

ADAS404: Isonuclear master data - extract from isoelectronic master data

The program implements a conversion of collisional-dielectronic data for iso-electronic sequences of ADAS data format *adf10* (iso-electronic master files) to data for an iso-nuclear sequence, that is for a specific element, of data format *adf11* (iso-nuclear master files). ADAS404 can handle both stage to stage (Standard) and metastable to metastable (Partial) forms. Also it permits contraction from the Partial form in the *adf10* input datasets to Standard form in the *adf11* output datasets. ADAS404 merges the actions of two codes (ADAS403 and ADAS404) in IBM-ADAS. It is anticipated that ADAS404 will be supplanted in the future by a more advanced code allowing 'flexible partitioning' between Resolved and Unresolved data in iso-nuclear master files.

Background theory:

The principal archiving of collisional radiative data generated by the populations codes and external interface codes of the Atomic Data and Analysis Structure is by iso-electronic sequence. These archived files are called *iso-electronic master files*. In applications, it is generally most useful to have available at the one time the collisional radiative data for every ion of a particular element under study. Such data collections are also archived and called *iso-nuclear master files*. In general, the iso-electronic data form the primary collection and the iso-nuclear data are generated from them by the code ADAS404. It should be noted that some iso-nuclear data are produced directly without an origin in iso-electronic data. The iso-electronic master files may contain ordinary stage to stage (unresolved) collisional radiative coefficients, called *standard files* (S) or generalised metastable distinguished (resolved) collisional radiative coefficients, called *partial files* (P). ADAS404 accepts iso-electronic data of either form and prepares the corresponding *standard* or *partial iso-nuclear master files*.

The classes of data available in the partial iso-electronic master files include the collisional-dielectronic recombination coefficient (ACD), the collisional-dielectronic ionisation coefficient (SCD), the collisional-radiative charge exchange recombination coefficient (CCD), the collisional-dielectronic recombination / cascade / bremsstrahlung radiated power coefficient (PRB), the collisional-radiative charge exchange recombination / cascade power coefficient (PRC), the collisional-radiative metastable cross-coupling coefficient (QCD) and the collisional-dielectronic parent cross-coupling coefficient (XCD), the collisional-radiative excitation total line power coefficient (PLT) and the collisional-radiative excitation specific line power coefficient (PLS). Standard iso-electronic files of the the QCD and XCD data classes do not occur. There are therefore nine classes of data present in principle although the iso-electronic data from any particular source may omit some of the data classes. The internal organisation of the data in the iso-electronic master files is according to two categories namely *recombination/ionisation (RI)* and *line/power (LP)*. The classes are summarised below:

| Mnemonic | Class | Forms | Categories |
|----------|---|-------|------------|
| ACD | Coll.-diel. recom. coefft. | P & S | RI |
| SCD | Coll.-diel. ionis. coefft. | P & S | RI |
| CCD | Coll.-diel. charge exch. coefft. | P & S | RI |
| PRB | Coll.-diel. recom./brems. power coefft. | P & S | RI |
| PRC | Coll.-rad. charge exch. recom. power coefft. | P & S | RI |
| QCD | Coll.-rad. metastable cross coupling coefft. | P | RI |
| XCD | Coll.-diel. parent meta. cross-coupling coefft. | P | RI |
| PLT | Coll.-rad. excit. line power coefft. | P & S | LP |
| PLS | Coll.-rad. specific line excit. power coefft. | P & S | LP |

Iso-electronic sequence data consists of data for a set of ions.

| mnemonic | standard form | | | partial form | | | | |
|----------|-------------------------------------|----------------------------------|--------------------|--|----------------------------------|--------------------|-----------|-----------|
| | symbol | unit | data set | symbol | unit | data set | | |
| | | | sub-set identif. | | | sub-set identif. | 1st index | 2nd index |
| ACD | $\alpha_{CD}^{(z+1 \rightarrow z)}$ | $\text{cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | $\alpha_{CD,\rho' \rightarrow \rho}^{(z+1 \rightarrow z)}$ | $\text{cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | ρ' | ρ |
| SCD | $S_{CD}^{(z \rightarrow z+1)}$ | $\text{cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | $S_{CD,\rho \rightarrow \rho'}^{(z \rightarrow z+1)}$ | $\text{cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | ρ' | ρ |
| CCD | $C_{CD}^{(z+1 \rightarrow z)}$ | $\text{cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | $C_{CD,\rho' \rightarrow \rho}^{(z+1 \rightarrow z)}$ | $\text{cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | ρ' | ρ |
| PRB | $P_{RB}^{(z+1)}$ | $\text{erg cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | $P_{RB,\rho'}^{(z+1)}$ | $\text{erg cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | ρ' | |
| PRC | $P_{RC}^{(z+1)}$ | $\text{erg cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | $P_{RC,\rho'}^{(z+1)}$ | $\text{erg cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | ρ' | |
| QCD | | | | $Q_{CR,\rho \rightarrow \sigma}^{(z \rightarrow z)}$ | $\text{cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | ρ | σ |
| XCD | | | | $X_{CR,\rho' \rightarrow \sigma}^{(z+1 \rightarrow z+1)}$ | $\text{cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | ρ' | σ' |
| PLT | $P_{LT}^{(z)}$ | $\text{erg cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | $P_{LT,\rho}^{(z)}$ | $\text{erg cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | ρ | |
| PLS | $P_{LS}^{(z)}$ | $\text{erg cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | $P_{LS,\rho}^{(z)}$ | $\text{erg cm}^3 \text{ s}^{-1}$ | $z_1 \equiv z + 1$ | ρ | |

The source files to be accessed contain generalised (metastable resolved) collisional radiative coefficients for iso-electronic sequences and these are to be combined to provide ordinary (stage to stage) collisional radiative coefficient files. The files to be manipulated are generically called *iso-electronic master files*, with those of ordinary type called *standard files* (S) and those of generalised type called *partial files* (P) here. The classes of data in the partial files include the collisional-dielectronic recombination coefficient (ACD), the collisional-dielectronic ionisation coefficient (SCD), the collisional-radiative charge exchange recombination coefficient (CCD), the collisional-dielectronic recombination / cascade / bremsstrahlung radiated power coefficient (PRB), the collisional-radiative charge exchange recombination / cascade power coefficient (PRC), the collisional-radiative metastable cross-coupling coefficient (QCD) and the collisional-dielectronic parent cross-coupling coefficient (XCD), the collisional-radiative excitation total line power coefficient (PLT) and the collisional-radiative excitation specific line power coefficient (PLS). These constitute nine classes. For the standard files, the QCD and XCD data classes do not occur. The internal organisation of the data in the files is according to two categories namely *recombination/ionisation (RI)* and *line/power (LP)*. To allow the combining to take place, it is necessary to have an additional class of isoelectronic master file containing equilibrium metastable fractional populations. The relevant classes are summarised below:

| Mnemonic | Class | Forms | Categories |
|----------|---|-------|------------|
| ACD | Coll.-diel. recom. coefft. | P & S | RI |
| SCD | Coll.-diel. ionis. coefft. | P & S | RI |
| CCD | Coll.-diel. charge exch. coefft. | P & S | RI |
| PRB | Coll.-diel. recom./brems. power coefft. | P & S | RI |
| PRC | Coll.-rad. charge exch. recom. power coefft. | P & S | RI |
| PLT | Coll.-rad. excit. line power coefft. | P & S | LP |
| PLS | Coll.-rad. specific line excit. power coefft. | P & S | LP |
| MET | Equilibrium metastable fractions | P | LP |

Consider the populations of ions of an element X of nuclear charge z_0 in a plasma. The populations of excited states may be neglected compared with those of metastable and ground states of its ions. In statistical equilibrium in the plasma, let the latter populations for ionisation stages z and $z+1$ be

$$N_{\rho}^{(z)} : \rho = 1, \dots, M_z \quad \text{and} \quad N_{\rho'}^{(z+1)} : \rho' = 1, \dots, M_{z+1} \quad 5.4.1$$

respectively, where M_z is the number of metastable states (including the ground state) of ionisation stage z and M_{z+1} is the number of metastable states (including the ground state) of ionisation stage $z+1$. The whole stage populations are

$$N^{(z)} = \sum_{\rho=1}^{M_z} N_{\rho}^{(z)} \quad \text{and} \quad N^{(z+1)} = \sum_{\rho'=1}^{M_{z+1}} N_{\rho'}^{(z+1)} \quad 5.4.2$$

respectively. To combine metastable resolved collisional radiative coefficients, the assumption is made that the equilibrium metastable population fractions may be used. The unresolved coefficients are then obtained as

$$\begin{aligned} \text{ACD:} \quad \alpha_{CD}^{(z+1 \rightarrow z)} &= \left(\sum_{\rho'=1}^{M_{z+1}} N_{\rho'}^{(z+1)} \sum_{\rho=1}^{M_z} \alpha_{CD, \rho' \rightarrow \rho}^{(z+1 \rightarrow z)} \right) / N^{(z+1)} \\ \text{SCD:} \quad S_{CD}^{(z \rightarrow z+1)} &= \left(\sum_{\rho=1}^{M_z} N_{\rho}^{(z)} \sum_{\rho'=1}^{M_{z+1}} S_{CD, \rho \rightarrow \rho'}^{(z \rightarrow z+1)} \right) / N^{(z)} \end{aligned} \quad 5.4.3$$

$$\text{PRB:} \quad P_{RB}^{(z+1)} = \left(\sum_{\rho'=1}^{M_{z+1}} N_{\rho'}^{(z+1)} P_{RB, \rho'}^{(z+1)} \right) / N^{(z+1)}$$

$$\text{PLT:} \quad P_{LT}^{(z)} = \left(\sum_{\rho=1}^{M_z} N_{\rho}^{(z)} P_{LT, \rho}^{(z)} \right) / N^{(z)}$$

Class CCD is equivalent to ACD, PRC to PRB and PLS to PLT. There are no standard file classes QCD or XCD since such data only links metastables of the same ionisation stage.

This procedure is self consistent if the standard coefficients calculated above are then used in an ionisation balance calculation, provided the metastable fractions were calculated using the same set of partial coefficients. In practise, the standard coefficients are used in non-equilibrium diffusive or time dependent calculations. In these circumstances, the equilibrium assumption for the metastable fractions is unsound, especially for highly dynamic plasmas. The partial coefficients should then be used directly in the models. It is to be noted that substantial errors may be introduced by common assumptions about stage to stage rate coefficients. If it assumed that a stage population is effectively that of its ground state, then the effective stage to stage coefficient used is

$$\overline{\alpha}_{CD}^{(z+1 \rightarrow z)} = \sum_{\rho=1}^{M_z} \alpha_{CD, 1 \rightarrow \rho}^{(z+1 \rightarrow z)} \quad 5.4.4$$

If the resolved recombination coefficients from metastables other than the ground of the ionisation stage $z+1$ are very small (this occurs with strong secondary autoionisation channels) then

$$\alpha_{CD}^{(z+1 \rightarrow z)} \approx (N_1^{(z+1)} / N^{(z+1)}) \overline{\alpha}_{CD}^{(z+1 \rightarrow z)} \quad 5.4.5$$

Since the population ratio may be significantly less than one ($\sim 1/2$ for beryllium-like ions recombining) this can give a substantial error.

The equilibrium metastable fractions may be calculated in a simplified manner including only spontaneous emission and collisional excitation and de-excitation processes in a 'low level' population balance (cf. ADAS205) without severe error

The data sets of type ADF10 contain tabulations for several members of an iso-electronic sequence each in a two-dimensional array at a fixed 'standard' set of reduced electron temperatures and reduced electron densities. That is the tabulations are at the same z -scaled (reduced) temperatures $\theta = T_e / z_1^2$ and densities $\rho = N_e / z_1^7$ where $z_1 - 1 (= z)$ is the charge of the (recombined or ionising) ion.

The coefficient data in expressions 5.3.3 above are therefore all at the same real *and* z-scaled temperatures and densities. In the combining process, they do not need to be interpolated. However, the equilibrium metastable fractional population data for the recombining ion are at the real temperatures $T'_e = [(z+2)/(z+1)]^2 T_{e1}^2$ and densities $N'_e = [(z+2)/(z+1)]^7 N_e$ and must be interpolated. This is achieved by cubic spline interpolation in the order $z'_1 (= z_1 + 1)$, ρ, θ . For data of class MET, the spline end conditions are set to zero curvature.

For a selected element (nuclear charge), the code ADAS404 identifies the iso-electronic sequence to which each of the ions of the element corresponds. For each data class in turn, it cycles through the ions of the element, accessing the appropriate isoelectronic master file. It interpolates the iso-electronic master file data using cubic splines to provide results for that class of collisional-radiative coefficient for the correct charge state (for each metastable sub-class in the partial case), at a two-dimensional array of arbitrarily chosen electron temperatures and electron densities within the range of the datasets.

The three-way spline interpolation is a matter of importance and data organisation is designed to assist in this. The primary calculations of collisional-radiative data by ADAS2 population processing codes are carried out for a series of ions of an iso-electronic sequence at a grid of electron temperatures and electron densities. Advantage is taken of the regularity of coefficients along the sequence as well as in temperature and density to provide reasonably compact isoelectronic master files according to the data set format specification *adf10*. Particularly, the approximate z-scaling properties of collisional-radiative coefficients are taken into account. Firstly it is noted that comparison of data for different charge states should be done at equal z-scaled (reduced) temperatures $\theta = T_e / z_1^2$ and densities $\rho = N_e / z_1^7$ where $z_1 - 1$ is the charge of the (recombined or ionising) ion. Then a constant *s* may be identified such that $z_1^s R_{CR}(\theta, \rho, z_1)$ is a slowly varying function of z_1 (R_{CR} denotes any collisional-radiative coefficient). A standard set of reduced electron temperatures and densities is used for the calculation of collisional radiative data for the different members of an iso-electronic sequence present in an iso-electronic master file. The choice of a set of z_1 's to include in the file for satisfactory interpolability is also important. It is necessary for the set to be dense at low z_1 , particularly $z_1 = 1, 2, 3$ should be present. A typical set might then include $z_1 = 5, 7, 9, 14, 20, 30$. It is also helpful to supplement the data set with important ions such the carbon, oxygen, silicon, iron and nickel members as appropriate. For interpolation of data with an exponential threshold in temperature such as collisional-radiative excitation and ionisation, it is necessary to cancel the dominant temperature dependence by multiplying the coefficient values by a factor of the form $\exp((I / z_1^2) / k\theta)$, where *I* is an appropriate energy, prior to interpolation. The iso-electronic master files used in this work contain a set of such excitation or ionisation energies for every charge state of the iso-electronic sequence (extrapolated for $z_1 > 50$) when necessary. This is so for SCD, PLT, PLS and some QCD data sets.

| Iopt | Nopt | $\frac{dy}{dx} _1$ | $\frac{d^2y}{dx^2} _1$ | $\frac{dy}{dx} _n$ | $\frac{d^2y}{dx^2} _n$ | Extrapol. |
|------|------|--------------------|------------------------|--------------------|------------------------|-----------|
| < 0 | 0 | . | 0.0 | . | 0.0 | no |
| 0 | 0 | . | 0.0 | . | 0.0 | yes |
| 1 | 1 | . | 0.0 | -1.5 | . | yes |
| 2 | 2 | 0.0 | . | 1.0 | . | yes |
| 3 | 3 | -0.5 | . | -1.5 | . | yes |
| 4 | 4 | 0.0 | . | . | 0.0 | yes |

Subject to these provisions, data is interpolated by cubic splines in the order, z_1, ρ, θ . The span of ρ and θ values in the data set is designed to minimise the need for extrapolation. However the end conditions at the first and last spline knots are set to give continuity onto the asymptotic behaviours where known. For each class of

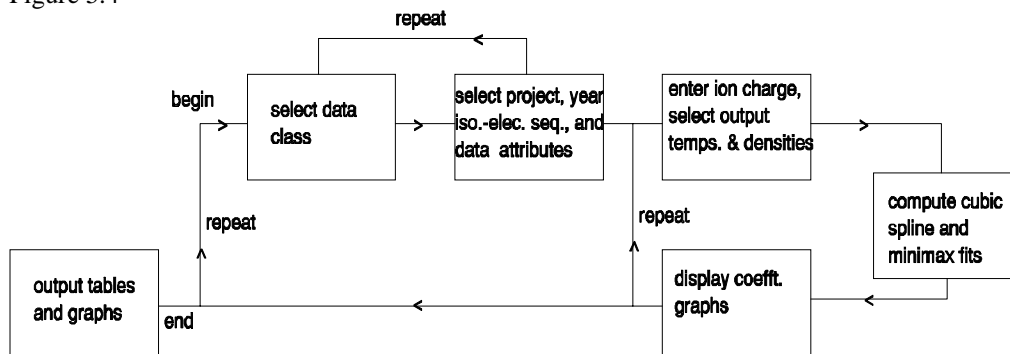
data the spline end conditions are individually set for asymptotic matching. The choices are as shown above. Iopt and Nopt are the controlling switches for extrapolation and end conditions permission respectively in the spline routines.

ADAS404 can accept a large grid of electron temperatures and electron densities at which the iso-nuclear collisional radiative coefficient data are produced. It is intended that subsequent application codes which make use of the iso-nuclear master files should need to give minimal attention to interpolation in temperature and density. Simple linear interpolation should be adequate and extrapolation not required. It is for these reasons that the ADAS404 code is elaborate in its spline interpolation and the specification of iso-electronic master files rigid.

Program steps:

These are summarised in figure 5.4.

Figure 5.4

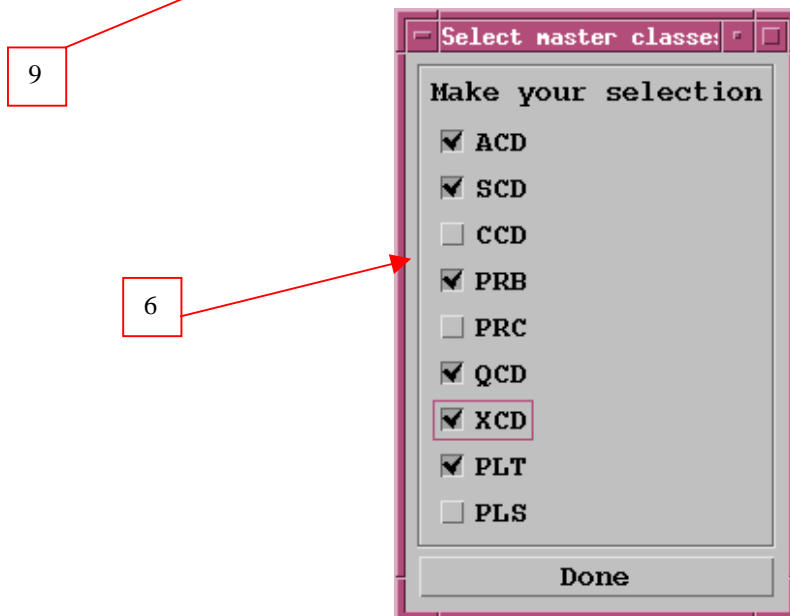
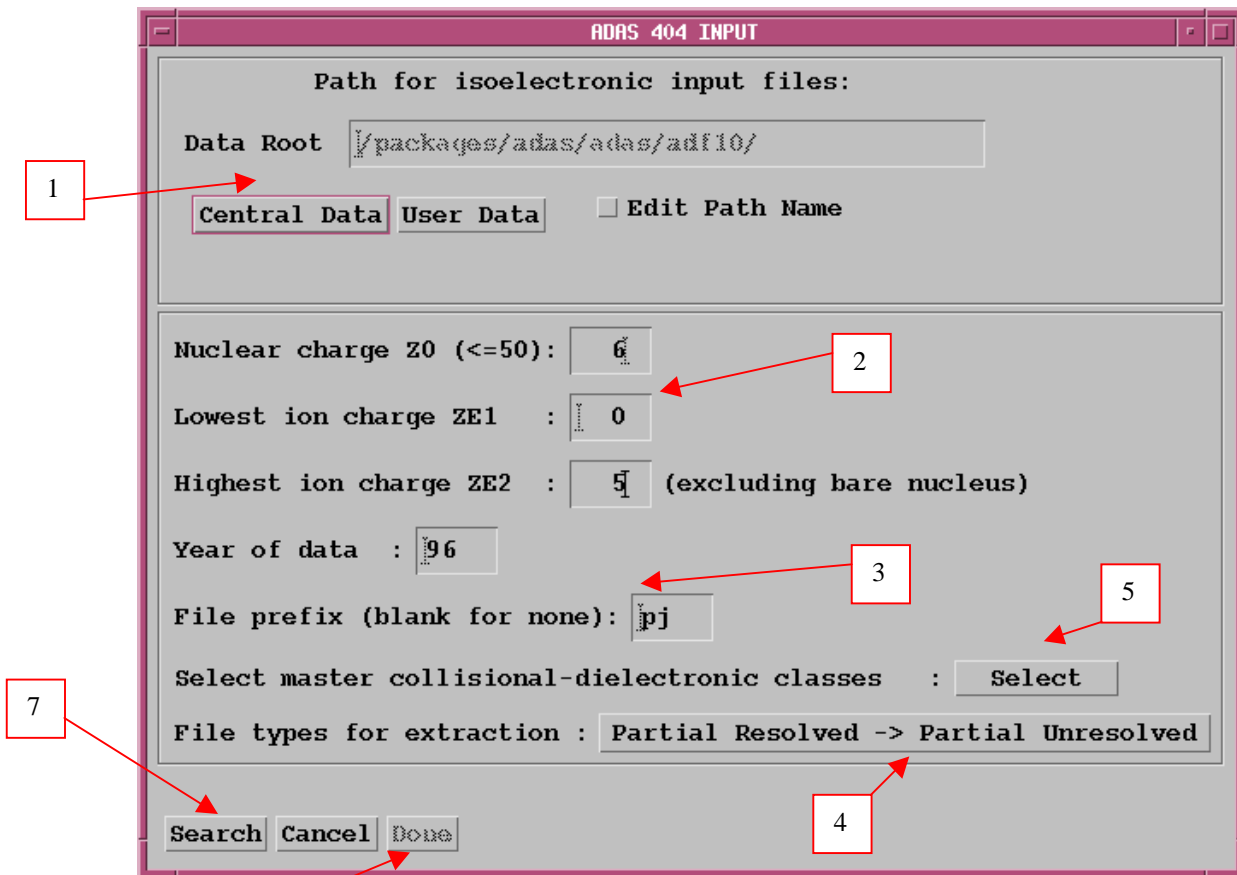


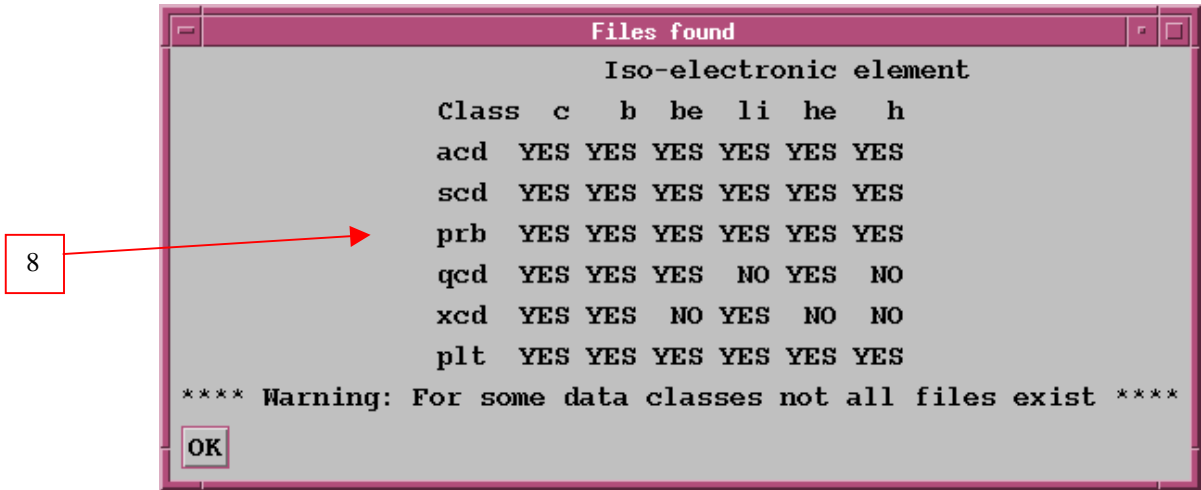
Interactive parameter comments:

Move to the directory in which you wish the standard ADAS created files to appear. For ADAS404 this is only the output text file produced after executing any ADAS program (*paper.txt* is the default). Initiate ADAS404 from the program selection menus in the usual manner.

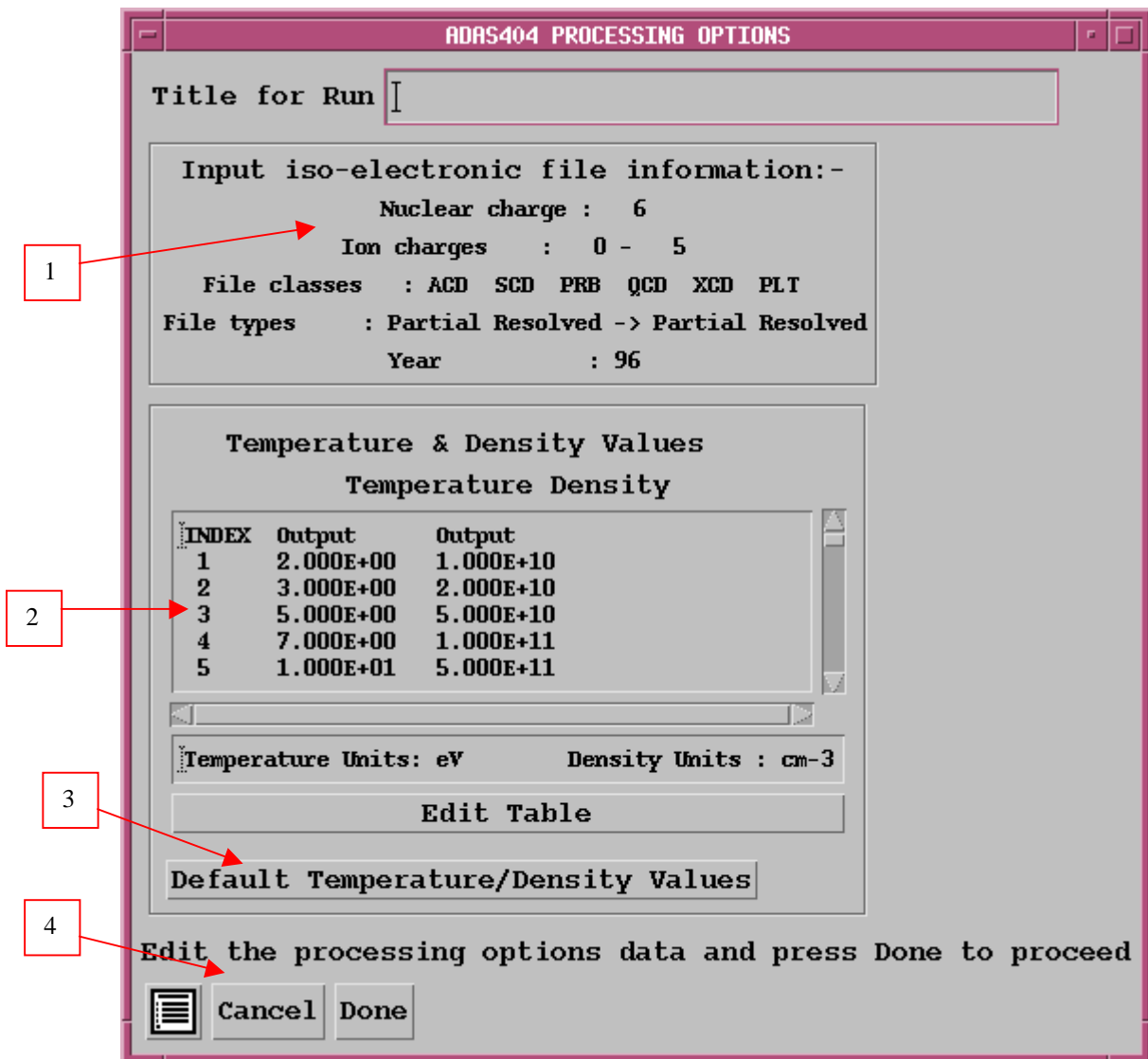
The **file selection window** appears first as illustrated below.

1. ADAS404 may access many datasets during its operation. Buttons are present to set the data root to that of the *Central data* or to your personal *User data* (provided it is in ADAS organisation. Alternatively the 'data root' may be edit explicitly.
2. Identify the iso-nuclear sequence by its *Nuclear charge* and the range of (contiguous) ions of the sequence to be included by *Lowest ion charge* and *Highest ion charge*.
3. Identify the primary *adf10* dataset source by specifying *Year of data* and *File prefix*.
4. Specify the mapping required by selecting appropriately from the drop-down menu at *File types for extraction*.
5. *Select* the iso-nuclear master collisional-dielectronic classes to be produced. A pop-up selection widget appears.
6. Click on the boxes for the classes desired. The boxes darken when selected. Then click *Done*.
7. Click on the Search button at the bottom left corner to check availability of the *adf10* datasets necessary for your requested *adf11* outputs.
8. A pop-up information widget shows the availability. Click OK
9. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous Series 4 menu.



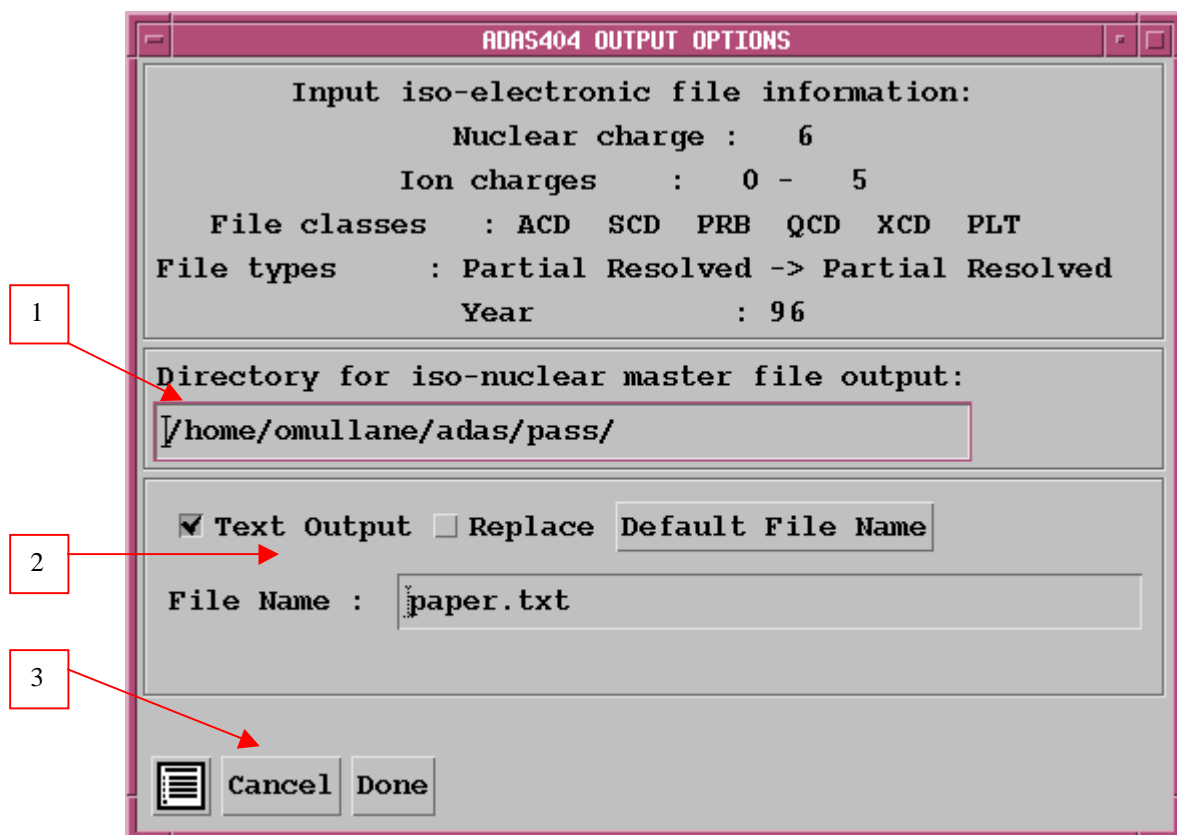


The processing options window has the appearance shown below



1. A summary of the selected element and data classes to be processed is given.
2. The selection of temperatures and densities pairs for output are made at b). The table may be edited by clicking on the *Edit Table* button.. The ADAS Table Editor window is then presented with usual set of editing operations available.
3. A default set of temperatures and densities suited to fusion applications is available. Click the *Default Temperature/Density Values* button to insert these in the table.
4. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window. The *Escape to Menu* icon is also available for a quick exit at the bottom left hand corner.

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



1. Specify the directory where you wish the iso-nuclear master files output by the program to be placed.
2. A text output file summarising the processing may be produced. Make the required selections.
3. Clicking the *Done* button causes the calculation to commence. Remember that *Cancel* takes you back to the previous window. The *Escape to Menu* icon is also available for a quick exit without execution.

Illustration:

Notes: