main ADAS User Manual. The final stage of this second stream is production of the most refined photon emissivity (PEC), and generalised collisional-radiative (GCR) data by the program ADAS208. This is an advanced version of ADAS205. A description of the use of ADAS208 is given in the last section of the present manual.

Figure 2.0


ADAS205
Process metastable and excited populations


ADAS207
Process
line emissivities

## ADAS205: Specific z excitation - process metastable and excited state populations

The program calculates excited state and metastable state populations of a selected ion in a plasma of specified temperatures and densities by drawing on fundamental energy level and rate coefficient data from a specific ion file of type ADF04.

## Background theory:

Consider ions $X^{+z}$ of the element $X$. The adjacent ionisation stages are $X^{+z+1}$ and $X^{+2-1}$. Let the levels of the ion $X^{+z}$ be separated into the metastable levels $X_{p}^{+1}$, indexed by Greek indices, and excited levels $X_{i}^{+;}$, indexed by Roman indices. The collective name metastable states as used here includes the ground state. The driving mechanisms considered for populating the excited levels $X_{i}^{+:}$are excitation from the metastable levels $X_{p}^{+8}$ and recombination from the ground level of the adjacent ion $X_{1}^{+z+1}$. The dominant population densities of the ions in the plasma are those of the levels $X_{\rho}^{+2}$ and $X_{1}^{+z+1}$, denoted by $N_{p}$ and $N_{1}^{+}$respectively. They, or at least their ratios 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 quasistatic 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. The statistical balance equations take the form

$$
\sum_{j=1}^{O} C_{i j} N_{j}=-\sum_{\sigma=1}^{M} C_{i \sigma} N_{\sigma}+N_{e} N_{i}^{+} r_{i}+N_{e} N_{H} q_{i}^{(c x)} \quad i=1,2, . .
$$

where the dominant populations (excluding the electron density) have been taken to the right hand side. The $C_{i j}$ and $C_{i \sigma}$ are elements of the collisional-radiative matrix, $r_{i}$ is the free electron recombination coefficient directly to the level $i$ and $q_{1}^{(C X)}$ is the charge exchange recombination coefficient from neutral hydrogen to the level $i$. The element $C_{i j}$ of the collisional-radiative matrix is composed as

$$
C_{i j}=-A_{j \rightarrow i}-N_{e} q_{j \rightarrow i}^{(e)}-N_{p} q_{j \rightarrow i}^{(p)} \quad i \neq j
$$

where $A_{j \rightarrow i}, q_{j \rightarrow i}^{(e)}$ and $q_{i \rightarrow i}^{(p)}$ are the rate coefficients for spontaneous transition, electron induced collisional transition and proton induced collisional transition respectively.

$$
C_{i i}=\sum_{j<i} A_{i \rightarrow j}+N_{e} \sum_{j \neq i} q_{i \rightarrow j}^{(e)}+N_{p} \sum_{j \neq i} q_{i \rightarrow j}^{(p)}+N_{e} q_{i}^{(I)}
$$

is the total loss rate from level $i$, with $q_{i}^{(\prime)}$ the electron impact ionisation rate coefficient.
The solution for the ordinary populations is

$$
\begin{align*}
N_{j}= & -\sum_{i=1}^{o} C_{j i}^{-1} \sum_{\sigma=1}^{M} C_{i \sigma} N_{\sigma}+\sum_{i=1}^{o} C_{j i}^{-1} r_{i} N_{e} N_{1}^{+} \\
& +\sum_{i=1}^{o} C_{j i}^{-1} q_{i}^{(C X)} N_{H} N_{1}^{+} \\
\equiv & \sum_{\sigma=1}^{M} F_{j o}^{(e x c)} N_{e} N_{\sigma}+F_{j}^{(n e c)} N_{e} N_{1}^{+}+F_{j}^{(C X)} N_{H} N_{1}^{+}
\end{align*}
$$

where the $F_{k}^{(e x c)}, F_{j}^{(r e c)}$ and $F_{j}^{(C X)}$ are the effective contributions to the excited populations from excitation from the metastables, from free electron capture and from charge exchange recombination from neutral hydrogen 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 all the level populations of the ion $X^{+z}$, that is of metastables as well as ordinary levels relative to metastables, may also be obtained from the equations

$$
\sum_{\sigma=1}^{M} C_{\rho \sigma} N_{\sigma}=-\sum_{j=1}^{o} C_{\rho j} N_{j}+N_{e} N_{1}^{+} r_{\rho}+N_{e} N_{H} q_{\rho}^{(C X)}
$$

Substitution of the quasi-equilibrium solution for the ordinary levels, eqn. 3.5.4, gives

$$
\begin{gather*}
\sum_{\sigma=1}^{M}\left(C_{\rho \sigma}-\sum_{j=1}^{o} C_{\rho j} \sum_{i=1}^{o} C_{j i}^{-1} C_{i \sigma}\right) N_{\sigma}=N_{e} N_{i}^{+}\left(r_{\rho}+\sum_{j=1}^{o} C_{\rho j} \sum_{i=1}^{o} C_{j i}^{-1} r_{i}\right) \\
+N_{H} N_{1}^{+}\left(q_{\rho}^{(C X)}+\sum_{j=1}^{o} C_{\rho j} \sum_{i=1}^{o} C_{j i}^{-1} q_{i}^{(C X)}\right)
\end{gather*}
$$

Solution of these equations gives an expression for the metastable populations $N_{\sigma}$ of the form

$$
N_{\sigma} \equiv F_{\sigma}^{(e x c)} N_{1}+F_{\sigma}^{(r e c)} N_{e} N_{1}^{+}+F_{\sigma}^{(C X)} N_{H} N_{1}^{+}
$$

The effective contributions to the metastable population densities (excluding the ground level) are expressed relative to the ground population density. Note also that a full equilibrium with respect to the adjacent $X^{+z+1}$ ion population density is not established. The ratio $N_{1} / N_{1}^{+}$ may be specified arbitrarily in establishing actual population densities. The metastable to ground fractions in equilibrium if only excitation is included are the $F_{\sigma}^{(e x c)}$. Substitution of eqn. 3.5 .7 in eqn. 3.5 .4 gives the full statistical equilibrium population densities for the ordinary levels in terms of the ground population density and adjacent ion population density.

$$
\begin{align*}
N_{j}= & \sum_{\sigma=1}^{M} F_{j \sigma}^{(e x c)} F_{\sigma}^{(e x c)} N_{e} N_{1}+\left(F_{j}^{(r e c)}+\sum_{\sigma=1}^{M} F_{j \sigma}^{(e x c)} F_{\sigma}^{(r e c)}\right) N_{e} N_{1}^{+} \\
& +\left(F_{j}^{(C X)}+\sum_{\sigma=1}^{M} F_{j \sigma}^{(e x c)} F_{\sigma}^{(C X X)}\right) N_{H} N_{1}^{+}
\end{align*}
$$

With densities $N_{e}, N_{p}$ and the ratios $N_{H} / N_{e}$ and $N_{1} / N_{1}^{+}$specified, the full equilibrium population densites relative to the ground level population density may be computed.

## 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 (appendix C). The scope of operation of ADAS205 is determined by the content of the specific ion file processed. The miminum 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 dexcitation 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. Proton induced rates, free electron recombination rates and charge exchange recombination rates may only be activated in the code if such data are 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. The code
sorts the transition lines in the specific ion file into the allowed categories. Specific ion files can include additional data for the more complex excited thate population calculations of code ADAS208. Such additional date, if present, are ignorod by ADAS205. Centrally supported, specific ion data collections are archived in pertitioned data sets. The status of these is described in the appendices.
Note that ADAS205 can only make use of free electron recombination data from the ground level of the adjacent stage. Data from metastable levels of both higher and lower adjecent stages can be present in specific ion files but the code ADAS208 must be used to access them. ADAS205 allows inclusion of a simple ionisation rate (ECIP approximation) from excited levels, however a self consistent three-body recombination coefficient in detailed balance is not calculated or included. Nor is there any correction for higher excited levels not explicitly included in the specific ion file. These more complete aspects are handled by the advanced excited population code ADAS208. Extra information, which must be present in specific ion files ADF04 to allow these extensions are ignored by ADAS205.

## Program steps:

These are summarised in fig. 2.5.
Figure 2.5

begin $>$\begin{tabular}{c}
Select specific <br>
ion file

,$\quad$

Read and verify <br>
specific ion <br>
file

$\quad A>$

Enter user <br>
data and <br>
selections

,$>$

Calculate <br>
population <br>
densities
\end{tabular}

## repeat

repeat
Output tables

and graphs end $\quad$\begin{tabular}{c}
Display <br>
population <br>
graphs

$<$

Select tabular <br>
and graphical <br>
output options
\end{tabular}$<$

## 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 .dot.
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. Clicking the Done button moves you forward to the next window. Clicking the Cancel button takes you back to the previous window


The processing options window has the appearance shown below

1. 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.
2. The densities table is handled in like manner. 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 $N_{H} / N_{e}$ and $N\left(z_{1}\right) / N(z)$ are only used if neutral hydrogen charge exchange data and free electron recombination data are present in input ADF04 file. These ratio vectors are specified at each electron density so the ratio 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 twodimensional electron temperature/electron density grid.
3. 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. See the main ADAS USER Manual for a detailed explanation of the handing of metastables in the collisional-radiative picture.
4. Various processes, supplementary to the primary electron excitation collisions and bound-bound radiative transitions, are activated as desired by clicking on the
appropriate buttons d). Nove again these onty have an efficet 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. Warniag-ionisation should not be switched on if you have included autoionising levels in your ADFO4 dataset but have omitted the details of alternative thresholds etc present in advanced ADF04 files.
5. 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 e).


The output options window has the appearance shown below

1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the Browse comments button is available.
2. 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.

3. Hard copy is activated by the Enable Hard Copy button c). The File name box then becomes editable. If the output graphic file already exits and the Replace button has not been activated, a 'pop-up' window issues a warning.
4. A choice of output graph plotting devices is given in the Device list window d). Clicking on the required device selects it. It appears in the selection window above the Device list window.
5. 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.
6. The Contour File button b) should be activated to write the passing file for use by the diagnostic line ratio program ADAS207. There is no arrangement for permanent storage of such files which reside only in a user's file space and are generally prepared for temporary immediate use. Usually in ADAS we store such temporary 'passed files' in a pass sub-library. You should create this at the first level within the adas database as

> /...../<uid>/adas/pass

By default ADAS205 sends the contour file to
/...../<uid>/adas/pass/contour.pass
7. The METPOP File button b) should be activated to write a passing file of metastable population fractions. It is of data format ADF11 and can be used in
ionisation/recombination applications of ADAS4 series programs. It goes by default into

## /...../<uid>/adas/pass/metpop.pass

8. The graph is displayed in a following Graphical Outpat when the Dove button is pressed.
9. 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.
10. Press the Next button to show the next graph in a sequence and the Previous button to show the previous graph.
11. Press the Print button to make a hard copy of the currently displayed picture.
12. Pressing the Done button restores the previous Output Options window.

## Illustration:

The output from the program is shown for the lithium-like ion $\mathrm{O}^{+5}$. The specific ion file is assembled from the data of Sampson and co-workers.
Figure 2.5a


The tabular output is shown in table 2.5.

Table 2.5


| nomx | coneroweation | (28+1) |  | ..... mand R (wave minter sc | (ryeberge) | macher ributive (wave mumber <c | tiow porimis (xymerga) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 2 | (2)01 | 0.51 | 0. | 0.0000000 | 1314000. | 10.1515370 |
| 2 | 1 | (2)11 | 0.51 | 96377. | 0.8782492 | 1017623. | 9.2732678 |
| 3 | 1 | (2) 11 | 2.51 | 96909. | 0.8631017 | 1017091. | 9.2684199 |
| 4 | 1 | (2)01 | 0.51 | 640009. | 5.1322054 | 473991. | 4.3193260 |
| 5 | 1 | (2)12 | 0.51 | 666185. | 6.0707356 | 447825. | 4.0807926 |
| 6 | 1 | (2) 21 | 1.51 | 666365. | 6.0723758 | 447635. | 4.0791523 |
| 7 | 1 | (2)21 | 2.5) | 674995. | 6.1510256 | 439005. | 4.0005099 |
| - | 1 | (2)21 | 2.5) | 675042. | 6.1514457 | 438958. | 4.0000816 |
| , | 1 | (2)01 | 0.51 | 852529. | 7.7688343 | 261471. | 2.3827003 |
| 10 | 1 | (2)11 | 0.51 | 863192. | 7.0659938 | 250809. | 2.2855409 |
| 12 | 1 | (2)11 | 1.5) | 863267. | 7.1866966 | 250733. | 2.2848484 |
| 12 | 1 | (2)21 | 1.5) | 867030. | 7.9009738 | 246970. | 2.2505574 |
| 13 | 1 | (2)21 | 2.5) | 867050. | 7.9011542 | 246950. | 2.2503751 |
| 14 | 1 | (2)31 | 2.5) | 168022. | 7.9100145 | 245978. | 2.2415176 |
| 15 | 1 | (2)31 | 3.5) | 168032. | 7.9101038 | 245968. | 2.2414265 |
| 16 | 1 | (2)01 | $0.5)$ | 948412. | 1.6425836 | 165588. | 1.5089496 |
| 17 | 1 | (2)11 | 0.5) | 953761. | 0. 6913238 | 160239 | 1.4602060 |
| 18 | 1 | (2)11 | 1.5) | 953798. | 6. 6916637 | 160202. | 1.4598688 |
| 19 | 1 | (2)21 | 2.5) | 955738. | 8. 7093432 | 158262. | 1.4421902 |
| 20 | 1 | (2)21 | 2.5) | 955748. | 8.7094334 | 158252 | 1.4420991 |
| 21 | 1 | (2)31 | 2.5) | 956201. | 8.7135633 | 157799. | 1.4379710 |
| 22 | 1 | (2)31 | 3.5) | 956205. | 8.7136034 | 157795. | 1.4379346 |
| 23 | 1 | (2)41 | 3.5) | 956672. | 8.7178535 | 157328. | 1.4336790 |
| 24 | 1 | (2)41 | 4.5) | 956674. | 8.7178736 | 157326. | 1.4336607 |


| ruoux | (kalvin) | (ov) | (reduced) |
| :---: | :---: | :---: | :---: |
| 1 | $1.000 \cdot 04$ | 1.55D+00 | 5.00D+02 |
| 2 | 3.600+04 | 3.10D+00 | 1.00D+03 |
| 3 | $7.200+04$ | 6.20D+00 | $2.00 \mathrm{D}+03$ |
| 4 | 1.200005 | $1.55 \mathrm{D}+02$ | 5.00D+03 |
| 5 | 3.600+05 | 3.100+01 | 1.00D+04 |
| 6 | $7.20 \mathrm{D}+05$ | 6.20D+01 | $2.00 \mathrm{D}+04$ |
| 7 | 1.400.06 | 1.55D+02 | 5.000+04 |
| - | 3.600.06 | 3.10D+02 | 1.00D+05 |


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## Notes:

## ADAS207: Metastable and excited population process line emissivities

The program evaluates and displays line emissivities and their ratios for an ion. It uses a passing file of excited population data from the code ADAS205.

## Background theory:

Consider emissivities of spectrum lines arising from a single ionisation stage. Ratios of such lines are frequently used as temperature, density or transient state diagnostics in plasmas. The primary advantage of seeking such ratios of lines from a single ionisation stage is that they are independent of the stage to stage ionisation balance (often uncertain). In general it is matter of some investigation to identify the most diagnostically useful ratios. The present program is designed to aid such investigation.

A necessary preliminary to evaluating line emissivities is a calculation of populations of excited states of the ion as a function of plasma parameters. This is provided by ADAS205 which must be executed before ADAS207. In practice, problems of line blending and the spectral resolution of spectrometers mean that it is useful to work with line groups rather than just individual lines. A line group is a set of lines conveniently or necessarily measured together. ADAS207 deals with two line groups which are built up by the user in the data entry section of the code.
From equation 2.5.4, the solution for the ordinary populations is

$$
N_{j}=\sum_{\sigma=1}^{M} F_{j \sigma}^{(e x c)} N_{e} N_{\sigma}+F_{j}^{(r e c)} N_{e} N_{i}^{+}+F_{j}^{(C X)} N_{H} N_{i}^{+}
$$

where the $F_{j \sigma}^{(e x c)}, F_{j}^{(r e c)}$ and $F_{j}^{(c x)}$ are the effective contributions to the excited populations from excitation from the metastables, from free electron capture and from charge exchange recombination from neutral hydrogen 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.
Consider a set of individual lines, or line group, $G$ with upper levels $I_{;}$and lower levels $J_{G}$. Let $A_{i \rightarrow j}$ be the spontaneous emission coefficient for the line $i \rightarrow j$. Then the composite emissivity for the line group is

$$
\begin{aligned}
& \varepsilon_{G}=\sum_{j \in \epsilon_{G}, j \in \epsilon_{G}} \varepsilon_{j \rightarrow i}=\sum_{j \in J_{G}, j \in \epsilon_{G}} A_{j \rightarrow 1} N, \\
& =\sum_{j \in J_{G}, \dot{\in} \epsilon_{G}} A_{j \rightarrow i}\left(\sum_{\sigma=1}^{M} F_{j \sigma}^{(e x c)} N_{e} N_{\sigma}+F_{j}^{(r e c)} N_{e} N_{1}^{+}+F_{j}^{(C X)} N_{H} N_{1}^{+}\right)
\end{aligned}
$$

expressed in terms of the ratios $N_{\sigma} / N_{1}, N_{1}^{+} / N_{1}$ and $N_{H} / N_{1}$. The photon emissivity coefficient for the line group is $\varepsilon_{G} / N_{e} N_{1}$. The coefficient depends on electron density and temperature in general. Ratios of line group emissivities cancel the leading $N_{e} N_{1}$ dependence. The code prepares and operates primarily with a ratio $\varepsilon_{G_{1}} / \varepsilon_{G_{2}}$.

## Program steps:

These are summarised in the figure 2.7.

Figure 2.7


## Interactive parameter comments:

The file selection window has the appearance shown below

1. The program requires selection of the 'contour' data file prepared as output from ADAS205 (see description of ADAS205). There is no arrangement for central ADAS storage of such files which reside only in a user's file space and are generally prepared for immediate use. Usually in ADAS we store such temporary 'passed files' in a pass sub-library. You should create this at the first level within the adas database as
/...../<uid>/adas/pass
to which the program looks by default.


The procemang options whelow has the appearmose shown below. It displays information from the comour file together with information from the ADFO4 file used in the prior ADAS205 program run.


1. Select Non-equilibrium or Equilibrium conditions by clicking the appropriate case in the list a). The selection made is shown in the selection window above. Note that a non-equilibrium choice is only meaningful if there is more than one metastable. The metastables selected in the ADAS205 run are shown in the adjacent window b). This window becomes active when non-equilibrium conditions are selected. The values to be entered for each metastable is a multiplier on the equilibrium metastable population. Thus 1.00 for each metastable gives the equilibrium case.

2. A 'line ratio' in the present context is a ratio of line groups. The current line groups are shown in the list windows. The columns of the each row show the transition index and then for the upper and lower levels of the transition, the level index, configuration designation and the outer quantum numbers. These data are taken from the associated ADF04 file.
3. Each line group is assembled by clicking on the appropriate Selection button c) or d). A new window is presented with all available transitions listed. This is shown above. Clicking on the button alongside a transition a) allows it to be selected or de-selected.

The output options window appearance is shown below.

1. The limits of the calculated line group ratio are shown on the output window a). It is important to check this range. Subsequent plots may be selected as logarithmic and it is easy to obtain vanishing line ratios by choice of abnormally low temperatures in the ADAS205 run. In these circumstances meaningless contour plots may be produced.

2. There are three distinct types of plot of the line ratio allowed b), namely contours, plots as a function of temperature and plots as a function of density. Click on the appropriate buttion. The further options selection window c) changes according to this choice.
3. For the contour piot caea, logmithmic or linear choices of contour me parmined. Click on the required type in the lower list window d). The chocen type appears in the selection window sbove.
4. The displayed graph has the usual overall layouth but with supplementury information on the right side listing the line group assemblies and metastable fraction multipliers.

## Illustration:

The output from the program is illustrated for the ion $\mathrm{O}^{+5}$. Figure 2.7a shows a contour plot on the temperature/density plane of the emissivity ratio

$$
\varepsilon_{2 s_{\sqrt{ }}-2 p_{1 / 2}}\left(T_{e}, N_{e}\right) / \varepsilon_{2 p_{\sqrt{2}}-3 d_{v 2}}\left(T_{e}, N_{e}\right)
$$

Figure 2.7a


The tabular output is shown in table 2.7.
Table 2.7




## Notes:

## Ionisation balance

The programs of series ADAS4 are concerned with the distribution of atoms between their ionisation stages. The key data required to establish this are effective recombination and ionisation coefficients between ions. Associated data are the total radiated power and its components by ions. The main storage of data of this type, ready for applications, called isonuclear master files in ADAS, is by iso-nuclear sequence and they may be in a resolved metastable picture or in an unresolved (stage to stage) picture. These data sets are of type ADF11 and necessary sub-types in this picture are general collisional radiative ionisation coefficients (SCD), free electron recombination coefficients (ACD), charge exchange recombination coefficients (CCD), free electron recombination + cascade + bremsstrahlung power coefficients (PRB), charge exchange recombination + cascade power coefficients (PRC), low level line power coefficients (PLT), metastable cross coupling coefficients (QCD) and parent cross coupling coefficients (XCD). In addition, archiving of the radiated power in one standard resonance line for each ionisation stage (PLS) is useful.

ADAS4 series provides an ionisation equilibrium model, program ADAS405. It operates in the resolved or unresolved pictures. The primary output of ADAS405 is ionisation balance fractional abundances as functions of temperature and density. It can however produce radiated power functions and has an advanced capability for computing emission functions (and their composition). It addresses this by drawing on collections of emission coefficient data from the ADAS database (type ADF15, called 'pec'data - see the main ADAS User Manual and the last chapter of this manual).

Figure 3.0


# ADAS405: Equilibrium ionisation - process metastable populations and emission functions 

The program calculates the fractional abundances of resolved metastable or unresolved stage populations of the ions of an element in equilibrium in a thermal plasma. It also evaluates the radiated power function and line emission contribution functions ( $G\left(T_{\rho}\right)$ ). The evaluation of emission functions (and ratios of emission functions between lines os possibly different ions of the same element) is controlled by a 'script file'. This specifies the composition of the lines required.

## 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

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

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

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

subject to the normalisation

$$
N_{t o t}=\sum_{z=0}^{z_{0}} N^{(z)}
$$

where $N_{t o t}$ is the number density of ions of element $X$ in any ionisation stage. The equilibrium fractional abundances $N^{(z)} / N_{\text {tor }}$ at a set of temperatures and densities are sought. The code accesses standard isonuclear master file data of type ADF11 to obtain the coefficients of equations 3.5.3. 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 triagonal 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 $P_{\text {tor }}$, is calculated as

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

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 $\mathbf{G}\left(\mathrm{T}_{\mathrm{e}}\right)$ 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. PEC coefficients in the metastable resolved case - see the descriptions of ADAS503 and ADAS208 in the last chapter) They occur in independent parts $\varepsilon_{i \rightarrow j}^{e x c}, \varepsilon_{i \rightarrow j}^{n c}$ 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 timescales. 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

$$
\begin{aligned}
& d / d N_{\rho}^{(z)}=N_{c} \sum_{\rho^{\prime}=1}^{M_{c-1}} S_{C D \rho^{\prime} \rightarrow \rho}^{(z-1 \rightarrow z)} N_{\rho^{\prime}}^{(z-1)} \\
& -\left(N_{e} \sum_{\rho^{*}=1}^{M_{r+1}} S_{C D \rho_{\rho} \rightarrow \rho^{+}}^{(z \rightarrow z+1)}+N_{e} \sum_{\rho^{\prime}=1}^{M_{t-1}} \alpha_{C D \rho \rightarrow \rho^{\prime}}^{(z \rightarrow z-1)}+N_{H} \sum_{\rho^{\prime}=1}^{M_{z-1}} C_{C D \rho \rightarrow \rho^{\prime}}^{(z \rightarrow z-1)}\right. \\
& \left.+N_{e} \sum_{\sigma=1}^{M} Q_{C D_{\rho \rightarrow 0}}^{(z \rightarrow z)}+N_{e} \sum_{\rho^{\prime}=1}^{M_{z}} X_{C D_{\rho} \rightarrow 0}^{(z \rightarrow z)}\right) N_{\rho}^{(z)} \\
& +N_{e} \sum_{\rho^{*}=1}^{M_{2+1}} \alpha_{C D p^{m} \rightarrow p}^{(z+1 \rightarrow z)} N_{\rho^{+}}^{(z+1)}+N_{H} \sum_{\rho^{p}=1}^{M_{r+1}} C_{C p^{*} \rightarrow p}^{(z+1 \rightarrow z)} N_{\rho^{*}}^{(z+1)} \\
& +N_{e} \sum_{\sigma=1}^{M_{3}} Q_{C D \sigma \rightarrow p}^{(z \rightarrow z)} N_{\sigma}^{(z)}+N_{e} \sum_{\sigma=1}^{M_{1}} X_{C D, \sigma \rightarrow p}^{(z \rightarrow z)} N_{\sigma}^{(z)}
\end{aligned}
$$

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

3.5.9
which must be interpreted for the metastable resolved case. Each element of the matrix in eqns. 3.5 .9 is now itself a matrix extending over the metastable sets of the ionisation stage involved. Thus

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

and

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

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

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

$$
N_{t o t}=\sum_{z=0}^{z_{0}} \sum_{\rho=1}^{M_{z}} N_{\rho}^{(i)}
$$

The equilibrium fractional abundances $N_{\rho}^{(z)} / N_{\text {te }}$ at a set of temperatures and densities are sought. The code accesses partial isonuclear master file data of type ADF11 to obtrain the coefficients of the equations 3.5.9. 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

$$
P_{t o t}=\sum_{s=0}^{z_{0}} \sum_{p=1}^{M_{z}}\left[P_{L T_{p}}^{(z)}+P_{R B_{p}}^{(z)}+\left(N_{H} / N_{e}\right) P_{R C_{p}}^{(z)}\right]\left(N_{\rho}^{(z)} / N_{t o t}\right)
$$

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

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

(c.f. the description of ADAS208 in the last chpater of this manual). In practice, there may be very many choices of $G\left(T_{e}\right)$ functions of interest.

## Program steps:

These are summarised in figure 3.5.
Figure 3.5


## Interactive parameter comments:

The program which makes use of data from archived ADAS datasets initiates an interactive dialogue with the user in three parts, namely, input data file selection, entry of user data and display/disposition of output.

The file selection window appears first as illustrated below

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 Joiat Undertaking effective rediated power coefficients ('prb', 'plt' and 'prc') are often made available both as the whole emitred power and as the power which would pass through certuin filers (such as Bo/Si windows). The fither is specified either simply as an energy cut-off (eg. ev2000) or as filter specification (eg. f11235). These codes appear as an extension in the relevant master file names. Specify the filter choice at (b). Note the present IDL-ADAS databsece contains very littie filtered power data but it can be added if there is an interest amonget users.
5. The remainder of the file identification (c) follows the general patter. 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. ' $p j^{\prime}$ ') which may be present in the final part of a file name (eg. '/../acd93r/acd93r_pj"c.dar').
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 urresolved. 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 at (e). The structure of script file is shown below. We have found it convenient to group script files in a personal ADAS database under a subdirectory classification $/$ scripts 405 i. 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.
10. Details of the species, number of (composite) lines and line ratios to be obtained are at the head of the file (SPECIES, NLINE, NRATIO). Note that you must follow the positional layout exactly. Emissivity coefficient data are obtained from 'pec' files of ADAS format ADF15. The number of such files to be searched in the ADAS database are specified at NFILE and the full Unix paths to the files themselves in following lines at PHOTON EMISSIVITY FILE NAMES. The subsequent table identifies the index number of the pecs in these files required to build the particular line emission function. The lines are indexed at ILINE, the number of component parts of each line is at NCOMP, the charge of the ion to which the component attaches is at IZION and the components simply indexed at ICOMP. The metastable of the ion to which the component is attached is specified by its ranked index number at IMET (the ground state is 1). INDPH gives the selection index of the component pec in the ADF15 file identified at IFILE from the list given earlier. Note the letter qualification on the INDPH index to distinguish electron collision driven pecs and charge exchange driven pecs. The composite lines may be ratioed as specified by IRATIO, an index number of the ratio; ILINE, the upper composite line of the ratio; JLINE, the lower composite line of the ratio. All other text is for information. Note that a 'c---.-' line is used to separate comments which follow it. Each comment line begins with ' $c$ ' and we conventionally put in a'c-..-' terminator line for the comments section.


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 dataset display and selection windows in the input option window of a code such as ADAS205 (see chapter 2). 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 pairs for data output are made at (e). The table may be edited by clicking on the Edit Table button.. The ADAS Table Editor window is then presented with the same set of editing operations available as are described in the introductory chapter. Electron temperatures should be monotonic increasing. It has proved helpful to add a Clear Table button (f) to remove all entries in the temperature and density output fields.
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.

1. 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.
2. 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.
3. 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.
4. The 'Goft Passing File' is the name used for the output dataset of calculated contribution functions. It is organised according to an ADAS data format ADF16. The output file name is specified at (e). Note that $G(T e)$ functions of type ADF20 (gf) are organised differently and have a slightly different definition from the output here of generalised contribution functions of type ADF16 (gcf). The expected practice is that ADAS405 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.


## Illustration:

The output from the program is illustrated for carbon in the resolved case. Figure 3.5 a 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 $10^{+13} \mathrm{~cm}^{-3}$. Figure 3.5 b shows shows 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 5.5 c shows the equilibrium generalised contribution function for the CI 1561 A resonance line. As can be seen from the script file, contributions from each of the four $\mathrm{C}^{+0}$ metastables are included. The contribution function omits the $N(C) / N(H)$ and $N(H) / N e$ factors usually included in the solar coronal $\mathrm{G}(\mathrm{Te})$ function definition.


Figure 3.5b
BCWER FUMCTOON YS ELECTBON TEMPERATURE; CABBON DEMONSTBATION
DATE: 05/08/94
ADAS : ADAS RELEASE:ADASO1 V1.11 PROGPAM: ADAS405 V1.0 DATE: 05/0804 TIME: 18.03 FILE : IJETSHPADASAO5.DATA(SCRIC) SPECIES: CARBON YEAR: 93 DEFAULTYEAR: 93 KEY : (FUL LINE-TOTAL) (DASH UNE-PARTIAL)


Figure 3.5c


Table 3.5a shows the tabular output from the carbon equilibrium ionisation balance. The option to calculate a ratio of contribution functions for two lines is tabulated but is not available graphically. FILTER applies only to radiated power. Isoelectronic master files which include the effect of an energy filter are of two qualities, namely, precisely estimated for a window of specified thicknesses of beryllium and quartz (FT)and secondly a simple sharp energy cut-off (EV). FILTER gives the master file name subfield of the form $\mathrm{EV}<\mathrm{nnnn}>$ or $\mathrm{FT}<1 \mathrm{l}><\mathrm{mm}>$ by which they identified.

Table 3.5a

DAS RELEASE: ADAS91 V1.11 PROGRAM: ADAS405 V1.0 DATE: 05/0B/94 TIME: $18: 17$
************ TABULAR OUTPUT FROM EQUILIBRIUM IONISATION AND EMISSION PROGRAM: ADAS405 - DATE: OS/OB/94
**************

CARBON DEMONSTRATION



| 15 | Frus |
| :---: | :---: |
| -- | ---- |
| 1 |  |
| 2 | JTxaup. PBCs3事C. DRTA (PJRAC1) |
| 3 | Jixskep IOMELSC. DATA (PICHC3) |
|  | Jwrenp. Iownhec . DATA (PECWC4) |



| UCLTAR CImPas | 6 |
| :---: | :---: |
| Owner canact smat | 0 |
| Iorast chnacs state | 6 |
| Uriste of exacis | 7 |
| Unima or mexactable | - 13 |


| M10Ex | $\begin{aligned} & \text { ELSCTRON } \\ & \text { (kelvin) } \end{aligned}$ | $\begin{aligned} & \text { THPMPRATURE } \\ & \text { (eV) } \end{aligned}$ | $\begin{aligned} & \text { ELABCTROA } \\ & \text { DEASITY (cm-3) } \end{aligned}$ | $\begin{aligned} & \text { HYDROGEN } \\ & \text { DENSITY (Cm-3) } \end{aligned}$ |
| :---: | :---: | :---: | :---: | :---: |
| 2 | $1.280+04$ | 1.100+00 | $1.000+10$ | $0.000+00$ |
| 2 | 1.51D+04 | 1.300+00 | $1.000+10$ | $0.00 D+00$ |
| 3 | 1.74D+04 | 1.500 +00 | $1.000+10$ | $0.00 D+00$ |
| 4 | 2.32D+04 | 2.00D+00 | 1.000+10 | $0.000+00$ |
| 5 | 3.48D+04 | $3.000+00$ | $1.00 \mathrm{D}+10$ | $0.000+00$ |
| 6 | $5.80 D+04$ | $5.000+00$ | $1.000+10$ | $0.000+00$ |
| 7 | 8.12D+04 | $7.00 \mathrm{D}+00$ | $1.000+10$ | $0.000+00$ |
| 8 | 1.16D+05 | 1.00D+01 | $1.000+10$ | $0.00 \mathrm{D}+00$ |
| 9 | 1.51D+05 | $1.300+01$ | $1.000+10$ | $0.000+00$ |
| 10 | 1.74D+05 | $1.50 D+01$ | 1.00D+10 | $0.00 D+00$ |
| 11 | 2.32D+05 | 2.00D+02 | 1. $000 \mathrm{D}+10$ | $0.000+00$ |
| 12 | 3.48D+05 | $3.00 D+01$ | $1.000+10$ | $0.00 \mathrm{D}+00$ |
| 13 | $5.80 \mathrm{D}+05$ | $5.00 D+01$ | $1.00 D+10$ | $0.00 D+00$ |
| 14 | 8.12D+05 | $7.00 \mathrm{D}+01$ | $1.000+10$ | $0.000+00$ |
| 15 | 1.16D+06 | $1.00 D+02$ | $1.000+10$ | $0.00 \mathrm{D}+00$ |
| 16 | 1.51D+06 | 1.30D+02 | $1.000+10$ | $0.00 D+00$ |
| 17 | 1.74D+06 | 1.50D+02 | $1.000+10$ | $0.00 D+00$ |

QUILIBRIUM FRACTIONAL ABUNDANCES, GCF PUNCTIONS AND LINE RATIOS:


|  | 2 | 0 | 2 | 548 | 1) | 5.86D-12 | 4.02D-12 | 2.51D-12 | 1.08D-12 | 1.77D-13 | 5.410-15 | 3.26D-16 | 3.100-18 | 5.54D-20 | 6.870-21 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 3 | 0 | 3 | 1078 | 1) | 2.04D-13 | 1.33D-13 | 7.78D-14 | 2.88D-14 | 3.770-15 | 8.82D-17 | 4.67D-18 | 4.03D-20 | 6.85D-22 | 8.320-23 |
| 1 | 4 | 0 | 4 | 1608 | 1) | 2.37D-12 | 1.65D-12 | 1.010-12 | 4.23D-13 | 6.950-14 | 1.94D-15 | 9.960-17 | 7.59D-19 | 1.13D-20 | 1.270-21 |
| 2 | CII |  |  | 9048 |  | 3.16D-13 | 2.46D-12 | 8.68D-12 | 6.22D-11 | 1.72D-10 | 5.310-11 | 1.09D-11 | 3.49D-13 | 1.44D-14 | 2.80D-15 |
| 1 | 1 | 1 | 1 | 38 | 2) | 2.65D-13 | 2.13D-12 | 7.74D-12 | 5.76D-11 | 1.62D-10 | 5.09D-11 | 1.06D-11 | 3.410-13 | 1.42D-14 | 2.76D-15 |
|  | 2 | 1 | 2 | 258 | 2) | 5.17D-14 | 3.36D-13 | 9.41D-13 | 4.61D-12 | 1.000-11 | 2.17D-12 | 3.21D-13 | 7.18D-15 | 2.270-16 | 3.78D-17 |

PBCTRAL LINE RATIOS:

```
R JL KL
```



QUILIBRIUM FRACTIONAL ABUNDANCES, GCF FUNCTIONS AND LINB RATIOS:

| E (eV) | 2.00D+01 | $3.00 \mathrm{D}+01$ | $5.000+01$ | $7.000+01$ | 1.000 + 02 | $1.300+02$ | 1. 50D +02 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| B ( $\mathrm{cm}-3$ ) | $1.000+10$ | $1.00 \mathrm{D}+10$ | 1.00D+10 | 1.00D+10 | $1.000+10$ | 1.000 + 10 | 1.000 |
| H (cm-3) | $0.000+00$ | $0.00 D+00$ | $0.00 D+00$ | $0.000+00$ | $0.000+00$ | $0.000+00$ | $0.00 \mathrm{D}+00$ |
| ND ION MET |  |  |  |  |  |  |  |
| $1 \mathrm{C}+0$ (1) |  |  |  |  |  |  |  |
| $2 \mathrm{c}+0$ (2) |  |  |  |  |  |  |  |
| $3 \mathrm{C}+0(3)$ |  |  |  |  |  |  |  |
| $4 C+0$ (4) |  |  |  |  |  |  |  |
| $5 C+1(1)$ | 5.78D-09 | 1.65D-10 | 6.36D-12 |  |  |  |  |
| $6 c+1(2)$ | 1.12D-09 | 2.73D-11 |  |  |  |  |  |
| $7 \mathrm{C}+2(1)$ | 1.49D-05 | 9.93D-07 | 9.91D-08 | 2.43D-08 | 3.60D-09 | 6.08D-10 | 2.200-10 |
| $8 \mathrm{C}+2(2)$ | 1.44D-05 | 9.19D-07 | 8.76D-08 | 2.11D-08 | 3.07D-09 | 5.08D-10 | 1.82D-10 |
| $9 C+3(1)$ | 9.26D-03 | 2.17D-03 | 7.41D-04 | 3.41D-04 | 8.39D-05 | 1.87D-05 | 7.69D-06 |
| $0 \mathrm{C}+4(1)$ | 9.91D-01 | 9.98D-01 | 9.23D-01 | 5.31D-01 | 1.25D-01 | 2.64D-02 | 1.090-02 |
| $1 C+4(2)$ | 1.63D-08 | 8.63D-07 | 6.57D-05 | 1.89D-04 | 1.210-04 | 4.48D-05 | 2.400-05 |
| $2 C+5(1)$ | 2.52D-07 | 2.29D-04 | 7.58D-02 | 4.45D-01 | 5.22D-01 | 2.57D-01 | 1.55D-01 |
| $3 C+6(1)$ |  | 4.10D-10 | 1.59D-04 | 2.41D-02 | 3.53D-01 | 7.17D-01 | 8.34D-01 |
| RB (W cm3) | 1.08D-29 | 9.86D-30 | 1.85D-29 | 4.27D-29 | 9.11D-29 | 9.900-29 | 9.29D-29 |
| LT ( W cm 3 ) | 9.08D-28 | 2.31D-28 | 2.19D-28 | 5.13D-28 | 6.98D-28 | 5.63D-28 | 4.52D-28 |
| RAD (W cm3) | 9.18D-28 | 2.41D-28 | 2.38D-28 | 5.56D-28 | 7.89D-28 | 6.62D-28 | 5.45D-28 |

PBCTRAL LINE GCF FUNCTIONS (cm3 s-1):

| $\mathrm{E}(\mathrm{eV})$ | $2.00 \mathrm{D}+01$ | $3.00 \mathrm{D}+01$ | $5.00 \mathrm{D}+01$ | $7.00 \mathrm{D}+01$ | $1.00 \mathrm{D}+02$ | $1.30 \mathrm{D}+02$ | $1.50 \mathrm{D}+02$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathrm{E}(\mathrm{cm}-3)$ | $1.00 \mathrm{D}+10$ | $1.00 \mathrm{D}+10$ | $1.00 \mathrm{D}+10$ | $1.00 \mathrm{D}+10$ | $1.00 \mathrm{D}+10$ | $1.00 \mathrm{D}+10$ | $1.00 \mathrm{D}+10$ |
| $\mathrm{H}(\mathrm{cm}-3)$ | $0.00 \mathrm{D}+00$ | $0.00 \mathrm{D}+00$ | $0.00 \mathrm{D}+00$ | $0.00 \mathrm{D}+00$ | $0.00 \mathrm{D}+00$ | $0.00 \mathrm{D}+00$ | $0.00 \mathrm{D}+00$ |



PECTRAL LINE RATIOS:

| R JL KL |  |  |
| :--- | :--- | ---: |
| 1 | 1 | 2 |

ABLE KEY:

| B | = ELECTRON TEMPERATURE | NE | - ELECTRON DENSITY |
| :---: | :---: | :---: | :---: |
| E | = HYDROGEN DENSITY | IND | - STAGE/METASTABLE COUNT |
| ON | - ION SPECIPICATION | MET | - METASTABLE INDEX |
| RB | - RBCONB. + BREMS. POWER FUNCTION | PRC | = CHARGE EXCHANGE RECONB. POWER PUNCTION |
| LT | - LINB RADIATED POWER FUNCTION | PRAD | = TOTAL RADIATED POWER FUNCTION |
| L | = SPECTRUM LIME INDEX | IC | - SPECTRUM LINE COMPONEAT COUNT |
| 2 | - ASSOCIATED ION POR LIRE COMPONENT | IM | - ASSOCIATED METASTABLE POR LINE COMPONEAT |
| P | = PHOTON EMISSIVITY PILE SELECTION INDEX | IP | - EMISSIVITY PILE INDEX |
| R | - SPECTRUM LINB RATIO INDEX | JL | - NUNERATOR SPECTRUM LIRE IRDEX |
| L | = DEACMINATOR SPECIRUA LIEE INDEX |  |  |

Notes:

# Differential emission measure and emission functions 

The programs of series ADAS5 are all interactive interrogation codes on elements of the fundamental and derived databases. This supplementary series has been found of use in analysis and interpretation. The particular type of data of relevance here are the $\mathrm{G}(\mathrm{Te})$ functions which merge the photon emissivity coefficients of lines of an ion with an equilibrium ionisation balance of the ion with respect to the total abundance of the species. These data (type ADF20) are of the form and definition usual in astrophysics. They are interrogated by program ADAS506.
The programs of series ADAS6 are data analysis codes fully integrated within the ADAS structure. ADAS601 evaluates an estimate of the emission measure differential in temperature from observed spectral intensities, assumed elemental abundances and a collection of $\mathrm{G}(\mathrm{Te})$ functions. This latter is directly produced by the interrogation program ADAS506 for the spectral lines of interest. The structure of ADAS601, unlike other ADAS programs, is not sequential. This is to give some agility in the analysis, allowing one to change any of the input data sets (elemental abundances, observed spectral intensities, collection of $\mathrm{G}(\mathrm{Te})$ functions), examine the $\mathrm{G}(\mathrm{Te})$ functions, change options, evaluate the differential emission measure, and display or print the output at any time during the analysis.

A schematic of the programs and dataset types interrogated is shown in figure 4.0.

Figure 4.0


## ADAS506: GFT - graph and fit G(Te) functions

The program interrogates GFT files of type ADF20. The $G\left(T_{e}\right)$ function is extracted for a selected radiative transition of an ion. The data may be interpolated using cubic splines at selected electron temperatures. A minimax polynomial approximation is made to the interpolated data. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the polynomial approximation.

## Background theory:

One of the most widely used methods available for the interpretation of astronomical spectral intensities is the emission measure technique. This method is less familar in spectroscopic studies of fusion plasma. However it and variants designed to determine impurity concentration, impurity variation in time and impurity influx are applicable in fusion.

The intensity of a spectral line from a column of optically thin plasma of cross-sectional area $A$ and due to a transition from upper level $j$ to lower level $k$ may be written as

$$
I_{j \rightarrow k}=\frac{1}{4 \pi \mathrm{~A}} \iiint A_{j \rightarrow k} N_{j} d z d y d x
$$

where $N_{j}$ denotes the population density of ions in the upper state $j, A_{j \rightarrow k}$ is the radiative transition probability for the transition and the integral is taken over the volume of the plasma viewed.

The excited population may be expressed in terms of the ground and metastable populations of the ionisation stage to which it belongs and to those of the adjacent higher ionisation stage by a quasi-equilibrium collisional radiative calculation as

$$
N_{j}=\sum_{\sigma=1}^{M_{z}} \mathcal{f}_{j \sigma}^{(e x c)} N_{e} N_{\sigma}+\sum_{v^{\prime}=1}^{M_{z+1}} f_{j^{\prime}}^{(r e c)} N_{e} N_{v^{\prime}}^{+}
$$

Usually contributions to the population of the excited state by excitation from the metastables of its own ionisation stage only need to be considered so that

$$
N_{j}=\sum_{\sigma=1}^{M_{2}} \mathscr{F}_{j \sigma}^{(e x c)} N_{e} N_{\sigma}
$$

In differential emission measure analysis, the assumption of ionisation balance is normally made. Although a time dependent ionisation could be used, the method would be specific to a particular model for the dynamic behaviour of the plasma and the universality of the emission measure technique would be lost. Thus it is convenient to write.

$$
N_{\sigma} \equiv N_{\sigma}^{(z)}=\frac{N_{\sigma}^{(z)}}{N_{t o t}} \frac{N_{t o t}}{N_{H}} \frac{N_{H}}{N_{e}} N_{e}
$$

where the ratio $N_{\sigma}^{(z)} / N_{t o t}$ is evaluated in equilibrium at the local temperature and density. For the solar plasma, the generally accepted assumption is that the abundance of the element $N_{t o t} / N_{H}$ does not vary through the depth of the atmosphere. Then gathering terms

$$
A_{j \rightarrow k} N_{j}=\frac{N_{t 01}}{N_{H}} N_{e}^{2} G\left(T_{e}, N_{e}\right)
$$

where

$$
G_{j \rightarrow k}\left(T_{e}, N_{e}\right)=A_{j \rightarrow k} \frac{N_{H}}{N_{e}} \sum_{\sigma=1}^{M_{z}} \mathcal{J}_{j \in}^{(e x c)} \frac{N_{\sigma}^{(x)}}{N_{1 o t}}
$$

Then the spectral intensity may be written as

$$
I_{j \rightarrow k}=\frac{1}{4 \pi \mathrm{~A}} \frac{N_{m}}{N_{H}} \iiint G_{j \rightarrow k}\left(T_{e}, N_{e}\right) N_{e}^{2} d z d y d x
$$

It is convenient to change the variable of the integral to electron temperature. However the atomic coefficient depends on both electron temperature and electron density so it is necessary to make some assumption about the relation between them. A common assumption is that the plasma pressure is constant over the relatively small range of temperature where the $G\left(T_{e}, N_{e}\right)$ function has significant values. In any event a model assumption is made even though the $G\left(T_{e}\right)$ function is usually written as function of temperature alone. Also introduce the concept of surfaces of constant temperature of which there may be more than one in the viewed volume. The intensity then may be rewritten as

$$
I_{j \rightarrow k}=\frac{1}{4 \pi \mathrm{~A}} \frac{N_{t o x}}{N_{H}} \int_{T_{1}}^{T_{2}} G_{j \rightarrow k}\left(T_{e}, N_{e}\right) \sum_{l} \int_{S_{l}\left(T_{e}\right)}\left|\nabla T_{e}\right|_{l}^{-1} N_{e}^{2} d S_{l} d T_{e}
$$

The limits of the integral $T_{1}$ and $T_{1}$ are the minimum and maximum electron temperatures in the part of the atmosphere contrinbuting to the spectrum. Introduce the differential emission measure, $\phi\left(T_{e}\right)$, defined by

$$
\phi\left(T_{e}\right)=\frac{1}{\mathbf{A}} \sum_{l} \int_{S_{i}\left(T_{e}\right)}\left|\nabla T_{e}\right|_{l}^{-1} N_{e}^{2} d S_{l}
$$

where the sum is taken over all $l$ of the isothermal surfaces $S_{l}\left(T_{e}\right)$ and $\left|\nabla T_{e}\right|_{l}$ is the modulus of the temperature gradient perpendicular to the surface. By this definition $\phi\left(T_{e}\right)$ is the average value for the differential emisison measure over the area viewed by the spectrometer. It is noted that $\phi\left(T_{e}\right)$ is the part of the integral it is sought to extract since it is the part which gives infromation about the structure of the atmosphere. The above analysis leads to the following expression for the spectral intensity

$$
I_{j \rightarrow k}=\frac{1}{4 \pi} \frac{N_{t o 1}}{N_{H}} \int_{T_{1}}^{T_{2}} G_{j \rightarrow k}\left(T_{e}, N_{e}\right) \phi\left(T_{e}\right) d T_{e}
$$

The program interrogates $G\left(T_{e}\right)$ data sets prepared according to the prescription of equation 6.6.6. Details of the model relating temperature, density, pressure and hydrogen to electron number densities are stored in the $G\left(T_{e}\right)$ datasets and this information is accessed simultaneoulsy with the $G\left(T_{e}\right)$ in the interrogation. Interpolation of the $G\left(T_{e}\right)$ to arbitrary temperatures is done by cubic splines. This implies an implicit interpolation in the other model parameters. For completeness these model parameters are also explicitly interpolated as a function of temperature.

## Program steps:

These are summarised in figure 4.6.
Figure 4.6


## Interactive parameter comments:

The file selection window has the appearance shown below:.


Browse Comments Cancel Done

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 ADF20 (' $\mathrm{G}(\mathrm{Te}$ ) 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. They are named by iso-electronic sequence (eg. gfi95\#li). specific file names include a source identifier (eg. $a l$ ) the specific ion symbol (eg.c3) and the pressure (eg. p3e14).
4. 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 (eg. gft95\#li_al\#c3_p3el4.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 has gone into the dataset and the attribution of the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the Done button moves you forward to the next window. Clicking the Cancel button takes you back to the previous window

The processing options window has the appearance shown below.


1. Transitions for which $\mathrm{G}(\mathrm{Te})$ data are available in the data set are displayed in the line list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a line to select it. The selected transition appears in the selection window a) just above the line list display window.
2. Your settings of electron temperatures (output) are shown in the temperature display window d). The temperature values at which the $\mathrm{G}(\mathrm{Te})$ coefficients are stored in the datafile (input) are also shown for information.
3. The program recovers the output temperatures you used when last executing the program. Pressing the Defoult Temperature values button inserts a default set of temperatures equal to the input temperatures
4. The Temperature Values are editable. Click on the Edit Table button if you wish to change the values. A 'drop-down' window, the ADAS Table Editor window: It follows the same pattern of operation as described in bulletin.
5. Clicking the Done button causes the next output options window to be displayed. Remember that Cancel takes you beck to the previous window.

The output options window has the appearance shown below.

6. The graph is displayed in a following graphical output window.
7. Writing to the collection file is activated by clicking the Collection File button at a). The operation is slightly different from the usual text output. The collection file is composed of blocks of data for each spectrum line. Each block includes a header line which enables the code to construct an indexed list of lines present in the collection file. A line which is already present in the collection is replaced if the Replace button is activated, otherwise it is disallowed. Thus the $\mathrm{G}(\mathrm{Te})$ collection file contains any one line only once.

## Illustration:

Figure 4.6a shows the $\mathrm{G}(\mathrm{Te})$ function for 150.1 A line of OVI. The GFT data set was prepared for a constant pressure model at $3 \times 10^{+14} \mathrm{~K} \mathrm{~cm}-3$. The model includes the variation of the ratio $N_{H} / N_{e}$ in the solar atmosphere with temperature in the $\mathrm{G}(\mathrm{Te})$ functions.
Figure 4.6a

Figure 4.6a

$$
\begin{aligned}
& \text { ADAS : ADAS RELEABE: ADNSO1 V1.10 PROCRMM: ADASE0S V1.0 DATE: 100MOA TMEE: } 10.51
\end{aligned}
$$

M MMMX : LOCNFT - DEGFEE=13 ACCUPACY =47.25\% END GRADIENT: LOWER=120.01 UPPERe-14.19
KEY ; (CHOBeEs - MPUT DATA) (FUL LINE - BPLINE) (DASH LINE - Mmmand


The tabulation is given in table 4.6a. For completeness, interpolation with temperature of the model electron density, electron pressure and $N_{H} / N_{e}$ is given in the table.
Table 4.6a


| $7.000+06$ $1.0007+07$ | $6.03 D+02$ $8.62 D+02$ | $1.94 D+05$ $2.78 D+05$ | $\begin{aligned} & 2.97 D-16 \\ & 4.38 D-17 \end{aligned}$ | $\begin{aligned} & 6.290+07 \\ & 3.000+07 \end{aligned}$ | $\begin{aligned} & 3.000+14 \\ & 3.000+14 \end{aligned}$ | $\begin{gathered} \text { C.29D-02 } \\ \text {. 29D-02 } \end{gathered}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| OMINIMAX POLYNOMLN - TAYLOR COMFFICIENTS : LOG10 (GFI) Ve. LOG10 (Trapckelvins) |  |  |  |  |  |  |
|  | 1) $=7.3$ | $63053 D+08$ | $\boldsymbol{\lambda}$ | = -1.525 | 210+09 |  |
|  | 3) $=1.4$ | 24362D+09 | $\boldsymbol{\lambda}$ | $=-8.3191$ | 5290+08 |  |
|  | 5) $=3.2$ | $57026 D+08$ | A | - -9.070 | 808D+07 |  |
|  | 7) $=1.8$ | $22456 D+07$ |  | . -2.865 | 607D+06 |  |
|  | 9) $=3.2$ | $65908 D+05$ | $\boldsymbol{\lambda}$ | - -2.768 | 18D+04 |  |
|  | 1) $=1.6$ | $59108 D+03$ | A | $=-6.854$ | 225D+01 |  |
|  | $3)=1.70$ | $82983 D+00$ |  | - -1.95 | 669D-02 |  |
| LOGFIT - DEGREE $=13$ ACCURACY = 47.45\% END GRADIENT: LOWER = 120.01 UPPER= -14.19 |  |  |  |  |  |  |

## Notes:

## ADAS601: Differential emission measure analysis

Given a set of observed spectral intensities, $G\left(T_{e}\right)$ functions and elemental abundances, the program evaluates an estimate for the emission measure differential in temperature, using the integral inversion algorithm of $\mathbf{A}$. M. Thompson. Selection of the input data files for elemental abundances, $G\left(T_{e}\right)$ functions, and observed spectral intensities can be made at any time during the analysis. The output consists of displays of the differential emission measure vs. electron temperature and the reconstructed observed spectral intensity ratios. A tabulation of these quantities is also produced. The input set of $G\left(T_{e}\right)$ functions can be displayed and examined at any time.

## Background theory:

In order to derive the emission measure differential in temperature, we require to solve the integral equation

$$
I_{u \rightarrow 1}=\frac{1}{4 \pi} \phi(Z) \int_{0}^{\infty} G_{u \rightarrow 1}\left(T_{e}\right) \phi\left(T_{e}\right) d T_{e}
$$

for a set of, say, $m$ spectral lines. In 4.1.1, $I_{w \rightarrow l}$ is the intensity of a spectral line from a column of optically thin plasma due to a transition from upper level $u$ to lower level $l$, $\star(Z) \equiv N_{\text {tol }} / N_{H}$ is the fractional elemental abundance assumed to be known, $Z$ the element's nuclear charge, $\phi\left(T_{e}\right)$ the emission measure differential in temperature, as defined in the ADAS506 section.

Note that in equation 4.1.1 the dependence on the electron density has been dropped, which would have lead to the formulation of the bi-variate integral inversion problem. $G$ and $\phi$ would then have been functions of electron temperature and electron density, and the integral over both variables. The simplified formulation expressed by equation 4.1.1 is achieved by selecting only those spectral lines whose $G$-functions have a slow dependence on electron density, at least in the physical range of interest. Resonance lines have such properties in most cases. However, in order to achieve the best approximation for the $G$-functions, the slow dependence on the electron density is taken into account by assuming an approximate constant pressure or constant density for the plasma. This is equivalent to selecting an approximate dependence $N_{e}=N_{e}\left(T_{e}\right)$, so that the $G$-functions can be considered effectively dependent on $T_{e}$ only. $G$-functions stored as ADF20 are computed for a grid of constant electron pressure for this purpose.

Equation 4.1.1 is solved by the data adaptive smoothing approach of A. M. Thompson. The integral is discretised (product integration method) as

$$
\begin{align*}
I_{u \rightarrow 1} & =\frac{1}{4 \pi} A(Z) \int_{0}^{\infty} G_{u \rightarrow 1}\left(T_{e}\right) \phi\left(T_{e}\right) d T_{e} \\
& =\frac{1}{4 \pi} A(Z) \sum_{i=1}^{N} \int_{T_{j-1}}^{T_{j}} G_{u \rightarrow 1}\left(T_{e}\right) \phi\left(T_{e}\right) d T_{e} \\
& =\frac{1}{4 \pi} A(Z) \sum_{j=1}^{N} \phi_{j}^{*} \int_{T_{j-1}}^{T_{j}} G_{m \rightarrow 1}\left(T_{e}\right) \phi_{0}\left(T_{e}\right) d T_{e}
\end{align*}
$$

where

$$
\phi_{j}^{*} \equiv \frac{\int_{T_{j-1}}^{T_{j}} G_{m \rightarrow 1}\left(T_{e}\right) \phi\left(T_{e}\right) d T_{e}}{\int_{T_{j-1}}^{T_{j}} G_{m \rightarrow 1}\left(T_{e}\right) \phi_{0}\left(T_{e}\right) d T_{e}}
$$

represents a weighted average of $\phi\left(T_{e}\right) / \phi_{0}\left(T_{e}\right)$ between $T_{j-1}$ and $T_{j} \cdot \phi_{0}\left(T_{e}\right)$ is an initial estimate of $\phi\left(T_{e}\right)$ towards which we shall smooth the solution. This process can be viewed as scaling the solution using an expected gross behaviour of $\phi\left(T_{e}\right)$ as represented by $\phi_{0}\left(T_{e}\right)$. The advantage is to reduce the dynamic range of the problem before the actual regularised solution (see below) is obtained. This has been proven to prevent uneven smoothing, with the solution being over-smoothed at large values of $\phi$ and under-smoothed at low values, when the source function (the differential emission measure) span a large dynamic range.

The prior function $\phi_{0}\left(T_{e}\right)$ is evaluated as follows. $\quad G_{\mu \rightarrow 1}\left(T_{e}\right)$ is approximated by $\bar{G}_{u \rightarrow 1} \delta\left(T_{e}-T_{u \rightarrow 1}^{\max }\right)$, where

$$
\bar{G}_{u \rightarrow 1} \equiv \int_{0}^{\infty} G_{u \rightarrow 1}\left(T_{e}\right) d T_{e}
$$

$T_{u \rightarrow l}^{\max }$ being the temperature corresponding to the maximum of $G_{u \rightarrow 1}\left(T_{e}\right)$ and $\delta$ the Dirac's delta function. A crude estimate of $\phi$ is then

$$
\bar{\phi}\left(T_{u \rightarrow 1}^{\max }\right)=\frac{4 \pi}{\Delta(Z)} \frac{I_{u \rightarrow 1}}{\bar{G}_{u \rightarrow 1}}
$$

A cubic B-spline is now fitted to the values $\log \left(\bar{\phi}\left(T_{w \rightarrow 1}^{\max }\right)\right)$ to obtain a smooth representation for $\phi_{0}\left(T_{e}\right)$. This representation can only yields features comparable to the typical kernel in width (estimated, to this purpose, to be $\approx 1 / 2$ decade). The knot points of the B -spline representation are therefore selected approximately $\approx 1 / 2$ decade apart. In other words, we obtain

$$
\log \left(\phi_{0}\left(T_{e}\right)\right) \equiv S\left(\log \left(T_{e}\right)\right)
$$

where $S\left(\log \left(T_{e}\right)\right)$ denotes the B -spline representation with interior knots about $\approx 1 / 2$ decade apart.

The B-spline fit described above provides a satisfactory estimate of $\phi_{0}\left(T_{c}\right)$ between the maximum and minimum values of $T_{u \rightarrow 1}^{\max }$. It is necessary, however, to extrapolate $\phi_{0}\left(T_{e}\right)$ beyond these boundaries. This is done as follows.

For

$$
\left.T>\max \left[T_{u \rightarrow 1}^{\max }\right] \quad \text { and } \quad\left[d \phi_{0} / d T_{e}\right]_{\max [[x \rightarrow 1}\right]<0
$$

or

$$
T<\min \left[T_{x \rightarrow 1}^{\max }\right] \quad \text { and } \quad\left[d \phi_{0} / d T_{e}\right]_{\min [m=10]}>0,
$$

$\log \left(\phi_{0}\left(T_{c}\right)\right)$ is extrapolated linearly. This allows the value of $\phi_{0}\left(T_{e}\right)$ to decrease smoothly while ensuring that it is always positive.

For

$$
T>\max \left[T_{u \rightarrow l}^{\max }\right] \quad \text { and } \quad\left[d \phi_{0} / d T_{e}\right]_{\max \left[T_{u \rightarrow 1}\right]}<0
$$

or

$$
T<\min \left[T_{w \rightarrow 1}^{\max }\right] \quad \text { and } \quad\left[d \phi_{0} / d T_{e}\right]_{\min \left[T_{x \rightarrow 1}^{\max }\right]}<0
$$

$\phi_{0}\left(T_{e}\right)$ is extrapolated linearly. This is done because any rapid power law variation in $\phi_{0}\left(T_{e}\right)$ beyond the maximum and minimum of $T_{u \rightarrow 1}^{\max }$ is likely to lead a gross inconsistency between the values of $\bar{\phi}\left(T_{n \rightarrow l}^{\max }\right)$ and the corresponding averaged value of $\phi_{0}\left(T_{e}\right)$.
Equation 4.1.1 is then written as

$$
g_{i}=\sum_{j=1}^{N} H_{i j} f_{j}+\varepsilon_{i} \quad(i=1,2, \ldots, m)
$$

which is the canonical form for inverse problems. In 4.1.7, $f_{j} \equiv \phi_{j}^{*}$ is the quantity to be estimated at the recovery points $T_{j}(j=1,2, \ldots, N), g_{i} \equiv I_{\mu \rightarrow l} / s_{i}$ is the data, $\varepsilon_{i} * s_{i}$ is the data noise so that $\varepsilon_{i}$ can be regarded as a Gaussian error of constant variance and $s_{i}$ a weighting parameter or an estimate of the noise variance on the $i$-th spectral line, and

$$
H_{i j} \equiv \frac{A(Z)}{4 \pi} \frac{1}{s_{i}} \int_{T_{j-1}}^{T_{j}} G_{i}\left(T_{e}\right) \phi_{0}\left(T_{e}\right) d T_{e}
$$

Equation 4.1 .7 is solved by a regularisation approach. In the method of regularisation the extra information required to stabilise the inversion is introduced by a smoothness condition on the source function. A solution is obtained by solving the optimisation problem

$$
\min _{\lambda}\left\{\sum_{i=1}^{m}\left(g_{i}-\sum_{j=1}^{N} H_{i j} \hat{f}\right)^{2}+\lambda \Phi(\hat{f})\right\}
$$

where $\lambda$ is a smoothing parameter representing the weight attached to the smoothing constraint $\Phi(\hat{f})$ (a linear functional of $f$, and $\hat{f}$ is the estimate of $f$. The functional $\Phi(\hat{f})$ represents a prior information about the function $f$. A choice for this functional derives from the minimisation of the norm of the second derivative of the solution. In other words, of all the solutions that can fit the data the one is chosen that minimises

$$
\|\Phi \hat{f}\|_{2}^{2}=\left\|\hat{f}^{\prime}\right\|_{2}^{2}=\int\left|\hat{f}^{\prime \prime}(y)\right|^{2} d y
$$

This choice of the linear functional defines the second order regularisation problem and is the one adopted for the solution of equation 4.1.7.
Representing the second derivative by second - order differences, 4.1.9 can be written as

$$
\min _{\lambda}\left\{\sum_{i=1}^{m}\left(g_{i}-\sum_{j=1}^{N} H_{i j} \hat{f}\right)^{2}+\lambda\left(\sum_{j=1}^{N} \hat{f}_{j+1}-2 \hat{f}_{j}+\hat{f}_{j-2}\right)^{2}\right\}
$$

with an appropriate re-scaling of the regularisation parameter. In order to avoid explicit ead conditioning, $\hat{f}_{0}=\hat{f}_{N+1}=0$.
Equation 4.1.9 or 4.1.11 can be expressed in matrix form as

$$
\left(\mathbf{H}^{T} \mathbf{H}+\lambda \Phi\right) \hat{\mathbf{f}}=\mathbf{H}^{\boldsymbol{r}} \mathbf{g}
$$

The smoothing parameter $\lambda$ is selected according to

$$
\min _{\lambda} \frac{\| \hat{\mathbf{H}} \hat{\boldsymbol{f}}-\left.\boldsymbol{g}\right|^{2}}{\left(\operatorname{trace}\left[\mathbf{H}^{T} \mathbf{H}+\lambda \mathbf{C}\right]\right)^{2}}
$$

where $\mathbf{C}$ is the hessian matrix of $\Phi(\hat{f})$. This method has the attractive property that we do not need to know explicitly the value of the noise variance of the data point but only their ratio. That is if the true standard deviation of the noise on the $i$-th element is $\sigma_{i}=\sigma_{0} s_{i}$ then the scaling factor $\sigma_{0}$ can be calculated a posteriori using

$$
\sigma_{0}^{2} \frac{\|\mathbf{H} \hat{\mathbf{f}}-\boldsymbol{g}\|^{2}}{\left(\operatorname{trace}\left[\mathbf{H}^{\top} \mathbf{H}+\lambda \mathbf{C}\right]\right.}
$$

## Program steps:

These are summarised in figure 4.1.
Figure 4.1


## Interactive parameter comments:

The organisation of the interactive windows differs in ADAS601 from the ADAS norm. Initiate ADAS601 from the ADAS6 series menu. The 'control window' is displayed first.

The Control window has the appearance shown below:

| $\nabla 1$ |  | PROGRAM : DEM V2.0 |
| :--- | :--- | :--- | :--- |
| Filo Weight Plot Run |  |  |

Abundance file :
/diak2/adaw/ada/arch601/abundance/abund.alan
Intemity file :
/diak2/adaa/adan/arch601/intensity/A.dat

Kernel file :
/dinh2/adad/adaa/arch601/kernel/goft.pmwa


The actions 'File' etc. are activated by clicking on the appropriate name. There are three input data file name information windows and then at the bottom of the control window, shorter information windows for the weighting stategy and the current activity. One can jump freely between actions, but on the first use of this program, the 'File' action must be taken first and files loaded sequentially (see below).

The File action drops down the menu shown below:


Clicking on the data type opens the usual form of ADAS file selection window shown below.


1. The data type sought is shown at a)
2. The central ADAS database has no formal data collections of the three types required here, but only sample data. It is suggested that you use the same organisation and main sub-directory naming as the ADAS example. Clicking the

Central data or User data buttons sets up a Data root b) of the ADAS pattern automatically. Personal data for the program ADAS601 should be held in the subdirectory
/disk2/<user>/adas/arch601
corresponding to the ADAS central subdirectory
/disk2/adas/adas/arch601.
Further subdirectories of /arch601 should be assigned, namely, labundance, /intensity and /kernel. Thus you abundance files should be held in the subdirectory
/disk2/<user>/adas/arch601/abundance/...
3. It is convenient to set up an additional subdirectory/run to hold output data from the progarm. Move to this subdirectory before initiating ADAS if you wish to ensure output files are placed directly into this subdirectory.
4. All three files must be identified before excuting the integral inversion.
5. The intensity file has the standard format shown below:

6. The abundance file is of the simple structure shown below:

| O | $2.470 \mathrm{E}-04$ |
| :--- | :--- |
| NE | $3.530 \mathrm{E}-05$ |
| SI | $3.920 \mathrm{E}-05$ |
| MG | $4.470 \mathrm{E}-05$ |
| S | $8.630 \mathrm{E}-06$ |
| FE | $3.920 \mathrm{E}-05$ |
| CA | $2.940 \mathrm{E}-06$ |

7. The kernel file is of the form produced directly as the collection file from ADAS506 above. Note that you must keep to precisely the same formatting conventions for you personal files of these types.
8. The Exit button terminates the program, saving the current settings in your defaults directory.

The Weight action drops down the menu shown below:


1. Click your choice for weighting of the observed intensities.
2. The last choice from the data file uses the variance estimate of the intensity measurement usually provided as part of the observed intensity data (see the structure of an intensity file). This is the default if no selection is made.

The Plot action drops down the menu shown below:

| Plot |
| :--- |
| graphical celection |
| plot kernel |
| plot DEM |

1. Clicking the graphical selection button pops up the standard ADAS output options window below:

2. Click the plot kernel button to show a simple graph of the $G(T e)$ functions available in the kernel file.
3. The DEM plot is only available once the integral inversion has been performed once (see below).

The Run action drops down the menu shown below:

| Run |
| :--- |
| execute integral inversion |

1. Click on the execute button to initiate the integral inversion calculation.
2. After completion of at least one calculation the differential emission measure becomes available for plotting as above.

## Illustration:

Figure 4.1a shows a plot of kemel data, that is the set of $\mathrm{G}(\mathrm{Te})$ functions contained in the selected kernel file. Figure 4.1.b show the resulting differential emission measure for the demonstration case in ADAS. Table 4.1.a shows the standard text output from the code.

Figure 4.1a


Figure 4.1b


## Notes:

## Coping with large quantities of data

The programs in this group belong to series ADAS2 and both are interactive processing codes on elements of the fundamental database. A schematic of the programs and dataset types interrogated is shown in figure 5.0. Each program extracts specific ion file data from the relevant data collection, acquires information from the user on his/her stategy for associating levels and then outputs the modified data set. No graphical display is produced. The output datasets are organised for direct entry into the user's personal ADAS fundamental database.

ADAS209 is designed to help with the problem of being overwhelmed with data when studying the excited populations and emissivities of complex ions. One seeks to simplify by grouping excited populations of similar levels or of levels of minor importance. We call this 'working at different resolution levels' in excited population structure. A specific situation is that in astrophysical studies where intermediate coupling LSJ resolution of populations is usual, even for light species, to assist high resolution spectroscopy. From the population structure point of view LS resolution is adequate. In fusion, LS resolution is usual for light species. The new code allows controlled 'bundling' of level populations. It does this by operating on a specific ion file (type ADF04) of high resolution and generating a new file of the same type but of lower resolution as prescribed by the user. Such an algorithm is also of value with very many level systems where there is a need to focus on the most important levels, for example metastables, and treat other levels more grossly.

ADAS210 is designed to help with the problem of handling data when studying the excited populations and emissivities of ions at different degrees of fineness (resolution levels) in excited population structure. One seeks to change between resolution levels easily. The astrophysical example is again apposite. One may have data of high quality at LS resolution for some ions which it is desired to convert to LSJ resolution for special studies. The new code allows controlled 'unbundling' of level populations. It does this by operating on a specific ion file (type ADF04) of low resolution and generating a new file of the same type but of higher resolution as prescribed by the user. Such a procedure is of course not a substitute for original high resolution cross-section data. However the procedure tries to maintain precision by using a 'template' file of high resolution (also of type ADF04) to aid in the 'unbundling' of the low resolution source ADF04 file.

Such algorithms are also of value with very many level systems where there is a need to focus on the most important levels perhaps at high resolution while treating other levels more grossly.

Figure 5.0


## ADAS209: General level bundling

The program processes specific ion files of type ADF04. The specific ion file is convertod to a smaller file of similar organisation according to a level 'bundling' stategy. The output file is is of type ADF04 and suitable for direct entry in the user's ADAS database. There is no graphical output.

## Background theory:

Consider the electron impact excitation reaction between two excited levels $i$ and $j$, of an ion $X^{+Z}$, of an element $X$;

$$
X_{i}^{+z}\left(E_{i}\right)+e\left(\varepsilon_{i}\right) \rightarrow X_{j}^{+z}\left(E_{j}\right)+e\left(\varepsilon_{j}\right)
$$

where $E_{i}\left(E_{j}\right)$ is the exitation energy of level $i(j)$, and $\varepsilon_{i}\left(\varepsilon_{j}\right)$ is the incident (scattered) electron energy.Then, the Maxwell averaged (effective colllision strength)

$$
\gamma_{\mathrm{ij}}=\int_{0}^{\infty} \Omega_{\mathrm{ij}}\left(\varepsilon_{\mathrm{j}}\right) \exp \left(-\varepsilon_{\mathrm{j}} / \mathrm{k} \mathrm{~T}_{\mathrm{e}}\right) \mathrm{d}\left(\varepsilon_{\mathrm{j}} / \mathrm{kT} T_{\mathrm{e}}\right)
$$

where $\Omega_{\mathrm{ij}}$ is the collision strength. If we now consider a transition I to J in LS coupling then the 'LSJ bundled' effective collision strength is a summation over the effective collision strengths between J-resolved fine structure levels, such that,

$$
\gamma_{\mathrm{J}}=\sum_{i \in 1} \sum_{j \in J} \gamma_{i j}
$$

Spontaneous emission coefficients (Einstein A-values) corresponding to the new 'bundled' transition are given by,

$$
A_{J \rightarrow I}=\sum_{i \in l} \sum_{j \in J} \omega_{j} A_{j \rightarrow i} / \omega_{j}
$$

where,

$$
\omega_{\mathrm{J}}=\sum_{\mathrm{j} \in \mathrm{~J}} \omega_{\mathrm{j}}
$$

The ADAS209 code makes use of the above expressions in calculating the user selected bundies.

In ionisation and recombination reactions it is proper to distinguish metastable states as potential final states for ionisation and initial states for recombination. In this context, parent states of the $\mathrm{X}^{+\mathrm{Z}+1}$ ion are identified in advanced format ADF04 files, and these too can be bundled if specific studies require only consideration of the ground states, or, if LSJ parent information is available. Three types of parent metastable information are identified which appear on the first line of the ADF04 file. These are 'term parents' with code ' $(<2 \mathrm{~S}+1>\mathrm{L})$ ), 'level parents' with code ' $(<2 \mathrm{~S}+1>\mathrm{L}<2 \mathrm{~J}+1>$ )' and unidentified parents '(<stat. weight.)'. The latter occur when mixed symmetry metastable parents are combined. In all these cases, the parent energy (relative to the lowest level of the ion) is calculated in the same way as the excitation energy ( $\mathrm{E}_{\mathrm{i}}$ ) for each of the levels of $\mathrm{X}^{+\mathbf{z}}$, namely,

$$
E_{J \rightarrow 1}=\sum_{i \in l} \sum_{j \in J} \omega_{j} E_{j \rightarrow i} / \omega_{j}-E_{\text {shif }}
$$

where $E_{\text {shift }}$ is the relative change in energy between the lowest states of $\mathbf{X}^{+\mathbf{z}}$ and $\mathbf{X}^{+\mathbf{z + 1}}$ and is therefore zero for all excited levels of $\mathrm{X}^{+\mathbf{z}}$.

The code is arranged to be quite flexible in its bundling strategy in that any levels may be grouped. However this can lead to difficulties when levels of different symmetries and configurations are bundled. This is especially the case when the levels of such a bundle span a target state for spontaneous emission from or to the bundle. A warning is issued by the code in these circumstances. It is essential to look at the output ADF04 file in such cases since spurious Einstein coefficients may be inserted and the same transition may appear twice but
with upper and lower bundle indices interchanged. In fact these correspond to the uppward and downward division. The safest stategy is usually to delete the spontaneous coefficients and add the upsilons.

## Program steps:

These are summarised in figure 5.9.
Figure 5.9


## Interactive parameter comments:

Programs of this series (ADAS2) which make use of data from archived ADAS datasets initiate an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output.
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 ADFO4 ('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. Clicking the Done button moves you forward to the next window. Clicking the Cancel button takes you back to the previous window

The processing options window has the appearance shown below

8. At a), two buttons are present to allow bundling of the levels of the selected ion and then bundling of the parents of these levels. The parents are the ground and metastable levels of the next higher ion to which ionisation may take place or from which recombination may take place. For basic studies, you will probably be using ADF04 datasets which omit recombination and assume ionisation only to the ground state of the next higher ion. Then the subtleties of parents may be ignored. This parent bundling option is non-trivial only when the advanced ADF04 specification is being used. More details are given in the ADAS Manual.

Click the appropriate button to fill the left side level display window b) and the right side Bundling window d).
9. The level list displayed in the window at a) is for information only and is a simple transcription of the list from the head of the source ADF04 file.
10. Note that the Data File Name at the left side is the same as the Data file at c ) on the right side.
11. In the Level Bundling window, the index number, configuration specification, ( $2 \mathrm{~S}+1$ ) $\mathrm{L}(\mathrm{J})$ quantum numbers and the level energy ( $\mathrm{cm}-1$ ) are given for each level in a separate display window with an editable box to its right d). The editable box is for entering a bundle index number. That is levels which are to be grouped are given the same bundle index number. If no index number is given for a level, then the code treats the level as a distinct bundle. The code reindexes bundles as necessary for consistency. Remember to press Return after entering each bundle index.
12. When you have finished the level bundling allocation, click the Parent Bundling button at a) to execute parent bundling. Note you may proceed to the next screen directly by clicking the Done button after level bundling. The code then puts in the default parent.
13. On clicking the Parent Bundling button the windows at $b$ ) and $d$ ) are filled with the corresponding parent information. The display is illustrated below. It generally has less than five entries and if the advanced ADF04 format is not in use then only one. The information format is a little different from that of the levels. The first value is the index number, followed by the parent term character string (in brackets) as given on the top line of the ADF04 file. The numerical value of the parent statistical weight follows with finally the parent energy (cm-1) relative to the lowest level of the ion. In the single parent case therefore this is just the ionisation potential.

14. Note that the organisation of all ADF04 datasets at present is such that although energy levels may be at the J-resolved intermediate coupling resolution, the parents are at term resolution. Thus there is usually no need to bundle parents unless there is a wish to focus for example on just the ground parent (lowest ionisation continurum). The latter may be the case if one wishes to bypass the
complexities of metastables. ADAS209 does however have the capability of dealing specifically with J-resolved parents.
15. Note the icon for Exit to Menu at (e). This quits the program and returns you to the ADAS series 2 menu. Remember that Done takes you forward to the next screen while Cancel takes you back to the previous screen

The output options window is of restricted form. It only offers the option of an output file. This part is of the same layout as codes previously described.
Figure 5.9d


1. The name of the source data file which has been bundled is repeated at a) for information. The output file is the bundled ADF04 file and it is of the correct format for re-entry in the ADF04 database. However, if you have used the defaults on parent bundling, it is advisable to check the top line of the file to see that the term allocation of the ground state is what you wish. The comments section at the end of the output ADF04 file details the source ADF04 file and the bundling imposed.
2. By default the output file is sent to your /pass file subdirectory as bundle.pass. You should ensure that you have created a /pass sub-directory of you personal /adas directory to receive such files.
3. There is no graphical output option.

## Illustration:

Figure 5.9a shows the input ADF04 file for $\mathrm{O}^{+4}$ in LSJ-resolution. Figure 5.9 b shows the bundled ADF04 file resulting from combining levels of the same triplet terms. Note that the bundled groups are distinguished by a '*' and that the configuration name is simply that of the first level which enters the bundle. Note that on the top line the parent term is a default one '(1S)' since the original source file contained no details of the ground state parent but only its ionisation potential. In the comments section at the end of the data, the bundling details are recorded by giving the Original level indexing and the Selection vector. Note that the Parent bundling vector is ' 0 ' recognising that no parent bundling was done.

Table 5.9a

| $0+4$ | 8 | 5 | 918657. |
| ---: | :--- | :--- | :--- |
| 1 | $2 S 2(1 S O)$ | $(1) 0(0.0)$ | 0.0 |
| 2 | $2 S 2 P(3 P O)$ | $(3) 1(0.0)$ | 81942.5 |
| 3 | $2 S 2 P(3 P 1)$ | $(3) 1(1.0)$ | 82078.6 |
| 4 | $2 S 2 P(3 P 2)$ | $(3) 1(2.0)$ | 82385.3 |
| 5 | $2 S 2 P(1 P 1)$ | $(1) 1(1.0)$ | 158797.7 |
| 6 | $2 P 2(3 P 0)$ | $(3) 1(0.0)$ | 213462.5 |
| 7 | $2 P 2(3 P 1)$ | $(3) 1(1.0)$ | 213618.2 |
| 8 | $2 P 2(3 P 2)$ | $(3) 1(2.0)$ | 213887.0 |
| 9 | $2 P 2(1 D 2)$ | $(1) 2(2.0)$ | 231721.4 |



Table 5.9b

| $0+4$ | 8 | 918657.0(15) |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1252 (150) |  | (1) 0 | ( 0.0 ) |  | 0. |  | \{1\} 1.000 |  |  |  |
|  | 2 2S2P(3P0) |  | - (3) 11 | ( 4.0$)$ |  | 32233. |  | \{1\}1.000 |  |  |  |
|  | 3 2S2P(1P1) |  | (1) 1 | $(1.0)$ |  | 58797. |  | \{1\}1.000 |  |  |  |
|  | 2P2(3PO) |  | - (3) 11 | ( 4.0 ) |  | 13750. |  | \{1\}1.000 |  |  |  |
| 5 | 5 2P2 (1D2) |  | (1) 2 | ( 2.0 ) |  | 31721. |  | \{1\}1.000 |  |  |  |
|  | 62 P 2 (150) |  | (1) 0 | ( 0.0) |  | 37910. |  | \{1\}1.000 |  |  |  |
| 7 | $72535(3 \mathrm{SI})$ |  | (3) 0 | $(1.0)$ |  | 46972. |  | \{1\}1.000 |  |  |  |
| 8 | 2S3S(150) |  | (1) 0 | ( 0.0) |  | 61276. |  | (1) 1.000 |  |  |  |
|  | 9 2S3P(1P1) |  | (1)1 | ( 1.0 ) |  | 30824. |  | (1)1.000 |  |  |  |
| 10 | 2S3P(3P0) |  | - (3) 11 | (4.0) |  | 32881. |  | \{1]1.000 |  |  |  |
| 11 | 1 2S3D(3D1) |  | * (3) 21 | ( 7.0 ) |  | 00766. |  | (1)1.000 |  |  |  |
| 12 | 2S3D(1D2) |  | (1) 2 | ( 2.0) |  | 2615. |  | (1)1.000 |  |  |  |
| -1 |  |  |  |  |  |  |  |  |  |  |  |
| 5.00 | 3 | 2.50+04 | 5.00 | 0+04 | $1.25+0$ | 052.5 | 50+05 | $5.00+05$ | 1.25+06 | $2.50+06$ | $5.00+06$ |
| 2 | $17.23+02$ | 6.12-01 | 15.39 | 9-01 | 4.49-0 | 13.8 | 0-01 | 3.06-01 | 2.05-01 | 1.37-01 | 8.26-02 |
| 3 | $12.86+09$ | $2.63+00$ | 02.67 | 7+00 | $2.81+0$ | 003.0 | 2+00 | $3.36+00$ | $4.03+00$ | 4.68+00 | 5.44+00 |
| 4 | 1 1.87-01 | 9.33-03 | 31.08 | 8-02 | 1.20-0 | 221.1 | 6-02 | 9.92-03 | 6.84-03 | 4.65-03 | 2.95-03 |
| 5 | $12.96+03$ | 1.10-01 | 11.13 | 3-01 1 | 1.17-0 | 11.1 | 6-01 | 1.10-01 | 9.09-02 | 7.28-02 | 5.54-02 |
| 11 | $26.85+10$ | $3.30+00$ | 03.30 | 0+00 | $3.33+00$ | 003.4 | $6+00$ | $3.78+00$ | $4.56+00$ | $5.41+00$ | $6.42+00$ |
| 10 | 4 5.27+07 | $2.09+00$ | 01.79 | +00 | $1.21+0$ | 007.7 | 2-01 | 5.35-01 | 7.72-01 | $1.32+00$ | $2.00+00$ |
| 11 | 4 3.00-30 | 2.13+00 | 11.85 | +00 | $1.33+00$ | 009.0 | 9-01 | 5.53-01 | 2.55-01 | 1.38-01 | 7.50-02 |
| 11 | 10 3.00-30 | $5.25+01$ | 15.70 | 0+01 | $8.07+0$ | 011.0 | 6+02 | $1.32+02$ | $1.61+02$ | $1.77+02$ | 1.89+02 |
| -1 |  |  |  |  |  |  |  |  |  |  |  |
|  | -1 |  |  |  |  |  |  |  |  |  |  |
| C |  |  |  |  |  |  |  |  |  |  |  |
| C File generated by compression of a J-resolved file |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |
| C Program: ADAs209 |  |  |  |  |  |  |  |  |  |  |  |
| c |  |  |  |  |  |  |  |  |  |  |  |
| C Source file: /home/brooks/adas/adf04/belike/belike_jl19940.dat |  |  |  |  |  |  |  |  |  |  |  |
| C Original level indexing: |  |  |  |  |  |  |  |  |  |  |  |
| C | 123 | 3 4 | 5 | 6 | 7 | 8 | 9 | 10 |  |  |  |
| c | $11 \quad 12 \quad 13$ | 314 | 15 | 16 | 17 | 18 | 19 | 20 |  |  |  |
| C Selection Vector: |  |  |  |  |  |  |  |  |  |  |  |
| c | 01 | 11 | 0 | 2 | 2 | 2 | 0 | 0 |  |  |  |
| c | $0 \quad 0 \quad 0$ | 03 | 3 | 3 | 4 | 4 | 4 | 0 |  |  |  |

```
Original parent metamtables:
    (1S)
parent bundling vector:
    O
Insert producer id here: D.H.Brooks
Date: 19/01/96
```


## Notes:

## ADAS210: General level unbundling

The program processes specific ion files of type ADF04. The specific ion source file is converted to a larger file of similar organisation according to a level 'unbundling' stategy. A template file of type ADF04 must also be available to support the processing. The output file is of type ADF04 and suitable for direct entry in the user's ADAS database. There is no graphical output.

## Background theory:

Consider the electron impact excitation reaction between two excited levels $I$ and $J$, of an ion $X^{+z}$, of an element $X$;

$$
X_{l}^{+z}\left(E_{\mathrm{l}}\right)+\mathrm{e}\left(\varepsilon_{\mathrm{l}}\right) \rightarrow \mathrm{X}_{\mathrm{J}}^{+\mathrm{z}}\left(\mathrm{E}_{\mathrm{J}}\right)+\mathrm{e}\left(\varepsilon_{\mathrm{J}}\right)
$$

where $E_{I}\left(E_{J}\right)$ is the excitation energy of level $I(J)$, and $\varepsilon_{\mathrm{I}}\left(\varepsilon_{\mathrm{J}}\right)$ is the incident (scattered) electron energy. If we have high precision calculation data for the effective collision strength associated with this transition, we may wish to obtain an 'LSJ unbundled' effective collision strength corresponding to the fine structure transition, $i \in I$ to $j \in J$, in LSJ intermediate coupling. In ADAS210 we use two methods to do this. First, we may already have lower quality data at LSJ resolution. If so, we can use ADAS209 to bundle this data and then form a ratio with our new data to use as a premultiplier to our lower quality data i.e. we normalise the J proportions of the lower quality, to that of the higher quality data. Therefore,

$$
\gamma_{\mathrm{ij}}^{\mathrm{Jn}}=\gamma_{\mathrm{ij}}^{\mathrm{Jo}} \gamma_{\mathrm{J}}^{\mathrm{LS}} / \gamma_{\mathrm{IJ}}^{\mathrm{BLSJ}}
$$

where $\gamma_{\mathrm{ij}}{ }^{\mathrm{Jn}}$ denotes the new LSJ effective collision strength, $\gamma_{\mathrm{ij}}{ }^{\mathrm{Jo}}$ denotes the lower quality LSJ value, $\gamma_{I I} \mathrm{LS}$ is the high quality LS resolved value and $\gamma_{I J} \mathrm{BLSJ}$ is the bundled lower quality values and is given by,

$$
\gamma_{\mathrm{J}}^{\mathrm{BLSJ}}=\sum_{\mathrm{i} \in \mathrm{l}} \sum_{\mathrm{j} \in \mathrm{~J}} \gamma_{\mathrm{ij}}
$$

The spontaneous emission coefficients (Einstein A-values), can be calculated in a similar manner such that,

$$
A_{j \rightarrow i}^{\mathrm{Jn}}=A_{j \rightarrow i}^{\mathrm{Jo}}\left(A_{J \rightarrow I}^{L S} / A_{J \rightarrow I}^{B L S J}\right) 0_{J}^{L S},
$$

where,

$$
A_{J \rightarrow I}^{B L S J}=\sum_{i \in I} \sum_{j \in J} A_{j \rightarrow i} \omega_{j}^{\mathrm{Jo}} / \omega_{j}^{\text {BLSJ }}
$$

with Jo and Jn referring to lower quality J-resolved data and new data respectively and superscript LS referring to the higher quality LS resolved data. In this case, the statistical weights have been included with analogous markings, and

$$
\omega_{j}^{B L S J}=\sum_{j \in J} \omega_{j}^{\mathrm{Jo}}
$$

Secondly, if we do not have any LSJ data, we use statistical splitting which gives

$$
\gamma\left({ }^{2 S+1} L_{J},{ }^{2 S^{\prime}+1} L^{\prime}{ }_{S}\right)=\sum_{J} \sum_{J^{\prime}}\left(\frac{2 J+1}{(2 L+1)(2 S+1)}\right)\left(\frac{2 J^{\prime}+1}{\left(2 L^{\prime}+1\right)\left(2 S^{\prime}+1\right)}\right) \gamma\left({ }^{2 S+1} L^{2 S^{\prime}+1} L^{\prime}\right)
$$

The $A$-values are zeroed in this case.

## Parent problems

In ionisation and recombination reactions it is proper to distinguish metastable states as well as ground states as potential final states for ionisation and initial states for recombination. For this reason, parent states of the $\mathbf{X}^{+\mathbf{Z}+1}$ ion are identified in the advanced format form of ADF04 files. These parents drive the population structure calculations and should be
included explicitly in any ionisation balance. For light ions LS term resolution of metesteble parents is adequate but a move to intermediate coupling may be required for highly ionised ions. This may also assist in high resolution spectroscopy. Consistency between resolution levels in fundamental and derived data is desirable. Bundling and unbundling allows us to 'work at different resolution levels'. ADAS210 can handie the unbundling of recombining ion parent metastables as well as the usual bound excited states of the recombined ion.
In unbundling, an additional template parent dataset at LSJ resolution is required and locatod by a search mechanism in ADAS210. If available, the parent configurations, parent energies and statistical weights are transcribed from the template following the selections entered by the user. Three types of parent metastable information are identified which appear on the first line of the source ADF04 file. These are 'term parents' with code ' $(<2 \mathrm{~S}+1>\mathrm{L}$ )', 'level parents' with code ' ( $<2 \mathrm{~S}+1>\mathrm{L}<2 \mathrm{~J}+1>$ )' and unidentified parents '(<stat. weight.)'. The latter occur when mixed symmetry metastable parents are combined. The energies are always adjusted to account for the energy shift relative to the lowest level of the ion. Only these forms are recognised by the subroutines which read ADF04 files.

In these cases the advanced specification ADF04 files are in use. Such files include information about the effective contributions to ionisation from each of the levels to each of the parent metastables (for more information see the description of ADAS208 in the last chapter of this manual and the specification of the ADF04 format in the Appendix).

## Program steps:

These are summarised in figure 5.10.
Figure 5.10


## Interactive parameter comments:

Programs of this series (ADAS2) which make use of data from archived ADAS datasets initiate an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output.
The file selection window has the appearance shown below


1. Selection of the source file to be unbundled is made in the top window. 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 c). 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 b) 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 the data files are 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. Selection of the 'template' file which assists in the unbunding is made in the lower window at d) and e) as for the source file. The information line refers to a 'Superstructure file' as template. We have mass produced such files at high resolution and they provide a good starting point. It is not obligatory to use an ADF04 file produced from the 'Superstructure' code as a template, but it must be drawn from a data collection with the same detailed naming conventions as the Superstructure collections. Incidentally such files are held in their own subdirectories of the /ADF04 directory according to isoelectronic sequence. Look for the code letter ' $j$ ' at the end of the ion name to tell you that the file is of high (ie. LSJ) resolution (eg. /.../adas/adas/adf04/copss\#be/copss\#be_ss\#odj.dat).
8. Clicking the Done button moves you forward to the next screen. Clicking the Cancel button takes you back to the previous screen

The processing options window has the appearance shown below


1. At a), two buttons are present to allow unbundling of the levels of the selected ion and then unbundling of the parents of these levels. The parents are the ground and metastable levels of the next higher ion to which ionisation may take place or from which recombination may take place. For basic studies, you will probably be using ADF04 datasets which omit recombination and assume ionisation only to the ground state of the next higher ion. Then the subtleties of parents may be ignored. This parent unbundling option is non-trivial only when the advanced ADF04 specification is being used. More details are given in the ADAS Manual. Click the appropriate button to fill the left side level display window $b$ ) and the right side Unbundling window $d$ ).
2. The level list displayed in the window at $b$ ) is from the source file which is to be unbundled and is for information only. It is a simple transcription of the list from the head of the source ADF04 file.
3. Note that the Data File at the right hand side c ) is the template file.
4. In the Level Unbundling window, the index number, configuration specification, $(2 S+1) L(J)$ quantum numbers and the level energy (cm-1) are given for each level in a separate display window with an editable box to its right d). The
editable box is for entering the index number of the source file level which you wish to associate with the high resolution template file level. Essentially the template levels are bundled first in the procedure for association with the low resolution source levels. That is template levels which are to be grouped are given the index number of their associated low resolution source file level. Then the low resolution level is unbundled in the proportions of the template file levels forming the group. Remember to press Return after entering each associated level index.
5. When you have finished the level allocation, click the Parent Unbundling button at a) to execute parent bundling. Note you may proceed to the next screen directly by clicking the Done button after level unbundling, but in this case a default '(1S)' parent is introduced. In this circumstance it is advisable to check that the top line of the output specific ion file is consistent with your intentions.
6. On clicking the Parent Unbundling button the window at b) is filled with the parent information from the source file. The window at d) by contrast is filled with level information from a template file for the adjacent higher ion of the same sub-directory class as the template file for the level unbundling. Thus if \%/../adas/adas/adf04/copss\#be/copss\#be_ss\#o4j.dat' was the level template then '.../adas/adas/adf04/copss\#li/copss\#li_ss\#o5j.dat' is the parent template. The information format is a little different from that of the levels. The first value is the index number, followed by the parent term character string (in brackets) as given on the top line of the ADF04 file. The numerical value of the parent statistical weight follows with finally the parent energy (cm-1) relative to the lowest level of the ion. In the single parent case therefore this is just the ionisation potential.
7. Note that the organisation of all ADF04 datasets at present is such that although energy levels may be at the J-resolved intermediate coupling resolution, the parents are at term resolution. The parent subject is of some depth and more details are given in the ADAS User Manual. For basic studies, these issues may be ignored.
8. Note the icon for Exit to Menu at (e). This quits the program and returns you to the ADAS series 2 menu. Remember that Done takes you forward to the next screen while Cancel takes you back to the previous screen

The output options window is of restricted form. It only offers the option of an output file. This part is of the same layout as codes previously described.

9. The name of the source data file which has been unbundled is repeated at (a) for information. The output file is the unbundled ADF04 file and it is of the correct format for re-entry in the ADF04 database. The comments section at the end of the output ADF04 file details the source ADF04 file and the unbundling imposed.
10. By default the output file is sent to your /pass file subdirectory as unbundle.pass. You should ensure that you have created a /pass sub-directory of you personal ladas directory to receive such files.

## 11. There is no graphical output option.

## Illustration:

An example of a source data set for unbundling is given in figure 5.10a and the unbundled output ADF04 file in figure 5.10b. The source sample here is in fact a bundied file from a prior ADAS209 run. In the comments section at the end of the unbundled data file, the un bundling details are recorded by giving the Template file indexing and the Source file assignment. Note that the Parent unbundling vector is blank recognising that no parent unbundling was done in this case. On the top line of the unbundled file '(IS)' is entered by default.
Table 5.10a


Table 5.10b


Notes:

# Advanced population and line emission studies 

This section introduces two programs from ADAS5 series and one from ADAS2 series as shown in figure 6.0 The programs are concerned with linking two streams of population modelling. The first stream is concerned with the modelling and prediction of detailed spectral line emission from plasmas commencing with a collection of 'complete' reaction data for an identified group of levels of an individual ion, called a specific ion file (type ADF04). Specific ion files have been encountered already in an earlier chapter and can include state selective recombination, charge exchange recombination, electron impact ionisation and ion impact excitation coefficient data, as well as the primary content of electron impact excitation data. . The derived data of most general value for spectral analysis are photon emissivity coefficients (PRC) and ionisations per photon (SXB).
The second stream is concerned with the modelling and prediction of effective recombination, ionisation and related coefficients in finite density thermal plasma. Such coefficients are required in a metastable resolved picture, rather than just the stage to stage form, for the most accurate studies. In practice the complete set of coefficients used in plasma modelling extends to collisional-radiative recombination (ACD), ionisation (SCD), charge exchange recombination (CCD), metastable cross-coupling (QCD), parent metastable cross-coupling (XCD), recombination-cascade power (PRB), charge exchange recombination power (PRC) and low-level line power (PLT). Collectively we call these the generalised collisional radiative (GCR) coefficients. In ADAS such data are first stored in an iso-electronic sequence collections of ADAS data format ADF10. Subsequently they are reassembled in an isonuclear form more suited to ionisation balance modelling.
The most refined photon emissivity (PEC) (type ADF15), ionisation per photon (SXB) (type ADF13) and generalised collisional-radiative (GCR) data are produced (the latter as a complete set of files of type ADF10) by the program ADAS208. This is an advanced version of ADAS205 which merges the key parts of the two streams. It draws necessary additional data on zero density ionisation coefficients (type ADF07), and two more complex data types called expansion data (ADF18) and condensation data (ADF17), which are beyond the scope of this discussion. SXB data is not used much in astrophysics and are not discussed further here (cf. the main ADAS User Manual).
The two other programs presented in this chapter are ADAS502 which is interrogative on the zero-density ionisation coefficient files of type ADF07, and ADAS503, which is interrogative on the photon emissivity files of type ADF15.

Figure 6.0


## ADAS502: SZD - graph and fit zero-density ionisation coefficients

The program interrogates zero-density electron impact ionisation rate coefficient (SZD) files of type ADF07. The data may be interpolated using cubic splines at selected electron temperatures. A minimax polynomial approximation is made to the interpolated data. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the polynomial approximation.

## Background theory:

Consider the ionisation reaction

$$
X_{\gamma}^{+z}+e \rightarrow X_{p_{r}}^{+z+1}+e+e
$$

where the ion $X^{+z}$ in initial state $\gamma$ is ionised leaving the residual ion $X^{+z+1}$ in the state $p_{p}$. Often ionisation from the ground state of the ion $X^{+2}$ only is present in sources of atomic data. Also the particular final state of the ion $X^{+\Sigma+1}$ is not specified, but rather a sum over final states is given. For more detailed studies, 'metastable resolved' ionisation data is required, that is where the states $\gamma$ and $p_{\rho}$ are metastable are required. If the ionisation crosssection for the reaction 6.2 .1 is $Q_{\gamma \rightarrow p_{r}}^{(z \rightarrow+1)}(\varepsilon)$, then the program accesses Maxwell averaged rate coefficients of the form

$$
\begin{align*}
S_{\gamma \rightarrow p_{p}}^{(z \rightarrow z+1)}\left(T_{e}\right)= & 2 \sqrt{\pi} \alpha c a_{o}^{2}\left(k T_{e} / I_{H}\right)^{1 / 2} \\
& \int_{I_{r, p_{\rho}} / k T_{e}}^{\infty} \frac{Q_{\gamma \rightarrow p_{\rho}}^{(z \rightarrow z+1)}(\varepsilon)}{\pi a_{o}^{2}}\left(\varepsilon / k T_{e}\right) \exp \left(-\varepsilon / k T_{e}\right) d\left(\varepsilon / k T_{e}\right)
\end{align*}
$$

where $2 \sqrt{\pi} \alpha c a_{o}^{2}=2.1716 \times 10^{-8} \mathrm{~cm}^{3} \mathrm{~s}^{-1}$.
In a plasma of zero density where there is no stepwise ionisation through excited states, the above ionisation rate coefficient is the effective ionisation rate coefficient from $\gamma$ to $p_{p}$. It is called the zero density ionisation rate coefficient. Collections of such coefficients are held in 'SZD' archived files of ADAS data format type ADF07. Each file is for an element and contains metastable resolved ionisation coefficients $S_{\gamma \rightarrow p_{f}}^{(x \rightarrow 2+1)}\left(T_{e}\right)$ and the summed ionisation coefficients

$$
S_{\gamma}^{(z \rightarrow z+1)}\left(T_{e}\right)=\sum_{p_{r}} S_{\gamma \rightarrow p_{r}}^{(z \rightarrow z+1)}\left(T_{e}\right)
$$

for each adjacent ion pair of the element.

## Program steps:

These are summarised in figure 6.2.


## Interactive parameter comments:

Programs of this series (ADAS5) which make use of data from archived ADAS datasets initiate an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output.
The file selection wiadow 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. Note that each type of data is stored according to its ADAS data format (adf number). Click the User Data button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first adas, to use this facility.
2. The Data root can be edited directly. Click the Edit Path Name button first to permit editing.

## N. B. Under the IDL Graphical User Interface which controls the window

operations, you must remember to prese the reburn key on the keyboard for any change to be recorded.
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. Clicking the Done button moves you forward to the next window. Clicking the Cancel button takes you back to the previous window

The processing options window has the appearance shown below

1. An arbitrary title may be given for the case being processed a). For information the full pathway to the dataset being analysed is also shown. The button Browse comments again allows display of the information field section at the foot of the selected dataset, if it exists.
2. The output data extracted from the datafile, in the case of ADAS502, an 'ionisation rate coefficient', may be fitted with a polynomial. This is as a function of temperature. Clicking the Fit polynomial button b) activates this. The accuracy of the fitting required may be specified in the editable box. The value in the box is editable only if the Fit Polynomial button is active. Remember to press the return key on the keyboard to record the value.
3. Available rate coefficients in the data set are displayed in the coefficient list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a coefficient to select it. The selected rate appears in the selection window c) just above the coefficient list display window.
4. Your settings of electron temperatures (output) are shown in the temperature display window d). The temperature values at which the ionisation rate coefficients are stored in the datafile (input) are also shown for information.
5. The program recovers the output temperatures you used when last executing the program. Pressing the Default Temperature values button inserts a default set of temperatures equal to the input temperatures.
6. The Temperature Values are editable. Click on the Edit Table button if you wish to change the values. A 'drop-down' window, the ADAS Table Editor window, appears as shown below:


The output options window appearance is shown below

1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the Browse comments button is available.
2. 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.

3. Hard copy is activated by the Enable Hard Copy button c). The File name box then becomes editable. If the output graphic file already exits and the Replace button has not been activated, a 'pop-up' window issues a warning.
4. A choice of output graph plotting devices is given in the Device list window d). Clicking on the required device selects it. It appears in the selection window above the Device list window.
5. 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.
6. The graph is displayed in a following Graphical Output window as shown below.

## Illustration:

Figure 6.2 a shows the zero density ionisation rate coefficient for the reaction $H e^{0}\left(1 s^{2} S\right)+e \rightarrow H e^{+1}\left(1 s^{2} S\right)+e+e$. The solid line is the spline fit used for the main interpolation and the dashed curve is the minimax fit.

Figure 6.2a


Table 6.2a

```
ADAS RELEASE: ADAS91 V1.10 PROGRAM: ADAS502 V1.1 DATE: 11/03/94 TIME: 13:19
** TABULAR OUTPUT FROM ZERO DENSITY IONIZATION RATE-COEFFICIENT INTERROGATION PROGRAM: ADAS502 - DATE: 11/03/94
**
---------------- HELIUM TEST
ZERO-DRNSITY IONIZATION RATB-COBFPICIENT AS A FUNCTION OF ELECTRON TEMPERATURE
FILE: JETSHP.IONBLEC.DATA(SZD\#HE) - DATA-BLOCK: 1
IONISING ION INFORMATION:
```

bLembnt Name
blemernt symbol
nuclezar charge
BFFECTIVE IONIZATION POTENTIAL $=198305.0 \mathrm{~cm}-1$
INITIAL STATE
ION
ION CHARGE
METASTABLE INDEX
PINAL STATE :
ION
ION CHARGE
meTASTABLE INDEX
$=\mathrm{HE}+\mathrm{O}$
(2)
$=1$
(21) $=\mathrm{HE}+$
$=12$
-...-...- BLECTRON TEMPERATURE $\qquad$
$\qquad$
$\mathrm{K} / 21 * 2$
kelvin ev
$2.321 D+04 \quad 2.000 D+00 \quad 2.321 D+04$
$3.482 \mathrm{D}+04 \quad 3.000 \mathrm{D}+00 \quad 3.482 \mathrm{D}+04$
$5.803 D+04 \quad 5.000 D+00 \quad 5.803 D+04$
$8.124 D+04 \quad 7.000 D+00 \quad 8.124 D+04$
CTRON TEMP
ZERO-DENSITY IONIZATION RATE-COBFPICIENT AS A FUNCTION OF ELECTRON TEMPERATURE

```
```

DATA GENERATED USING PROGRAM: ADAS502

```
```

DATA GENERATED USING PROGRAM: ADAS502

```
```

FILE: JETSHP.IONBLEC.DATA(SZD带HE) - DATA-BLOCK: 1 IONISING ION INFORNATION:

```

IONIZATION RATB-COEFFT cm**3/8ec.
4.921D-20
1.558D-14
1.187D-12
4.293D-11
2.152D-10
7.677D-10
3.928D-09
7.305D-09
1.265D-08
1.630D-08
1.980D-08
```

HOTE: - $\triangle$ IONIEATION RATE-COEFFTS. EXTRAPOHATED FOR RLECTROA TERPERATURE VALUR
MINIMRX POLYNONINL FIT - TAYIOR COBFFICIENSS

```


\section*{Notes:}

\section*{ADAS503: PEC - graph and fit photon emissivity coefficients}

The program interrogates photon emissivity (PEC) files of type ADF15. The coefficient is extracted for a selected radiative transition of an ion. The data may be interpolated using cubic splines at selected electron temperature/electron density pairs. A minimax polynomial approximation is made to the interpolated data. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the polynomial approximation.

\section*{Background theory:}

The emissivity in a transition \(j \rightarrow k\) of an ion may be written (see equation6.8.7) as
\[
\begin{align*}
& \left.\sum_{v^{\prime}=1}^{M_{z+1}^{\prime}} \mathcal{T}^{\prime}(C X) N_{j^{\prime}} N_{v^{\prime}}^{+}+\sum_{\mu^{\prime}=1}^{M_{z-1}} \mathcal{f}_{j^{\prime}}^{(i o n)} N_{e} N_{\mu^{\prime}}^{-}\right)
\end{align*}
\]
where \(N_{\sigma}\) denotes the population density of the specified ion in the metastable state \(\sigma, N_{g^{\prime}}^{+}\) denotes the population density of ions in the metastable state \(v^{\prime}\) of the adjacent higher ionisation stage and \(N_{\mu^{\prime}}^{-}\)denotes the population density of ions in the metastable state \(\mu^{\prime}\) of the adjacent lower ionisation stage. The \(\mathcal{F}_{j \sigma}^{(\text {exc })}, \mathcal{J}_{j, v^{\prime}}^{(r e c)}, \mathcal{J}_{j, v^{\prime}}^{\left(C^{\prime}\right)}\) and \(\mathcal{F}_{j, \mu^{\prime}}^{(i o n)}\) are the effective contributions to the population of the upper excited level \(j\) of the transition from excitation from the metastables, from free electron capture, from charge exchange recombination from neutral hydrogen and from ionisation respectively. All these coefficients depend on density as well as temperature. \(N_{e}\) is the electron density and \(N_{H}\) the neutral hydrogen density .

This allows specification of the excitation photon emissivity coefficient
\[
\operatorname{pEC}_{\sigma, j \rightarrow k}^{(\text {exc })}=\left(A_{j \rightarrow k} \mathcal{F}_{j \sigma}^{(\text {exc })}\right) / N_{e}
\]
the recombination photon emissivity coefficient
\[
\mathcal{P E} \mathcal{C}_{\sigma, j \rightarrow k}^{(e x c)}=\left(A_{j \rightarrow k} \mathcal{G}_{j \sigma}^{(e x c)}\right) / N_{e}
\]
the charge exchange photon emissivity coefficient
\[
\operatorname{PR}_{\sigma, j \rightarrow k}^{(e x c)}=\left(A_{j \rightarrow k_{j \sigma}}^{\mathcal{J}_{j \sigma}^{(e x c)}}\right) / N_{e}
\]
and the inner shell ionisation photon emissivity coefficient
\[
\operatorname{pEP}_{\sigma, j \rightarrow k}^{(e x c)}=\left(A_{j \rightarrow k_{j, ~}}^{\mathcal{F}_{j \sigma}^{(e x c)}}\right) / N_{e}
\]

PEC data are extracted from archived files of type ADF15. They are interpolated by cubic splines in electron temperature and density to provide results at an arbitrary set of temperature/density pairs. The interpolated data are approximated by a minimax polynomial and a graph produced. A tabulation of the the interpolated spline data and the minimax approximation is prepared.

\section*{Program steps:}

These are summarised in figure 6.3.

Figure 6.3


\section*{Interactive parameter comments:}

Programs of this series (ADAS5) which make use of data from archived ADAS datasets initiate an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output.

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. Note that each type of data is stored according to its ADAS data format (adf number). Click the User Data button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first adas, to use this facility.
2. The Data root can be edited directly. Click the Edit Path Name button first to permit editing.

\section*{N. B. Under the IDL Graphical User Interface which conatrols the window}
operations, you must remember to press the return key on the keyboard for any change to be recorded.
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. Clicking the Done button moves you forward to the next window. Clicking the Cancel button takes you back to the previous window

The processing options window has the appearance shown below
1. An arbitrary title may be given for the case being processed a). For information the full pathway to the dataset being analysed is also shown. The button Browse comments again allows display of the information field section at the foot of the selected dataset, if it exists.
2. The output data extracted from the datafile, in the case of ADAS503, an 'emissivity coefficient', may be fitted with a polynomial. This is as a function of temperature. Clicking the Fit polynomial button b) activates this. The accuracy of the fitting required may be specified in the editable box. The value in the box is editable only if the Fit Polynomial button is active. Remember to press the return key on the keyboard to record the value.
3. Spectrum lines for which emissivity coefficients are available in the data set are displayed in the line list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a line to select it. The selected line appears in the selection window c) just above the line list display window.
4. Your settings of electron temperature/electron density pairs (outputs) are shown in the temperature/density display window d). The temperature and density values at which the emissivity coefficients are stored in the datafile (inputs) are also shown for information. Note that you must give temperature/density pairs, ie. the same number of each as for a model. The underlying datafile has a two-dimensional storage as a function of temperature and density.
5. The program recovers the output temperature/density pairs you used when last executing the program. Pressing the Default Temperature values button inserts a default set of temperatures equal to the input temperatures, all at the same density. A choice of density from the input density set is allowed on a 'pop-up' window.
6. The Temperature \& Density Values are editable. Click on the Edit Table button if you wish to change the values. A 'drop-down' window, the ADAS Table Editor window, appears as shown below:


The output options window appearance is shown below
1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the Browse comments button is available.
2. 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.

3. Hard copy is activated by the Enable Hard Copy button c). The File name box then becomes editable. If the output graphic file already exits and the Replace button has not been activated, a 'pop-up' window issues a warning.
4. A choice of output graph plotting devices is given in the Device list window d). Clicking on the required device selects it. It appears in the selection window above the Device list window.
5. 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.
6. The graph is displayed in a following Graphical Output window.

\section*{Illustration:}

Figure 6.3a shows a PEC coefficient of excitation type, associated with the ground state (metastable 1) for the spectrum line BeI ( \(2 \mathrm{~s} 2 \mathrm{p}^{1} \mathrm{P} \cdot 2 \mathrm{~s}^{2}{ }^{1} \mathrm{~S}\) ) of neutral beryllium. The solid line connects the spline fit points obtained in the main interpolation and the dashed curve is the minimax fit.

Figure 6.3a


Table 6.3a


\section*{Notes:}

\section*{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.

\section*{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 \(X_{\rho}^{+z}\), 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 driving mechanisms considered for populating the excited levels \(X_{i}^{+z}\) are excitation from the metastable levels \(X_{\rho}^{+z}\), recombination from the metastable levels of the adjacent ion \(X_{\tau}^{+z+1}\), and ionisation form the metastable levels of the adjacent ion \(X_{\mu}^{+z-1}\). The dominant population densities of the ions in the plasma are those of the levels \(X_{\rho}^{+z}, X_{\tau}^{+z+1}\) and \(X_{\mu}^{+z-1}\), denoted by \(N_{\rho}, N_{\tau}^{+}\)and \(N_{\mu}^{-}\) 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 quasistatic 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 \(X^{+2}\). The ordinary levels are those identified explicitly in the specific ion file. Collectively, the metastable levels and ordinary levels of \(X^{+2}\) 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 \(X^{+2+1}\) ) and spin system. The grouped populations are called bundle-nS populations. The statistical balance equations for a specified parent, \(\tau\), and spin system, \(S\), take the form.

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 \(\mathrm{v}, \mathrm{v}^{\prime}\) denote metastable states of \(X^{+z+1}\) to which the specific parent \(\tau\) also belongs. The high n -shell populations are assumed in quasi-static equilibrium with the low \(n\)-shell populations and the adjacent stage metastables (parents). The high n -shell populations may be condensed onto the low \(n\)-shell populations to give

On the other hand the low level group population equations take the form
\[
\left.\left[\begin{array}{cccc}
\cdot & \cdot & 0 & 0 \\
N_{e} S_{\rho, \mu^{\prime}} & -C_{\rho, \sigma} & -C_{\rho, j} & N_{e} r_{\rho, v^{\prime}} \\
N_{e} S_{i, \mu^{\prime}} & -C_{i, \sigma} & -C_{i, j} & N_{e} r_{i, \nu^{\prime}} \\
0 & N_{e} S_{8, \sigma} & N_{e} S_{8, j} & -C_{v, v^{\prime}}
\end{array}\right] \begin{array}{c}
N_{\mu^{\prime}}^{-} \\
N_{\sigma} \\
N_{j} \\
N_{v^{\prime}}^{+}
\end{array}\right]=\left[\begin{array}{c}
\frac{d}{\partial} N_{\mu}^{-} \\
\frac{d}{d} N_{\rho} \\
0 \\
\frac{d}{\alpha} N_{v}^{+}
\end{array}\right]
\]
6.8.3
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 occuring 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. \(\mathbf{6 . 8} \mathbf{2}\) may be subtracted to leave only the indirect couplings, denoted by
\[
\left[\begin{array}{ll}
\overline{-C}_{\tau \bar{n} S, \pm \bar{n} ' S} & {\overline{N_{e} r_{n \bar{n} S}}} \\
{\overline{\bar{N},^{\prime}}}^{\bar{N}_{9, n \bar{n} ' S}} & \overline{-C}_{u, v^{\prime}}
\end{array}\right]
\]

The barred indirect matrices may be expanded over the low level manifold using level weighting factors as
\[
\begin{align*}
& \overline{\bar{C}}_{\mathrm{n} \bar{n}, \tau \bar{n}^{\prime} S} \rightarrow\left[\begin{array}{ll}
C_{\rho, \sigma}^{i n d i r} & C_{\rho, j}^{\text {indir }} \\
C_{i, \sigma}^{i n d i r} & C_{i, j}^{\text {indir }}
\end{array}\right] \\
& \bar{S}_{\vartheta, \tau \bar{n}: S} \rightarrow\left[\begin{array}{ll}
S_{v, \sigma} & S_{v, j}
\end{array}\right] \\
& \bar{r}_{\tau \bar{n} S, v^{\prime}} \rightarrow\left[\begin{array}{l}
r_{\rho, v^{\prime}} \\
r_{i, \Omega^{\prime}}
\end{array}\right]
\end{align*}
\]
and then added to equations. 6.8.3 to give
where \(\because \equiv C+C^{\text {indir }}, \overparen{ } \equiv r+r^{\text {indir }}, \quad \ell \equiv S+S^{\text {indir }}\) and \({ }_{v u^{\prime}} \equiv C_{u u^{\prime}}+\bar{C}_{\mathrm{uv}^{\prime}}\). These equations constitute the extension to the simpler low level population equations. . The solution for the ordinary populations is then
\[
\begin{align*}
& N_{j}=-\sum_{i=1}^{O}{ }_{j i} \sum_{\sigma=1}^{M}{ }_{i} N_{\sigma}+\sum_{v^{\prime}} \sum_{i=1}^{O}{ }_{j i}^{-1} x_{i^{\prime}} . N_{e} N_{v^{\prime}}^{+} \\
& +\sum_{v^{\prime}} \sum_{i=1}^{O}{ }_{0}^{0-1} 2_{i^{\prime}}^{(C X)} N_{H} N_{v^{\prime}}^{+}+\sum_{v^{\prime}} \sum_{i=1}^{O}{ }_{i j}^{-1} \varepsilon_{i \mu^{\prime}}^{(i o m)} N_{e} N_{\mu^{\prime}}^{-} \\
& \equiv \sum_{\sigma=1}^{M} \mathcal{f}_{j \sigma}^{(e x c)} N_{e} N_{\sigma}+\sum_{v^{\prime}} g_{j v^{\prime}}^{(r c)} N_{e} N_{v^{\prime}}^{+}+\sum_{v^{\prime}} g_{j^{\prime}}^{(C X)} N_{H} N_{v^{\prime}}^{+} \\
& +\sum_{\mathbf{0}^{\prime}} \mathscr{J}_{\boldsymbol{j}^{\prime}}^{\left(i \mu^{\prime}\right)} N_{e} N_{\mu^{\prime}}^{-}
\end{align*}
\]
where an additional term has been added arising from charge exchange recombination. The \(\mathcal{F}_{j c}^{(e x c)}, \mathcal{F}_{j^{\prime}}^{(r e c)}, \mathcal{F}_{j \nu^{\prime}}^{(C X)}\) and \(\mathscr{F}_{j \mu^{\prime}}^{(i o n)}\) 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 \(X^{+2}\) may also be obtained by setting \(\frac{d}{d t} N_{\rho}=0\) in equation 6.8.6
\[
\begin{align*}
\sum_{\sigma=1}^{M} C_{\rho \sigma} N_{\sigma}= & -\sum_{j=1}^{o} C_{\rho j} N_{j}+\sum_{v^{\prime}} Q_{\rho v^{\prime}} N_{e} N_{v^{\prime}}^{+} \\
& +\sum_{v^{\prime}} 2_{\rho v^{\prime}}^{(C X)} N_{H^{\prime}} N_{v^{\prime}}^{+}+\sum_{\mu^{\prime}} \delta_{\rho \mu^{\prime}}^{(i o n)} N_{e} N_{\mu^{\prime}}^{-}
\end{align*}
\]

Eliminating the ordinary level populations from the quasi-equilibrium solution of equation 6.8.7 in the matrix equations \(\mathbf{6 . 8 . 6}\) gives
\[
\left[\frac{\frac{d}{d \phi} N_{\mu}^{-}}{\frac{\frac{d}{d} N_{\rho}}{\frac{d}{d} N_{v}^{+}}}\right]=
\]

6.8.9

The partitioned matrix elements are the generalised collisional radiative coefficients. These are the ionisation coefficients
\[
S_{C D, \sigma \rightarrow 0}=\left(\delta_{v \sigma}-\sum_{j=1}^{o} b_{v j} \sum_{i=1}^{o} c_{j i}^{-1} c_{i \sigma}\right)
\]
the free electron recombination coefficients
\[
\alpha_{C D, v^{\prime} \rightarrow \rho}=\left(a_{\rho v^{\prime}}+\sum_{j=1}^{o} C_{\rho j} \sum_{i=1}^{o} C_{j i}^{-1} a_{i v^{\prime}}\right)
\]
the charge exchange recombination coefficients
\[
C_{C D, v^{\prime} \rightarrow p}=\left(2_{p v^{\prime}}+\sum_{j=1}^{o} C_{p^{j}} \sum_{i=1}^{o} C_{j i}^{-1} 2_{i^{\prime}}\right)
\]
the metastable cross-coupling coefficients
\[
X_{C D, \sigma \rightarrow \rho}=\left(C_{\rho \sigma}-\sum_{j=1}^{o} C_{\rho j} \sum_{i=1}^{o} C_{j i}^{-1} C_{i \sigma}\right)
\]
and the parent metastable cross-coupling coefficients.
\[
Q_{C D, v^{\prime} \rightarrow v}=\bar{C}_{v^{\prime} v}
\]

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
\[
P_{L T, \sigma}=\left(\sum_{k, j} \Delta E_{k j} A_{j \rightarrow k_{j}}^{7(e x c)}\right) / N_{e}
\]

The free electron recombination cascade bremsstrahlung power coefficients \(P_{R B, 8}\), and the charge exchange power coefficients \(P_{\text {R } ., s}\), 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 ( \(\beta\) ?:? and \(S / X B\) ratios ( \((X B)\) ). The reciprocals of the latter are also known as photon efficiencies. From equations 6.8.7, the emissivity in the spectrum line \(j \rightarrow k\) is
\[
\begin{align*}
& \varepsilon_{j \rightarrow k}=A_{j \rightarrow k}\left(\sum_{\sigma=1}^{M} f_{j c}^{(e x c)} N_{\sigma}+\sum_{v^{\prime}=1}^{M_{k+1}} \underset{j^{\prime}}{(r e c)} N_{e} N_{v^{\prime}}^{+}+\right. \\
& \left.\sum_{v^{\prime}=1}^{M_{z+1}} f_{j^{\prime}}(C X) N_{H} N_{v^{\prime}}^{+}+\sum_{\mu^{\prime}=1}^{M_{t-1}{ }_{j}(\text { iow })} N_{e} N_{\mu^{\prime}}^{-}\right)
\end{align*}
\]

This allows specification of the excitation photon emissivity coefficient
\[
\operatorname{pe}_{\sigma, j \rightarrow k}^{(e x c)}=\left(A_{j \rightarrow k}^{g_{j c}^{(e x c)}}\right) / N_{e}
\]
the recombination photon emissivity coefficient
\[
\operatorname{PE}_{\varepsilon_{v^{\prime}, j \rightarrow k}^{(r e c)}}^{(r c)} A_{j \rightarrow k^{\prime}}^{g_{j v^{\prime}}^{(r e c)}}
\]
the charge exchange photon emissivity coefficient
\[
\operatorname{pe}_{\mathcal{U}_{U^{\prime}, j \rightarrow k}}^{(C X)}=A_{j \rightarrow k^{\prime}, N^{\prime}}^{7}
\]
and the ionisation photon emissivity coefficient
\[
\operatorname{pse}_{\mu^{\prime}, j \rightarrow k}^{(i o n)}=A_{j \rightarrow k^{\prime} ; \mu^{\prime}} \tau^{(i o n)}
\]

The \(S\) / \(X B\) are only meaningful for the excitation part of the emissivity and are
\[
\ell X B_{\sigma, j \rightarrow k}=\sum_{\mathrm{v}=1}^{M_{x+1}} \mathbf{S}_{C D, \sigma \rightarrow 0} /\left(A_{i \rightarrow k^{\prime}}^{\mathrm{g}_{j \sigma}^{(e x c)}}\right)
\]

Each of these coefficients is associated with a particular metastable \(\sigma, v^{\prime}\) or \(\mu^{\prime}\) of the \(X^{+2}\), \(X^{+z+1}\) or \(X^{+z-1}\) ions respectively.

\section*{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 (appendix C). The scope of operation of ADAS208 is determined by the content of the specific ion file processed. The miminum 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 dexcitation 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 compex 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.

\section*{Program steps:}

These are summarised in figure 6.8.
Figure 6.8


\section*{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 Uiser 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 ADF14 (subdirectory /f18-p08) which cross-references projection matrices (ADF18) 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


The processing options window has the appearance shown below
1. 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.
2. 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 \(\mathrm{N}_{\mathrm{H}} / \mathrm{N}_{\mathrm{e}}\) 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.
3. 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. See the main ADAS USER Manual for a detailed explanation of the handling of metastables in the collisional-radiative picture.
4. Various processes, supplementary to the primary electron excitation collisions and bound-bound radiative transitions, are activated as desired by clicking on the appropriate buttons d). 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.
5. 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 Zeffective e).
6. The spawn ionisation coefficient search button activates a new process equivalent to to ADAS502.


The spawned ionisation rate coefficient acquisition windows are as follow:
1. 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.

2. 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.
3. 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.
4. 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.
5. 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.
6. 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.


The ADAS208 output options window has the appearance shown below
1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the Browse comments button is available.
2. 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.

3. Hard copy is activated by the Enable Hard Copy button c). The File name box then becomes editable. If the output graphic file already exits and the Replace button has not been activated, a 'pop-up' window issues a warning.
4. A choice of output graph plotting devices is given in the Device list window d). Clicking on the required device selects it. It appears in the selection window above the Device list window.
5. 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.
6. Three 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 file. These are of ADF15, ADF13 and ADF10 structure respectively. They go by defaults into
/...../<uid>/adas/pass/pec.pass

\section*{/...../<uid>/adas/pass/xxb.pass \\ /...../<uid>/adas/pass/gcf.pass} respectively.
7. The graph is displayed in a following Graphical Output when the Done button is pressed.
8. 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.
9. Press the Next button to show the next graph in a sequence and the Previous button to show the previous graph.
10. Press the Print button to make a hard copy of the currently displayed picture.
11. Pressing the Done button restores the previous Output Options window.

\section*{Illustration:}

The output from the program is shown for the lithium-like ion \(\mathrm{O}^{+5}\) in figure 6.8a. The specific ion file is assembled from the data of Sampson and co-workers.

Figure 6.8a
ROPUIATION DEPENDENCE ON MEIASTABIES: \(0+5\) EIECTRON TEMR \(=2.00 E+01\) (EV)
ADAS RELEASE: ADAS01 V1010 PROGRAM: ADAS205 V1.0 DATE: 26/05/93 TIME: 16:15
GRAPH TITLE : POPULATION GRAPH
INPUT FILE : /JETSHP.COPSMHLI.DATA(SMWO5) O+5 POPULATIONS


The tabular output is shown in below. Energies are in units of \(I_{H}\), excitation and deexcitation rate coefficients are in units of \(\mathrm{cm}^{3} s^{-1}\) and the A-coefficient is in units of \(s^{-1}\). IFPTS indicates the optimising level with FXC2 and FXC3 the optimised parameters. IBPTS \(=1\) if the bad point options is chosen, otherwise 0 . IDIFF \(=1\) if the difference option is chosen, otherwise 0

Table 6.8.






\begin{tabular}{ll} 
PROTON IMPACT COLLIEIONS & - WOT INCLUDED \\
IONIZATION RATES & - NOT INCLUDED \\
NEUTMAL HYDROGB CHARGE EXCHANOE - NOT INCLUDED \\
FREE ELECTRON RECOREINATION & - NOT INCLUDED
\end{tabular}

TABLE KEY
\begin{tabular}{|c|c|}
\hline NE & - LLECTRON DTESITY \\
\hline TE & - ELECTROET TPMPERATURE \\
\hline 1 & - mermey level index \\
\hline IMET & - metastable Index \\
\hline IORD & - ORDIMARY LEVEL INDE \\
\hline
\end{tabular}
\begin{tabular}{|c|c|c|}
\hline RUABERR OF PROTOA & IMPACT COLLISIONS & INCLUDED \\
\hline number of pres & ELECTRON RECOMBIAMATIONS & INCLUDED \\
\hline munbra of charcs & EXCHNASE RECOMBIETATIONS & INCLUDSD \\
\hline
\end{tabular}


EQUILIERTUM METASTABLE POPULATION DEPEADENCE ON DENSITY AT TE = \(1.558+00 \mathrm{EV}=1.80 \mathrm{E}+04\) KBLVIN InIT I
\(\begin{array}{lllllllllll}1 & 1 & 1.00008+00 & 1.00008+00 & 1.0000 \mathrm{~B}+00 & 1.0000 \mathrm{~B}+00 & 1.0000 \mathrm{~B}+00 & 1.0000 \mathrm{~B}+00 & 1.0000 \mathrm{E}+00 & 1.0000 \mathrm{~B}+00 & 1.0000 \mathrm{~B}+00\end{array}\)

POPULATIOA DEPENDENCT ON DENSITY AND METASTABLE 1
IORD I
\begin{tabular}{|c|c|c|c|c|c|c|c|c|c|c|}
\hline 1 & 2 & 6.19978-07 & 1.85478-06 & 6.12182-06 & 1.78688-05 & 5.4423E-05 & 1.31208-04 & 2.59788-04 & 3.61178-04 & 4.18408-04 \\
\hline 2 & 3 & 1.1657E-06 & 3.4877E-06 & 1.15188-05 & 3.36638-05 & 1.02908-04 & 2.49318-04 & 4.9604E-04 & 6.9123E-04 & 8.01558-04 \\
\hline 3 & 4 & 2.21818-28 & 6.6581E-28 & 2.22398-27 & 6.70928-27 & 2.27518-26 & 7.0657B-26 & 2.47768-25 & 7.5647E-25 & 2.3692E-24 \\
\hline 4 & 5 & 2.1908E-30 & 6.8041E-30 & 2.53502-29 & 9.8078E-29 & 5.5478E-28 & 3.08428-27 & 1.78688-26 & 6.88228-26 & 2.40908-25 \\
\hline 5 & 6 & 4.2994E-30 & 1.33518-29 & 4.97185-29 & 1.92248-28 & 1.08778-27 & 6.05918-27 & 3.51858-26 & 1.35618-25 & 4.74648-25 \\
\hline 6 & 7 & 1.68818-30 & 5.16885-30 & 1.84368-29 & 6.5287E-29 & 3.21718-28 & 1.63058-27 & 9.32658-27 & 3.87628-26 & 1.60748-25 \\
\hline 7 & 8 & 0 & 7.70198-30 & 2.74682-29 & 9.72708-29 & 4.79698-28 & 2.43688-27 & 1.3977B-26 & 5.82538-26 & 2.41018-25 \\
\hline 8 & 9 & 2.7627E-36 & 0.27948-36 & 2.75028-35 & 8.17885-35 & 2.67218-34 & 7.90808-34 & 2.69528-33 & 8.2808E-33 & 3.03788-32 \\
\hline 9 & 10 & 1.59038-37 & 4.92308-37 & 1.8146E-36 & 6.8416E-36 & 3.62458-35 & 1.79698-34 & 8.82098-34 & 3.11878-33 & 1.23388-32 \\
\hline 10 & 21 & 3.15322-37 & 9.75978-37 & 3 & 1 & 7.17608-35 & 3.56198-34 & 1.7516E-33 & 6.19878-33 & 32 \\
\hline 11 & 12 & 1.71948-37 & 5.26238-37 & 1.87418-36 & 6.6164B-36 & 3.24378-35 & 1.6319E-34 & 9.1844E-34 & 3.81708-33 & 1.71018-32 \\
\hline 12 & 13 & 2.5724E-37 & 7.87268-37 & 2.80342-36 & 9.89558-36 & 4.85258-35 & 2.44388-34 & 1.3768E-33 & 5.72308-33 & 2.5633E-32 \\
\hline 13 & 14 & 1.28578-37 & 3.90228-37 & 1.35392-36 & 4.52601-36 & 2.07558-35 & 1.12128-34 & 6.36248-34 & 4.44758-33 & 2.28318-32 \\
\hline 14 & 15 & 1.71618-37 & 5 & 1.30668-36 & 6.03668-36 & 2.76638-35 & 1.49498-34 & 1.11638-33 & 5.9366E-33 & 3.0453E-32 \\
\hline 15 & 16 & 7. & 2.35062-39 & 7.54002-39 & 2.07488-38 & 5.91938-38 & 1.64885-37 & 6.24965-37 & 2.27158-36 & 9.8429:-36 \\
\hline 16 & 17 & 8.5843E-41 & 2.69285-40 & 1.02198-39 & 3.89418-39 & 1.85938-38 & 7.86932-38 & 3.73768-37 & 1.44415-36 & 6.3723E-36 \\
\hline 17 & 10 & 1.70418-40 & 5.34638-40 & 2.02938-39 & 7.7355E-39 & 3.69418-38 & 1.56458-37 & 7.44148-37 & 2.67808-36 & 1.2705E-35 \\
\hline 18 & 19 & 1.08408-40 & 3.31985-40 & 1.18598-39 & 4.22758-39 & 2.09868-38 & 1.04391-37 & 5.78008-37 & 2.3842E-36 & 1.07958-35 \\
\hline 19 & 20 & 1.6302E-40 & 4.99068-40 & 1.78098-39 & 6.3346E-39 & 3.13628-38 & 1.5594E-37 & c.64738-37 & 3.57118-36 & 1.6178E-35 \\
\hline 20 & 21 & 1.30498-40 & 3.96568-40 & 1.38358-39 & 4.7302\%-39 & 2.33168-38 & 1.27358-37 & 7.82138-37 & 3.37575-36 & 1.55601-35 \\
\hline 21 & 22 & 1.73978-40 & 5.28678-40 & 1.84435-39 & 6.30438-39 & 3.10538-38 & 1.69518-37 & 1.04158-36 & 4.49785-36 & 2.07398-35 \\
\hline 22 & 23 & 1.99585-42 & 6.06928-41 & 2.12928-40 & 7.20085-40 & 3.47438-39 & 2.2297E-38 & 2.78238-37 & 2.59098-36 & .9725E-35 \\
\hline 23 & 24 & 2.49285-41 & 7.5798 ㅍ-41 & 2.64501-40 & e.98315-40 & 1.32048-39 & 2.77898-38 & 3.47838-37 & . 24278 & 2.46798-35 \\
\hline
\end{tabular}


\section*{Notes:}

\section*{Appendices}

\section*{ADAS data formats}

The various permanent data sets in ADAS fall into a number of categories with precisely defined organisation and formatting. The specifications of these are called 'ADAS data formats' or ADF's for short. The categories most relevant here are as follows:
\begin{tabular}{ll} 
ADF04 & resolved specific ion data collections \\
ADF07 & direct resolved electron impact ionisation coefficients \\
ADF11 & iso-nuclear master files \\
ADF15 & photon emissivity coefficients \\
ADF20 & G(Te) functions
\end{tabular}

\section*{ADF04}

Provides all required energy level and rate coefficient data for specified low levels of an ion. The data set is complete for a low level population calculation. Specific level selective free electron recombination and charge exchange recombination is included. Formatting conventions and variable storage are given below.

\section*{Utilising subroutines :}

ADAS201 ADAS205
ADAS206 ADAS208
Directories of formatted files to ADF04 specification :
/.../adas/adas/adf04/<seq>like/
/.../adas/adas/adf04/copss\#<seq>/
/.../adas/adas/adf04/copsm\#<seq>/
/.../adas/adas/adf04/copmm\#<seq>1
/.../adas/adas/adf04/copmm\#<el.no.>/
/.../adas/adas/adf04/coppm\#<seq>/
/.../adas/adas/adf04/copjl\#<seq>/
where <seq> is the isoelectronic sequence symbol
<el. no.> is the isonuclear charge number
Data lines :
SYM , IZ , IZ0, IZ1, BWNO1 , [(PTRM1), BWNO2, (PTRM2) .....] , ADFID until IND \(=-1\)

IND , SPEC , IS , IL , IJ , WNO , [(IP1) , IZTA1 , (IP2) , IZTA2 .....]
\(-1,(\operatorname{EORB}(\mathrm{I}), \mathrm{I}=1,14)\)
ZEFF , ITYP , (TEA(I), \(=1\), MAXT)
until INDU \(=-1\) and \(\operatorname{NDL}=-1\)
until INDU \(=-1\)
ICODE, INDU, INDL , AVAL, (GAM(I),I=1,MAXT)
\(\begin{array}{ll} & -1 \\ -1 & -1\end{array}\)
variable identification :
name meaning
SYM element symbol in form \#\#+
IZ charge of the ion
IZ0 nuclear charge
IZ1 ion charge +1
BWNO1 ionisation potential of lowest level (cm-1) rel. to 1st parent term.
[ PTRM1 term of the 1st parent
BWNO2 ionisation potential of lowest level (cm-1) rel. to 2nd parent term.
PTRM2 term of the 2nd parent


Items in square brackets are only used by program ADAS208. They are ignored by the other processing programs
Table B4c - example.
\begin{tabular}{|rllll|}
\hline\(H+0\) & & 1 & 1 & 109679 \\
1 & \(1 S\) & & \((2) 0(0.5)\) & 0. \\
2 & \(2 S\) & \((2) 0(0.5)\) & 82259. \\
3 & \(2 P\) & \((2) 1(2.5)\) & 82259. \\
4 & \(3 S\) & & \((2) 0(0.5)\) & 97492. \\
5 & \(3 P\) & & \((2) 1(2.5)\) & 97492. \\
\hline
\end{tabular}


\section*{ADF07}

Provides electron impact ionisation rate coefficients for ions optionally with resolution into metastable initial and final states. Formatting conventions and variable storage are given below.

Utilising subroutines:
ADAS208 ADAS502
Directories of formatted files to ADF07 specification :
/.../adas/adas/adf07/ionelec/
Data lines :
NSEL, TEXT
for \(\operatorname{ISEL}=1\) to NSEL
IZ , IZ1, NTE, BWNO, METI, METF, ISEL
(TEV(IT), \(\mathrm{IT}=1,24\) )
(SZD(IT), IT=1,24)
repeat
variable identification :
\begin{tabular}{ll} 
name & meaning \\
NSEL & number of reactions available \\
TEXT & information \\
IZ & initial ion charge \\
IZ1 & final ion charge \\
NTE & number of temperatures \\
BWNO & effective ionisation potential (cm-1) \\
METI & initial state metastable index \\
METF & final state metastable index \\
ISEL & transition index \\
TEV() & electron temperatures (eV) \\
SZD() & zero density ionisation rate coefficient (cm**3 sec-1)
\end{tabular}

Table B7c - example.
\[
\begin{aligned}
& 1.000 \mathrm{D}+002.000 \mathrm{D}+003.000 \mathrm{D}+004.000 \mathrm{D}+005.000 \mathrm{D}+007.000 \mathrm{D}+00 \\
& 1.000 \mathrm{D}+011.500 \mathrm{D}+012.000 \mathrm{D}+013.000 \mathrm{D}+014.000 \mathrm{D}+015.000 \mathrm{D}+01 \\
& 7.000 \mathrm{D}+011.000 \mathrm{D}+021.500 \mathrm{D}+02 \quad 2.000 \mathrm{D}+02 \quad 3.000 \mathrm{D}+024.000 \mathrm{D}+02 \\
& 5.000 \mathrm{D}+027.000 \mathrm{D}+021.000 \mathrm{D}+032.000 \mathrm{D}+03 \quad 5.000 \mathrm{D}+031.000 \mathrm{D}+04 \\
& 1.694 \mathrm{D}-12 \text { 2.947D-10 1.827D-09 4.741D-09 8.754D-09 1.733D-08 } \\
& \text { 3.016D-08 4.737D-08 5.983D-08 7.577D-08 8.506D-08 9.086D-08 } \\
& \text { 9.715D-08 1.008D-07 1.015D-07 1.002D-07 9.640D-08 9.266D-08 } \\
& \text { 8.932D-08 8.378D-08 7.750D-08 6.505D-08 4.975D-08 3.978D-08 } \\
& \mathrm{BE}+0 / \mathrm{BE}+1 / 24 / \mathrm{I} . \mathrm{P} .=253212.0 / \mathrm{ICODR}=2 / \mathrm{PCODE}=1 / \text { ISEL- } 2 \\
& 1.000 \mathrm{D}+002.000 \mathrm{D}+00 \quad 3.000 \mathrm{D}+004.000 \mathrm{D}+00 \quad 5.000 \mathrm{D}+00 \quad 7.000 \mathrm{D}+00 \\
& 1.000 \mathrm{D}+011.500 \mathrm{D}+012.000 \mathrm{D}+013.000 \mathrm{D}+014.000 \mathrm{D}+015.000 \mathrm{D}+01 \\
& 7.000 \mathrm{D}+011.000 \mathrm{D}+021.500 \mathrm{D}+02 \quad 2.000 \mathrm{D}+02 \quad 3.000 \mathrm{D}+024.000 \mathrm{D}+02 \\
& 5.000 \mathrm{D}+027.000 \mathrm{D}+021.000 \mathrm{D}+032.000 \mathrm{D}+03 \text { 5.000D }+031.000 \mathrm{D}+04 \\
& \text { 2.738D-11 1.313D-09 5.407D-09 1.148D-08 1.845D-08 3.271D-08 } \\
& \text { 5.189D-08 7.648D-08 9.407D-08 1.168D-07 1.3044-07 1.392D-07 } \\
& \text { 1.493D-07 1.556D-07 1.580D-07 1.568D-07 1.518D-07 1.437D-07 } \\
& \text { 1.412D-07 1.323D-07 1.221D-07 1.016D-07 7.663D-08 6.067D-08 }
\end{aligned}
\]


\section*{ADF11}

Isonuclear master file data. Formatting conventions and variable storage are given below.

Utilising subroutines:
ADAS405 ADAS406
Directories of formatted files to ADF07 specification :
/.../adas/adas/adf1 1/<class><yr>\#<el> /

> where <class> is the data class <yr> is the two digit year number <code> is the resolution letter ( \(r=>\) resolved, blank \(=>\) unresolved)

Data lines :
Resolved files
IZMAX, IDMAXD, ITMAXD, IZIMIN, IZIMAX
(NMETA(I),I=1,IZMAX+1)
(DDENSD(ID),ID=1,IDMAXD)
(DTEVD(IT),IT=1,ITMAXD)
for \(I Z 1=1, I Z M A X\)
for IPRT and IGRD
IPRT, IGRD [,WVLEN], IZI, DATE
for \(I T=1, I T M A X D\)
(DRCOFD \({ }^{*}\) (IT,ID),ID=1,IDMAXD)
repeat
repeat
repeat

Unresolved files
IZMAX, IDMAXD, ITMAXD, IZIMIN, IZIMAX
(DDENSD(ID),ID=1,IDMAXD)
(DTEVD(IT),IT=1,ITMAXD)
for \(\mathrm{IZ} 1=1, \mathrm{IZMAX}\)
[WVLEN,] IZI, DATE
for \(\mathrm{IT}=1\),ITMAXD
(DRCOFD \({ }^{*}\),IT,ID),ID=1,IDMAXD)
repeat
repeat
variable identification :
\begin{tabular}{ll} 
name & meaning \\
IZMAX & nuclear charge
\end{tabular}
\begin{tabular}{ll} 
IDMAXD & number of densities \\
ITMAXD & number of densities \\
IZ1MIN & lowest ion charge +1 \\
IZ1MAX & highest ion charge
\end{tabular}

NMETA( number of metastables for each ionisation stage
\begin{tabular}{ll} 
DDENSD0 & \(\log 10(\) electron density \((\mathrm{cm}-3))\) \\
DTEVDO & \(\log 10(\) electron temperature (K))
\end{tabular}
\begin{tabular}{lll} 
& IPRT & parent metastable index \\
IGRD & recombined ion metastable index & \\
[ & \\
WVLEN & specific line wavelength (Angstrom) & class 9 only] \\
IZ1 & recombining ion charge & \\
DATE & date
\end{tabular}

> DRCOFD(,) \(\quad \log 10\) (generalised collisional radiative coefficients)
> (units according to class)

\section*{Table Bllc - resolved data}
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline 426 & 351 & 4 & /BERYLLIUM & & \multicolumn{3}{|l|}{/DICKSON ET AL 1992} \\
\hline 21 & 21 & 1 & & & & & \\
\hline 10.00000 & 10.20003 & 10.40002 & 10.59999 & 10.80003 & 11.00000 & 11.20003 & 11.40002 \\
\hline 11.59999 & 11.80003 & 12.00000 & 12.20003 & 12.40002 & 12.59999 & 12.80003 & 13.00000 \\
\hline 13.20003 & 13.40002 & 13.59999 & 13.80003 & 14.00000 & 14.20003 & 14.40002 & 14.59999 \\
\hline 14.80003 & 15.00000 & & & & & & \\
\hline 0.00015 & 0.10016 & 0.20015 & 0.30015 & 0.40015 & 0.50015 & 0.60015 & 0.70015 \\
\hline 0.80015 & 0.90015 & 1.00015 & 1.10016 & 1.20015 & 1.30015 & 1.40015 & 1.50015 \\
\hline 1.60015 & 1.70015 & 1.80015 & 1.90015 & 2.00015 & 2.20015 & 2.40015 & 2.60015 \\
\hline 2.80015 & 3.00015 & 3.20015 & 3.40015 & 3.60015 & 3.80015 & 4.00015 & 4.20015 \\
\hline 4.40015 & 4.60015 & 4.70015 & & & & & \\
\hline \multicolumn{8}{|l|}{-.-.-.-------/ IPRT= 1 / IGRD= 1 /---.---/ Z1= 1 / DATE \(=16 / 11 / 93\)} \\
\hline \multicolumn{8}{|l|}{-11.57681-11.55926-11.53861 \(-11.51437-11.48604-11.45315-11.41518-11.37166\)} \\
\hline -11.32210 & -11.26598 & -11.20285 & -11.13244 & -11.05561 & -10.97341 & -10.88689 & -10.79719 \\
\hline & -10.61241 & -10.51952 & -10.42769 & -10.33806 & -10.25165 & -10.16957 & -10.09290 \\
\hline \[
-10.02268
\] & -9.96003 & & & & & & \\
\hline \multicolumn{8}{|l|}{-} \\
\hline \multicolumn{8}{|l|}{\(\cdot\)} \\
\hline \multicolumn{8}{|l|}{} \\
\hline -74.00000 & -74.00000 & -74.00000 & -74.00000 & -74.00000 & -74.00000 & -74.00000 & -74.00000 \\
\hline -74.00000 & -74.00000 & -74.00000 & -74.00000 & -74.00000 & -74.00000 & -74.00000 & -74.00000 \\
\hline -74.00000 & -74.00000 & -74.00000 & -74.00000 & -74.00000 & -74.00000 & -74.00000 & -74.00000 \\
\hline -74.00000 & -74.00000 & & & & & & \\
\hline \multicolumn{8}{|l|}{-} \\
\hline -9.42566 & -9.42504 & -9.42431 & -9.42348 & -9.42260 & -9.42169 & -9.42080 & -9.41994 \\
\hline -9.41916 & -9.41849 & -9.41796 & -9.41761 & -9.41747 & -9.41757 & -9.41794 & -9.41862 \\
\hline & -9.42102 & -9.42267 & -9.42448 & -9.42633 & -9.42810 & -9.42968 & -9.43096 \\
\hline \multicolumn{8}{|l|}{-9.43182-9.43215} \\
\hline \multicolumn{2}{|l|}{c} & \multicolumn{6}{|c|}{c} \\
\hline \multicolumn{8}{|l|}{\multirow[t]{2}{*}{}} \\
\hline & & & & & & & \\
\hline \multicolumn{8}{|l|}{c} \\
\hline \multicolumn{8}{|l|}{C PREPARED USING CODB JETXLE.IOABAL.PORT (MJD404R)} \\
\hline C & WILLIAM & J. DICRSON & 16/11/93 & & & & \\
\hline
\end{tabular}

Table B11d - unresolved data
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline 213 & \(51 \quad 1\) & 21 & /HELION & \multicolumn{4}{|l|}{} \\
\hline 4.00000 & 5.00000 & 6.00000 & 7.00000 & 8.00000 & 9.00000 & 10.00000 & 11.00000 \\
\hline 12.00000 & 13.00000 & 14.00000 & 15.00000 & 16.00000 & & & \\
\hline -0.06466 & 0.03533 & 0.13534 & 0.23535 & 0.33534 & 0.43534 & 0.53534 & 0.63534 \\
\hline 0.73534 & 0.83534 & 0.93534 & 1.03533 & 1.13534 & 1.23535 & 1.33534 & 1.43534 \\
\hline 1.53534 & 1.63534 & 1.73534 & 1.83534 & 1.93534 & 2.03533 & 2.13534 & 2.23535 \\
\hline 2.33534 & 2.43534 & 2.53534 & 2.63534 & 2.73534 & 2.03534 & 2.93534 & 3.03533 \\
\hline 3.13534 & 3.23535 & 3.33534 & 3.43534 & 3.53534 & 3.63534 & 3.73534 & 3.83534 \\
\hline 3.93534 & 4.03533 & 4.13534 & 4.23535 & 4.33534 & 4.43534 & 4.53534 & 4.63534 \\
\hline 4.73534 & 4.83534 & 4.93534 & & & & & \\
\hline & & & & & / 21-1 & / DATE \({ }^{\text {d }} 09\) & 9/11/90 \\
\hline -21.02274 & -21.02448 & -21.01428 & -20.98969 & -20.97136 & -20.98573 & -21.03465 & -21.02173 \\
\hline -20.82594 & -20.37585 & -19.79799 & -19.26837 & -18.92128 & & & \\
\hline -8.26043 & -8.26360 & -8.25394 & -8. 22642 & -8.19355 & -8.17223 & -8.17398 & -8.18895 \\
\hline -8.20194 & -8.20187 & -8.19411 & -8.18816 & -8.19132 & & & \\
\hline & & & & & -/ 21: 2 & 1 date \(=0\) & 9/11/90 \\
\hline -36.43890 & -36.43925 & -36.43584 & -36.42578 & -36.40593 & -36.37265 & -36.31938 & -36.23863 \\
\hline -36.10640 & -35.80753 & -35.19548 & -34.17990 & -32.98088 & & & \\
\hline -9.04721 & -9.04720 & -9.04707 & -9.04648 & -9.04495 & -9.04234 & -9.04021 & -9.04073 \\
\hline -9.04481 & -9.04660 & -9.03791 & -9.01206 & -8.97073 & & & \\
\hline
\end{tabular}

\section*{ADF15}

Provides photon emissivity coefficients. Formatting conventions and variable storage are given below.

Utilising subroutines:
ADAS405 ADAS406
ADAS503
Directories of formatted files to ADF15 specification:
/.../adas/adas/adf15/ionelec/
/.../adas/adas/adf15/pec<yr>\#<el>/
\[
\begin{aligned}
\text { where } & <y r>\text { is a two digit year number } \\
& <e l>\text { is the element symbol }
\end{aligned}
\]

Data lines:
```

    NSEL, TEXT
    for ISEL=1 to NSEL
        WLNG,NDENS, NTE ,FILMEM, TYPE , INDM, ISEL
        (DENS(IN), IN=1,NDENS)
        (TE(IT), IT=1,NTE)
        for IN =1 to NDENS
            (PEC(IN,IT),IT=1,NTE)
        repeat
    repeat
    ```
variable identification :
\begin{tabular}{ll} 
name & meaning \\
NSEL & number of transitions available \\
TEXT & information \\
WLNG & wavelength of transition (Ang) \\
NDENS number of densities \\
NTE & number of temperatures \\
FILMEM & \begin{tabular}{l} 
source specific ion excitation file
\end{tabular} \\
TYPE & \begin{tabular}{l} 
type of photon emissivity (excit, recomb, cx)
\end{tabular} \\
INDM & associated metastable index in source file \\
ISEL & \begin{tabular}{l} 
transition index \\
DENS()
\end{tabular} \\
TE() & \begin{tabular}{l} 
electron densities (cm-3)
\end{tabular} \\
PEC(,) & finite density photon emissivity coefficients (cm3 s-1)
\end{tabular}

Table B15c


\section*{ADF20}

Provides \(\mathrm{G}(\mathrm{Te}\) ) functions. Formatting conventions and variable storage are given below.

\section*{Utilising subroutines :}

ADAS506
Dinectories of formatted files to ADF20 specification:
/.../adas/adas/adf20/gft<yr>\#<seq>1
where <yr> is a two digit year number <seq> is the isoelectronic sequence symbol

Data lines:
EL, IZ, NLEVELS, NKNOTS, NLINES
SHFILE
SBFILE
SSFILE
PROG, DATE, UID
for \(i=1\), NLEVELS
IND, CODE, IS, IL, IJ
repeat
for \(\mathrm{it}=1\), NKNOTS
TE, DENS, P, RHE TM, TEL, DENSL, PL
repeat
SPSYMB
for \(\mathrm{itr} 0=1\), NLINES, 10
(WVLAP(itr), itr=itr0, itr0+9)
(WVLEX(itr), itr=itr0, itr0+9)
(LL(itr), LU(itr), itr=itr0, itr0+9)
for \(i t=1\), NKNOTS
TELV, (GFT(itr,it),itr=itr0,itr0+9)
repeat
repeat

DESCRIPTIVE TEXT
variable identification:
name
EL
IZ
NLEVELS
NKNOTS
meaning
two character element symbol
ion charge
number of energy levels for ion number of data values for a transition
\begin{tabular}{|c|c|}
\hline NLINES & number of transitions \\
\hline SHFILE & source file for hydrogen to electron number density ratio \\
\hline SBFILE & source files for ionisation balance calculation \\
\hline SSFILE & source specific ion file \\
\hline PROG & computer code used fro the data production \\
\hline DATE & date of production \\
\hline UID & user identifier of data producer \\
\hline IND() & index numbers of energy levels \\
\hline CODE( & arbitrary identifier string for energy levels \\
\hline IS() & multiplicity of level \\
\hline IL() & total orbital quantum number of level \\
\hline IJ() & (statistical weight-1)/2 for level \\
\hline TE() & electron temperatures ( K ) \\
\hline DENS() & electron densities (cm-3) \\
\hline P() & pressure ( \(\mathrm{K} \mathrm{cm}-3\) ) \\
\hline RHE() & hydrogen/electron number density ratio \\
\hline TM() & time (or unspecified counter) \\
\hline TEL() & \(\log 10\) ( electron temperature(K)) \\
\hline DENSL() & \(\log 10(\) electron density ( \(\mathrm{cm}-3)\) ) \\
\hline PL() & \(\log 10\) ( pressure ( \(\mathrm{Kcm}-3\) ) \\
\hline SPSYMB & spectroscopic notation for emitting ion \\
\hline WVLAP() & appproximate wavelength for line (Angstrom) \\
\hline WVLEX() & exact wavelength for line (Angstrom) \\
\hline LL() & lower level index for line \\
\hline LU() & upper level index for line \\
\hline TELV & \(\log 10\) (electron temperature ( K )) \\
\hline GFT(,) & \(\mathrm{G}\left(\mathrm{T}_{\mathrm{e}}\right)\) function ( \(\mathrm{cm} 3 \mathrm{~s}-1\) ) \\
\hline & 1st parameter - transition \\
\hline & 2nd parameter - temperature \\
\hline
\end{tabular}

Table B20c - example.



\section*{TRANSITION MAVELENGTHS ADJUSTED TO SPECTROSCOPIC VALUES IN KBLLY}
ADAS data status
recursor:
Sequence
Li-like
Be-like
B-like
C-like
F-like
Ne-like
Na-like

He-like
Be-like
O-like
Members
\(\mathrm{Be}-\mathrm{U}\)
\(\mathrm{B}-\mathrm{U}\)
\(\mathrm{C}-\mathrm{U}\)
\(\mathrm{N}-\mathrm{U}\)
\(\mathrm{Ne}-\mathrm{U}\)
\(\mathrm{Na}-\mathrm{U}\)
\(\mathrm{Mg}-\mathrm{U}\)

\(\mathrm{C}-\mathrm{Mo}\)
\(\mathrm{C}-\mathrm{Fe}\)
\(\mathrm{Ne}-\mathrm{Fe}\)
\begin{tabular}{|c|c|}
\hline Library & Comments \\
\hline rlidata & Sampson/Zhang( \(\mathrm{n}=2,3,4,5\) ) \\
\hline rbedata & Sampson/Zhang( \(\mathrm{n}=2\) ) \\
\hline rbdata & Sampson/Zhang( \(\mathrm{n}=2,3\) ) \\
\hline rcdata & Sampson/Zhang( \(n=2,3\) ) \\
\hline rfdata & Sampson/Zhang( \(\mathrm{n}=2,3\) ) \\
\hline medata & Sampson/Zhang( \(\mathrm{n}=3,4\) ) \\
\hline madata & Sampson/Zhang( \(\mathrm{n}=3,4,5\) ) \\
\hline adf05(helike) & Sampson/Zhang( \(\mathrm{n}=2,3\) ) \\
\hline adf05(belike) & Lang ( \(\mathrm{n}=2,3\) ) \\
\hline adf05(olike) & Lang/Summers( \(n=2\) ) \\
\hline
\end{tabular}
כen

2x!I-8
2x!I-9g
2x!I-! 7





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\(\mathrm{Be}, \mathrm{C}, \mathrm{N}, \mathrm{O}, \mathrm{Ne}, \mathrm{Mg}, \mathrm{Al}, \mathrm{Si}, \mathrm{S}, \mathrm{Ar}\) s.aдquaw
\begin{tabular}{|c|c|c|c|c|c|}
\hline C-like & N,O,Ne, Mg,Al,Si,S,Ar & copsm\#c & Sampson/Zhang( \(\mathrm{n}=2,3\) ) & j & medium \\
\hline & \(\mathrm{Ca}, \mathrm{Ti}, \mathrm{Fe}, \mathrm{Ni}\) & & & & \\
\hline F-like & Ne, Mg, Al, Si,S,Ar & copsm\#f & Sampson/Zhang( \(\mathrm{n}=2,3\) ) & j & medium \\
\hline & \(\mathrm{Ca}, \mathrm{Ti}, \mathrm{Fe}, \mathrm{Ni}\) & & & & \\
\hline Ne-like & \(\mathbf{M g}, \mathrm{Al}, \mathrm{Si}, \mathrm{S}, \mathrm{Ar}\) & copsm\#ne & Sampson/Zhang( \(\mathrm{n}=3,4\) ) & j & medium \\
\hline & \(\mathrm{Ca}, \mathrm{Ti}, \mathrm{Fe}, \mathrm{Ni}\) & & & & \\
\hline Na-like & Mg, Al,Si,S,Ar & copsm\#na & Sampson/Zhang( \(\mathrm{n}=3,4,5\) ) & j & medium \\
\hline & \(\mathrm{Ca}, \mathrm{Ti}, \mathrm{Fe}, \mathrm{Ni}\) & & & & \\
\hline Li-like & \(\mathrm{Be}, \mathrm{C}, \mathrm{N}, \mathrm{O}, \mathrm{Ne}, \mathrm{Mg}, \mathrm{Al}, \mathrm{Si}, \mathrm{S}, \mathrm{Ar}\) & copss\#li & Superst/dipole i.p. \(\mathrm{n}=2,3,4,5\) ) & j & low \\
\hline & \(\mathrm{Ca}, \mathrm{Ti}, \mathrm{Fe}, \mathrm{Ni}\) & & & & \\
\hline Be-like & \(\mathrm{C}, \mathrm{N}, \mathrm{O}, \mathrm{Ne}, \mathrm{Mg}, \mathrm{Al}, \mathrm{Si}, \mathrm{S}, \mathrm{Ar}\) & copss\#be & Superst/dipole i.p. \((\mathrm{n}=2)\) & j & low \\
\hline & \(\mathrm{Ca}, \mathrm{Ti}, \mathrm{Fe}, \mathrm{Ni}\) & & & & \\
\hline B-like & C,N,O,Ne, Mg, Al, Si,S,Ar & copss\#b & Superst/dipole i.p. \((\mathrm{n}=2,3\) ) & j & low \\
\hline & \(\mathrm{Ca}, \mathrm{Ti}, \mathrm{Fe}, \mathrm{Ni}\) & & & & \\
\hline C-like & N,O,Ne, Mg,Al,Si,S,Ar & copss\#c & Superst/dipole i.p. \((\mathrm{n}=2,3\) ) & j & low \\
\hline & \(\mathrm{Ca}, \mathrm{Ti}, \mathrm{Fe}, \mathrm{Ni}\) & & & & \\
\hline F-like & Ne,Mg,Al,Si,S,Ar & copss\#f & Superst/dipole i.p. \((n=2,3\) ) & j & low \\
\hline & \(\mathrm{Ca}, \mathrm{Ti}, \mathrm{Fe}, \mathrm{Ni}\) & & & & \\
\hline Ne-like & \(\mathbf{M g}, \mathrm{Al}, \mathrm{Si}, \mathrm{S}, \mathrm{Ar}\) & copss\#ne & Superst/dipole i.p. \((\mathrm{n}=3,4\) ) & j & low \\
\hline & \(\mathrm{Ca}, \mathrm{Ti}, \mathrm{Fe}, \mathrm{Ni}\) & & & & \\
\hline Na-like & \(\mathbf{M g}, \mathrm{Al}, \mathrm{Si}, \mathrm{S}, \mathrm{Ar}\) & copss\#na & Superst/dipole i.p. \((\mathrm{n}=3,4,5\) ) & j & low \\
\hline & \(\mathrm{Ca}, \mathrm{Ti}, \mathrm{Fe}, \mathrm{Ni}\) & & & & \\
\hline Be isonuc. & all ions & copmm\#4 & Cowan/Bom(n=2,3) & j \& ls & low \\
\hline
\end{tabular}
collisional radiative recombination／ionisation calculation with ADAS series 2 codes．


2．copmm files contain dipole and non－dipole non－spin change collision rate coefficients only．Exchange collisions are not present．
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Z
 Ar isonuc．
 －onuos！！ S

 \(z\)
Z
兑
C isonuc．


1．copss filess contain dipole collision rate coefficients only．They are often used for supplementation of higher quality data sets which
\[
\text { ( } \left.\varepsilon^{‘} \tau=\mathrm{u}\right) \text { шоя/иемоэ } \quad 9 \varepsilon \# \text { шudos }
\] 8z\＃umudos 9z\＃umudos 81\＃mudos LI\＃wumdos 91\＃umudos てI\＃umudos 01\＃ \(\mathbf{~ U u m d o s ~}\) 8\＃uudos 율
薄 o
昔
 （ \(\varepsilon^{\prime} \tau=\mathrm{u}\) ）шод／ивмоЈ （ \(\varepsilon^{\prime} \tau=\mathbf{u}\) ）шод／иемоэ （ \(\varepsilon^{\prime} \tau=\mathbf{u}\) ）шод／иемод （ \(\varepsilon^{\prime} \tau=\mathrm{u}\) ）шоя／иемој



 （ \(\varepsilon\)＇\(\tau=\mathbf{u}\) ）шоя／иемој
\[
\begin{aligned}
& \begin{array}{l}
\text { Quality } \\
\text { high } \\
\text { high } \\
\text { high } \\
\text { medium } \\
\text { high } \\
\text { medium } \\
\text { high } \\
\text { medium } \\
\text { high } \\
\text { high } \\
\text { high } \\
\text { medium } \\
\text { high }
\end{array} \\
& \begin{array}{l}
\text { Resolution } \\
\text { resolved } \\
\text { resolved } \\
\text { unresolved } \\
\text { resolved } \\
\text { unresolved } \\
\text { resolved } \\
\text { unresolved } \\
\text { resolved } \\
\text { unresolved } \\
\text { unresolved } \\
\text { resolved } \\
\text { unresolved } \\
\text { resolved }
\end{array} \\
& \begin{array}{l}
\text { Comments } \\
\text { CLM normalised, S\&H split } \\
\text { CLM normalised, S\&H split } \\
\text { CLM normalised } \\
\text { CLM normalised, S\&H split } \\
\text { CLM normalised } \\
\text { CLM normalised, S\&H split } \\
\text { CLM normalised } \\
\text { CLM normalised, S\&H split } \\
\text { CLM normalised } \\
\text { CLM normalised } \\
\text { Griffin, normalised } \\
\text { A\&R } \\
\text { Griffin, normalised }
\end{array} \\
& \begin{array}{l}
\text { Library } \\
\text { szd93\#h } \\
\text { szd93\#he } \\
\text { szd93\#li } \\
\text { szd93\#be } \\
\text { szd93\#b } \\
\text { szd93\#c } \\
\text { szd93\#n } \\
\text { szd93\#o } \\
\text { szd93\#f } \\
\text { szd93\#ne } \\
\text { szd93\#cr } \\
\text { szd93\#fe } \\
\text { szd93\#mo }
\end{array} \\
& \text { fe } \\
& \begin{array}{l}
\mathrm{cr}, \mathrm{cr} 0, \mathrm{cr} 1 \\
\mathrm{fe}
\end{array} \\
& \begin{array}{l}
\text { Members } \\
\text { h,h0 } \\
\text { he,he0,he1 } \\
\text { li } \\
\text { be,be0,bel, } \\
\text { b } \\
\text { c,c0,cl,c2,c } \\
\text { n } \\
\text { o,o0,ol,o2,0 } \\
\text { f } \\
\text { ne }
\end{array} \\
& \begin{array}{l}
0,00,01,02,03,04,05,06,07 \\
\text { f } \\
\text { ne }
\end{array} \\
& \text { mo,mon, mol } \\
& \begin{array}{l}
\text { Element } \\
\text { Hydrogen } \\
\text { Helium } \\
\text { Lithium } \\
\text { Beryllium } \\
\text { Boron } \\
\text { Carbon } \\
\text { Nitrogen } \\
\text { Oxygen } \\
\text { Fluorine } \\
\text { Neon } \\
\text { Chromium } \\
\text { Iron } \\
\text { Molybdenum }
\end{array} \\
& \begin{array}{lll}
\text { Comments } & \text { Resolution } & \text { Quality } \\
\text { CLM normalised, S\&H split } & \text { resolved } & \text { high } \\
\text { CLM normalised, S\&H split } & \text { resolved } & \text { high } \\
\text { CLM normalised } & \text { unresolved } & \text { high } \\
\text { CLM normalised, S\&H split } & \text { resolved } & \text { medium } \\
\text { CLM normalised } & \text { unresolved } & \text { high } \\
\text { CLM normalised, S\&H split } & \text { resolved } & \text { medium } \\
\text { CLM normalised } & \text { unresolved } & \text { high } \\
\text { CLM normalised, S\&H split } & \text { resolved } & \text { medium } \\
\text { CLM normalised } & \text { unresolved } & \text { high } \\
\text { CLM normalised } & \text { unresolved } & \text { high } \\
\text { Griffin, normalised } & \text { resolved } & \text { high } \\
\text { A\&R } & \text { unresolved } & \text { medium } \\
\text { Griffin, normalised } & \text { resolved } & \text { high }
\end{array} \\
& \begin{array}{l}
\text { Library } \\
\text { szd93\#h } \\
\text { szd93\#he } \\
\text { szd93\#li } \\
\text { szd93\#be } \\
\text { szd93\#b } \\
\text { szd93\#c } \\
\text { szd93\#n } \\
\text { szd93\#o } \\
\text { szd93\#f } \\
\text { szd93\#ne } \\
\text { szd93\#cr } \\
\text { szd93\#fe } \\
\text { szd93\#mo }
\end{array} \\
& \begin{array}{l}
\text { Members } \\
\text { h,h0 } \\
\text { he,he0,he1 } \\
\text { li } \\
\text { be,be0,bel, be2,be3 } \\
\text { b } \\
\text { c,c0,cl,c2,c3,c4,c5 } \\
\text { n } \\
\text { o,00,ol,o2,o3,o4,05,06,o7 } \\
\text { f } \\
\text { ne } \\
\text { cr,cr0, crl } \\
\text { fe } \\
\text { mo,mo0,mol }
\end{array} \\
& \begin{array}{l}
\text { Element } \\
\text { Hydrogen } \\
\text { Helium } \\
\text { Lithium } \\
\text { Beryllium } \\
\text { Boron } \\
\text { Carbon } \\
\text { Nitrogen } \\
\text { Oxygen } \\
\text { Fluorine } \\
\text { Neon } \\
\text { Chromium } \\
\text { Iron } \\
\text { Molybdenu }
\end{array} \\
& \begin{array}{l}
\text { Notes: } \\
\text { N }
\end{array} \\
& \text { Notes: 1. The element member contains a preferred compilation for all the ions of the element. The ion members contain just the individual ion resolved data. } \\
& \text { 2. CLM normalised refers to the Culham Laboratory Reports CLM-R216- \& CLM-R270 for the total stage to stage coefficients. } \\
& \text { 3. S\&H refers to splitting into metastable resolved ionisation coefficients using the method of Summers \& Hooper. Results are n } \\
& \text { to stage total. } \\
& \text { 4. Griffin refers to metastable resolved data extracted from the detailed adf23 data sets prepared by Griffin, Pindzola or Badnell. } \\
& \text { This data is also normalised as specified in the dataset comments. Griffin data will eventually replace all the S\&H split data. } \\
& \text { 5. A\&R refers to Arnaud \& Raymond (1992) Astrophys. J. 398, } 394 .
\end{aligned}
\]

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un! \(\|\) Kıg

 s|d'yd'und'qud'pכo'pos 'pos \begin{tabular}{l}
\(\%\) \\
6 \\
6 \\
\hline
\end{tabular} \(\%\)
\(\%\)
6
8 Hd'qud'pox'pob'pos 'pos spdivd'urd'qud'poo'pos'pos pos 'pose
pos 'pose s[d'yld'udd'qud'pos'pos 'pos pos' \(\mathbf{~ ' p o s}\) Hd'qud'pox'pob'pos 'pos s[d'7 Id'oId'qud'poo'pos 'pos Hfd'qud'pox'pob'pos 'pos \(^{\text {d }}\)
 pos 'pos
pos 'ров Hd'qId'pox'pob'pos 'pos sld 7 Id'odd'qud'pos'pos 'pse sassold



 1ep. \(0^{-} 68<\) SSE| \(\gg / 68<\mathrm{SSE} \mid \mathrm{D}>1\) IEP \(\cdot 0^{-}\)S8<SSB|O>/S8<SSE|O>/

 IEP \(\cdot q^{-} \downarrow L<\) SSE \(\mid \gg / \downarrow L<\) SSE \(\mid ग>/\) 1ер. 2 q \(^{-}\)- \(\varepsilon 6<\) SSR|ग>/IE6<SSEID>/ IEP \(\cdot\) q \(^{-} 68<\) SSE \(\mid 0>/ 68<\) SSE \(\mid \gg /\)
 1ер. 2 - \(^{-} 68<\) SSE \([0>/ 68<S S E \mid 0>/\) 1EP \(\cdot 2 \cdot प^{-}\)S8<SSE[0>/S8<SSE \(0>1\)



\(0 z\) - sosppueddy

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Summers, c-r
I-0 's0ZSVGV
วu! วseq LGf
J-9's0ZSVGV
JET base line
 d-9 'sıəuums
d-9'80ZSVGV

sıизшиол
penjosarun
E
\(\frac{1}{6}\)
\(\frac{6}{2}\)
8
E
\(\frac{1}{6}\)
\(\frac{8}{6}\)
8
panjoson
pasjosajun panjosarun
ponjosarun
ponjosanun
ponjosarun
ponjosad
panjoserun
ponjosod ponjosenun

panjososun
pasjosal
panjosarun
uoinmosay

\begin{tabular}{|c|c|c|c|}
\hline <class>74/<class>74_o.dat & Summers, c-r & unresolved & \\
\hline /<class>85/<class>85_o.dat & Armaud \& Rothenflug *HPS c-r & unresolved & medium \\
\hline /<class>89/<class>89_0.dat & JET base line & unresolved & low \\
\hline /<class>93r/<class>93r_o.dat & ADAS208, c-r & resolved & high \\
\hline /<class>74/<class>74_f.dat & Summers, c-r & unresolved & medium \\
\hline <<class>85/<class>85_f.dat & Arnaud \& Rothenflug *HPS c-r & unresolved & medium \\
\hline /<class>89/<class>89_f.dat & JET base line & unresolved & low \\
\hline /<class>74/<class>74_ne.dat & Summers, c-r & unresolved & medium \\
\hline /<class>85/<class>85_ne.dat & Arnaud \& Rothenflug *HPS c-r & unresolved & medium \\
\hline <<class>89/<class>89_ne.dat & JET base line & unresolved & low \\
\hline /<class>74/<class>74_na.dat & Summers, c-r & unresolved & medium \\
\hline <class>85/<class>85_na.dat & Arnaud \& Rothenflug *HPS c-r & unresolved & medium \\
\hline <class>74/<class>74_mg.dat & Summers, c-r & unresolved & medium \\
\hline /<class>85/<class>85_mg.dat & Amaud \& Rothenflug *HPS c-r & unresolved & medium \\
\hline /<class>74/<class>74_al.dat & Summers, c-r & unresolved & medium \\
\hline /<class>85/<class>85_al.dat & Armaud \& Rothenflug *HPS c-r & unresolved & medium \\
\hline
\end{tabular}
\(\left.\begin{array}{ll}\text { Oxygen } & \text { acd, scd } \\
\text { Oxygen } & \text { acd, scd } \\
\text { Oxygen } & \text { acd, scd,ccd,prb,prc,plt,pls } \\
\text { Oxygen } & \text { acd, scd,qcd,xcd,prb,plt }\end{array}\right]\)\begin{tabular}{ll} 
& \\
Fluorine & acd, scd \\
Fluorine & acd, scd \\
Fluorine & acd, scd,ccd,prb,prc,plt,pls \\
Neon & acd, scd \\
Neon & acd, scd \\
Neon & acd, scd,ccd,prb,prc,plt,pls \\
\hline Sodium & acd, scd \\
Sodium & acd, scd \\
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Notes: 1. Summers denotes Summers (1974) Appleton Laboratory Report IM3657. Arnaud \& Rothenflug denotes
2. c-r denotes collisional radiative data with density dependence. *HPS c-r indicates Summers (1974) density variation imposed on zero density data. 3. JET base line denotes simplified calculations reproducable by ADAS408 using adf03 data sets.
4. \(r\) denotes resolved data format generated by ADAS208 in combination with ADAS204 to give adf10 iso-electronic data type, post-processed with ADAS404 to give adfll isonuclear data type.



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