

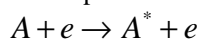
# Introduction

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 three components of the package are an interactive system, a library of key subroutines, and a very large database of fundamental and derived atomic data. The interactive part provides immediate display of important fundamental and derived quantities used in analysis together with a substantial capability for preparation of derived data. It also allows exploration of parameter dependencies and diagnostic prediction 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. The database spans most types of data required for fusion and astrophysical application

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## General principles

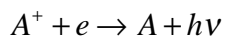
The broad mechanism for radiation emission from a hot tenuous plasma is simple. Thermal kinetic energy of electrons in the plasma is transferred by collisions to the internal energy of impurity ions:



where  $A^*$  denotes an excited state and  $A$  the ground state of the impurity ion. This energy is then radiated as spectrum line photons which escape from the plasma volume



Similarly ions increase or decrease their charge state by collisions with electrons



where  $A^+$  denotes the next ionisation stage of impurity ion  $A$ . In this case the escaping photon is a continuum one. The picture is often loosely referred to as the 'coronal model'. A detailed quantitative description is complicated because of the need to evaluate individually the many controlling collisional and radiative processes, a task which is compounded by the variety of atoms and ions which participate. The coronal model has been the basis for the description of impurities in fusion plasmas for many years. However, the progress towards ignition and to higher density plasmas, the use of neutral heating and diagnostic beams and the importance of divertors for impurity control suggest that a description beyond the coronal approximation is now appropriate. The Atomic Data and Analysis Structure is centred on generalised collisional radiative theory. The theory is outlined in the following sub-sections, in which it is shown that consideration of relaxation time-scales, metastable states, secondary collisions etc. - aspects rigorously specified in collisional-radiative theory - allow an atomic description suitable for modelling the newer areas above (McWhirter & Summers, 1984).

## Time constants

The lifetimes of the various states of atoms, ions and electrons in a plasma to radiative or collisional processes vary enormously. Of particular concern for spectroscopic studies are those of translational states of free electrons, atoms and ions and internal excited states (including states of ionisation) of atoms and ions. These lifetimes determine the relaxation times of the various populations, the rank order of which, together with their values relative to observation times and plasma development times determines the modelling approach. The key lifetimes divide into two groups, namely, the intrinsic atomic group comprising metastable radiative decay,  $\tau_m$ , ordinary excited state radiative decay  $\tau_o$  and auto-ionising state decay  $\tau_a$ , and the extrinsic collisional group comprising free electron thermalisation  $\tau_{e-e}$ , positive ion thermalisation  $\tau_{i-i}$ , ion-electron equilibration  $\tau_{i-e}$  and ionisation  $\tau_{ion}$ . Evidently, the first group are purely atomic parameters while the latter depend on plasma conditions. The intrinsic group are ordered as

$$\tau_a \ll \tau_o \ll \tau_m \quad 1.1$$

Typical values for them are given by

$$\begin{aligned} \tau_m &\sim 10^1 / z^8 \quad s \\ \tau_o &\sim 10^{-8} / z^4 \quad s \end{aligned} \quad 1.2$$

The extrinsic group are ordered as

$$\tau_{ion} \gg \tau_{i-e} \gg \tau_{i-i} \gg \tau_{e-e} \quad 1.3$$

in general. The expressions for these time constants are as follows

$$\begin{aligned} \tau_{ion} &\sim [10^7] (z+1)^2 (I_H / kT_e)^{1/2} \exp(\chi / kT_e) (cm^{-3} / N_e) \quad s \\ \tau_{i-i} &\sim [7.0 \times 10^7] (m_i / m_p)^{1/2} (kT_i / I_H)^{3/2} (1 / z^4) (cm^{-3} / N_i) \quad s \\ \tau_{i-e} &\sim [1.4 \times 10^9] (m_i / m_p) ((kT_e / I_H) + 5.4 \times 10^{-4} (kT_i / I_H) (m_p / m_i))^{3/2} \\ &\quad (1 / z^2) (cm^{-3} / N_i) \quad s \\ \tau_{e-e} &= [1.6 \times 10^6] (kT_e / I_H)^{3/2} (cm^{-3} / N_e) \quad s \end{aligned} \quad 1.4$$

where the ions are of charge  $z$ . The ion mass is  $m_i$ , the proton mass  $m_p$ , the ionisation potential  $\chi$ , the ion density  $N_i$ , the electron density  $N_e$ , the ion temperature  $T_i$  and the electron temperature  $T_e$ . The intrinsic and extrinsic groups are to be compared with each other and with times for plasma ion diffusion across temperature or density scale lengths,  $\tau_{dif}$ , the relaxation times of transient plasma phenomena under study,  $\tau_{phen}$  and instrumental observation sampling times  $\tau_{obs}$ . For fusion plasmas, usually

$$\tau_{dif} \sim \tau_{ion} \sim \tau_m \gg \tau_o \gg \tau_{e-e} \quad 1.5$$

## Basic assumptions

From these time-scales, it may be assumed in most circumstances that the free electrons have a Maxwellian distribution and that the dominant populations of impurities in the plasma are those of the ground and metastable states of the various ions. The dominant populations evolve on time-scales of the order of plasma diffusion time-scales and so should be modelled dynamically, that is in the particle number continuity equations, along with the momentum and energy equations of plasma transport theory. The excited populations of impurities on the other hand may be assumed relaxed with respect to the instantaneous dominant populations, that is they are in a *quasi-equilibrium*. The quasi-equilibrium is determined by local conditions of electron temperature and electron density. So, the atomic modelling may be partially de-coupled from the impurity transport problem into local calculations which provide quasi-equilibrium excited ion populations and emissivities and then effective source coefficients (collisional-radiative coefficients) for dominant populations which must be entered into the transport equations. The solution of the transport equations establishes the spatial and temporal behaviour of the dominant populations which may then be re-associated with the local emissivity calculations for matching to and analysis of observations.

## Generalised collisional-radiative theory

The basic model was established by Bates et al. (1962). The ion in a plasma is viewed as composed of a complete set of levels indexed by  $i$  and  $j$  and a set of radiative and collisional couplings between them denoted by  $C_{ij}$  (an element of the 'collisional-radiative matrix' representing transition from  $j$  to  $i$ ) to which are added direct ionisations from each level of the ion to the next ionisation stage (coefficient  $q_i^{(i)}$ ) and direct recombinations to each level of the ion from the next ionisation stage (coefficient  $r_i$ ). There is no loss of

generality in the present discussion in ignoring other ionisation stages provided couplings to and from them are only via ground states. For each level, there is a total loss rate coefficient for its population denoted by

$$-C_{ii} = \sum_{j \neq i} C_{ji} + N_e q_i^{(i)} \quad 1.6$$

The population of any level is determined by the balance of processes populating and depopulating it. Suppose the dominant populations are a recombined ion ground state ( $i = 1$ ) and a recombining ion ground state denoted by  $+$ . These states alone are assumed significantly populated. Excited level populations (that is  $N_i$  for  $i > 1$ ) are small in comparison. Then the quasi-equilibrium statistical balance is

$$\begin{aligned} \frac{d}{dt} N_1 &= \sum_{j \neq 1} C_{1j} N_j + C_{11} N_1 + N_e N_+ r_1 \\ 0 &= \sum_{j \neq 1} C_{ij} N_j + C_{i1} N_1 + N_e N_+ r_i \quad , \quad i = 2, \dots \end{aligned} \quad 1.7$$

In matrix form these become

$$\begin{bmatrix} \frac{d}{dt} N_1 \\ 0 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{1j} \\ C_{i1} & C_{ij} \end{bmatrix} \begin{bmatrix} N_1 \\ N_j \end{bmatrix} + N_e N_+ \begin{bmatrix} r_1 \\ r_i \end{bmatrix} \quad 1.8$$

The populations of the excited levels in quasi-equilibrium,  $N_j^{eq}$  are given by

$$N_j^{eq} = -N_e N_+ \sum_{i \neq 1} C_{ji}^{-1} r_i - \sum_{i \neq 1} C_{ji}^{-1} C_{i1} N_1 \quad 1.9$$

Substitution of equations 1.9 in equation 1.7 for  $N_j$ , allows identification of a collisional-dielectronic ionisation coefficient

$$S_{CD} = C_{11} - \sum_{j \neq 1} \sum_{i \neq 1} C_{1j} C_{ji}^{-1} C_{i1} \quad 1.10$$

and collisional-dielectronic recombination coefficient

$$\alpha_{CD} = r_1 - \sum_{j \neq 1} \sum_{i \neq 1} C_{1j} C_{ji}^{-1} r_i \quad 1.11$$

Physically, the collisional-dielectronic coefficients give the contributions to the effective growth rates for the ground state population due to recombination from and ionisation to the state  $+$ , so that the time dependent equation for  $N_1$  becomes

$$\frac{d}{dt} N_1 = -N_e S_{CD} N_1 + N_e \alpha_{CD} N_+ \quad 1.12$$

The ionisation balance of Summers (1973) adopted this approach with the excited state populations combined into principal quantum shell populations (the 'bundle-n' method) and used 'matrix condensation' (Burgess and Summers, 1969) to allow very large numbers of principal quantum shells to be included in the calculations. The deficiencies mentioned in the introduction are apparent. Populated metastable states can exist and there is no real distinction between them and ground states. We use the term 'metastables' to denote both ground and metastable states and index them by  $\rho$  for the recombined ion, and by  $\nu$  for the recombining ion. Therefore the ion of charge state  $z$  has metastable populations  $N_\rho^{(z)}$  and the recombining ion population,  $N^+$ , must be subdivided into the set  $N_\nu^{(z+1)}$ . We sometimes call the recombining ion metastable states 'parent' states.

## Resolution, condensation and expansion

There is a practical problem. Evidently, discussion of metastables requires a detailed specific classification of the level structure of ions (for example  $LS$  or  $LSJ$  resolution) whereas to cope with the very many principal quantum shells participating in the calculations of collisional-dielectronic coefficients at finite density necessitates a grosser viewpoint (such as 'bundle-n'). Furthermore, addressing radiated power, each ion tends to have a limited set of low levels principally responsible for the dominant spectrum line power emission for which the 'bundle-n' approach is too imprecise, that is, averaged energies, oscillator strengths and collision strengths do not provide a good representation. Note also that key parent transitions for dielectronic recombination span a few low levels for which precise atomic data are necessary. In the recombined ion, parentage gives approximate quantum numbers, that is, levels of the same  $n$  divide into those based on different parents. Lifetimes of levels of the same  $n$  but different parents can vary strongly (for example through secondary autoionisation). Also the recombination population of such levels is generally from the parent with which they are classified. We therefore recognise three sets of non-exclusive levels of the recombined ion

- (i) Metastable levels - indexed by  $\rho$ ,  $\sigma$ .

- (ii) Low levels - indexed by  $i, j$  in a resolved coupling scheme, being the complete set of levels of a principal quantum shell range  $n: n_0 \leq n \leq n_1$ , including relevant metastables and spanning transitions contributing substantially to radiative power or of interest for specific observations.
- (iii) Bundle- $n$  levels - segregated according to the parent metastable upon which they are built and possibly also by spin system.

Viewed as a recombining ion, the set (i) must include relevant parents and set (ii) must span transitions which are dielectronic parent transitions. Time dependence matters only for the populations of (i), high precision matters only for groups (i) and (ii) and special very many level handling techniques matter only for group (iii). To satisfy the various requirements and to allow linking of population sets at different resolutions, a series of manipulations on the collisional-radiative matrices are performed (see for example equations 1.6 to 1.12) (Summers and Hooper, 1983). To illustrate this, suppose there is a single parent metastable state. Consider the collisional-radiative matrix for the recombined ion and the right hand side (see equation 1.8) in the bundle- $n$  picture, and a partition of the populations as  $[n, \bar{n}]$  with  $n: n_0 \leq n \leq n_1$  and  $\bar{n}: n_1 < \bar{n}$ . Elimination of the  $N_{\bar{n}}$  yields a set of equations for the  $N_n$ . We call this a 'condensation' of the whole set of populations onto the  $n$  populations. The coefficients are the effective ionisation coefficients from the  $n$ , the effective cross-coupling coefficients between the  $n$  and the effective recombination coefficients into the  $n$ , which now include direct parts and indirect parts through the levels  $n$ . Exclusion of the direct terms prior to the manipulations yields only the the indirect parts. Call these  $C_{mn}^{indir}$  and  $r_n^{indir}$ . We make the assumption that  $C_{mn}^{indir}$  and  $r_n^{indir}$  may be *expanded* over the resolved low level set using statistical weight factors alone, since the collisional mixing of substate populations with  $n > n_1$  is generally large. The expanded indirect matrix  $C_{ij}^{indir}$  and  $r_i^{indir}$  where  $i$  and  $j$  span the resolved low level set (ii) are then combined with higher precision direct couplings  $C_{ij}^{dir}$  and  $r_i^{dir}$  so that

$$C_{ij} = C_{ij}^{indir} + C_{ij}^{dir} \quad 1.13$$

and

$$r_i = r_i^{indir} + r_i^{dir} \quad 1.14$$

If there is more than one recombining ion metastable state (indexed by  $\nu$ ) then the procedure must be performed for each parent and possibly spin system separately to assemble the final  $C_{ij}$ .  $r_i$  is replaced by its generalisation  $r_\nu$  and equations (1.9) are replaced by

$$N_j^{eq} = -N_e \sum_{i \neq \rho'} \sum_{\nu} C_{ji}^{-1} r_{i\nu} N_\nu^+ - \sum_{i \neq \rho'} \sum_{\rho} C_{ji}^{-1} C_{i\rho} N_\rho \quad 1.15$$

The process may be continued (without the statistical expansion) condensing the low level set onto the metastable set. The generalised collisional-dielectronic coefficients are the result. The time dependent and/or spatial non-equilibrium transport equations which describe the evolution of the ground and metastable populations of ions in a plasma use these generalised coefficients. Following solution, the condensations can be reversed to recover the complete set of excited populations and hence any required spectral emission. The progressive condensation described above can be viewed as simply one of a number of possible paths which might be preferred because of special physical conditions or observations, such as  
 high bundle- $n$  ---> intermediate bundle- $n_1$  ---> low LS resolved ---> metastable states  
 high bundle- $n$  ---> low Stark resolved states ---> ground state  
 Four types of bundling and condensation are distinguished in this work.

- (a) Ground parent, spin summed bundle- $n$  ---> lowest  $n$ -shell
- (b) Parent and spin separated bundle- $n$  ---> lowest spin system  $n$ -shell
- (c) Parent and spin separated bundle- $n$  ---> low LS resolved ---> metastable states
- (d) Low LS resolved ---> metastable states

Type (a) corresponds to the approach used in Summers (1973). Type (d) corresponds to the usual population calculation for low levels in which normally recombination and ionisation are ignored. It establishes the dependence of each population on excitation for the various metastables only, together with equilibrium metastable fractional populations and metastable cross-coupling effective rate coefficients. Types (b) and (d) are the principal procedures to be exploited in this work for large scale computation and type (c) for special specific studies. These elaborations are developed more fully in the theoretical background description given with each ADAS code in later sections.

## Features and superfeatures

To make effective use of an atomic modelling system of the present kind, it is helpful to consider the relationship of calculated spectral features to observed features. The starting point is the emission associated with a particular impurity excited level. It is called a *feature primitive*. It is the set of transition energies

and transition probabilities originating from the level. These purely atomic quantities determine positions and relative emissivities of spectrum lines driven by the level population. The level and its population may be a bundled one. All the component lines associated with the bundle constitute the feature primitive in this case, statistical weights alone determining their relative emissivities. No knowledge of the excited state population structure is required to prepare feature primitives.

A local quasi-equilibrium population calculation establishes the dependence of the populations of excited levels on each metastable state. In turn this allows combination of feature primitives to form a *feature*. A feature is the set of line positions and local emissivities associated with a metastable and is determined by a local population calculation.

A *superfeature* is a set of line of sight integrals of spectral emission. It is obtained by combining features with the line of sight distribution of metastable populations derived from an impurity transport calculation. A superfeature includes line broadening and distortions due to the dynamics of the plasma along the line of sight. It is at the superfeature level that the confrontation of experiment and theory takes place. The series 1, series 2 and series 4 codes of the Atomic Data and Analysis Structure may be viewed as providing the tools for

*feature primitive* → *feature* → *superfeature*

spectral synthesis. Series 6 provides spectral analysis by employing synthetic features.

## Zeeman and Stark manifolds

It is most common in spectroscopic studies of fusion plasmas to consider isolated atom or ion spectral emissions, that is j-resolved line components or LS multiplets. The relatively strong magnetic fields in these plasmas does cause Zeeman splitting of spectral lines of low ionisation stages of ions near or in the plasma boundary. There is no explicit calculation of separate m-subshell populations of thermal ions in the present issue of ADAS. Thus population alignment is not addressable. In most circumstances, however, m-substates are equally populated and no alignment is evident. The Zeeman manifold then forms a feature primitive in the nomenclature of the previous subsection and is within the scope of ADAS.

The situation of neutral atoms in beams is a special one in fusion plasmas. Neutral beams are used as heating beams as well as dedicated diagnostic beams for the central plasma and scrape-off-layer. The only species used at the present time are isotopes of neutral hydrogen, helium and lithium. Atoms in the fast penetrating heating beams experience large motional Stark electric fields in their frame of  $\sim 100\text{kV/cm}$ . For neutral hydrogen this resolves the level degeneracy and the full Stark multiplets are observed. A Stark basis of states is necessary for population structure analysis of beam atoms. This is adopted in the beam modelling codes of ADAS series 3. It is to be noted that the principles of condensation, expansion and superfeature construction apply equally to this situation and is within the scope of the Atomic Data and Analysis Structure.

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## 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 further 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 code series

ADAS as a whole is organised into the seven code series shown below. In technical terms their 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 most of the rest of ADAS. ADAS1 does not provide *ab initio* calculations of fundamental reaction cross-sections. Rather ADAS1 allows preparation and assessment of such data from other sources for inclusion in the ADAS database. Unit conversions, data display, comparison with, and adjustment of, simple expected functional forms for the data, Maxwell averaging, control of asymptotic behaviour and interpolation onto user preferred or ADAS standard temperature ranges are the main objectives. Types of fundamental data addressed include electron impact excitation cross-sections (ADAS101), electron impact excitation rate coefficients (ADAS102), dielectronic recombination (ADAS103), radiative recombination (ADAS104), electron impact ionisation cross-sections

(ADAS105), electron impact ionisation rate coefficients (ADAS106) and charge exchange recombination (ADAS107).

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 (called a specific ion file of type *adf04*) 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. The specific ion reaction data collections can be interrogated and displayed (ADAS201). Approximate excitation cross-section data for a specific ion may be prepared from an interpolable data collection for the iso-electronic sequence (ADAS203). A similar procedure can be performed for recombination and ionisation (ADAS202). This routine also prepares the input for a bundle-nS generalised collisional dielectronic recombination and ionisation coefficient calculation (ADAS204). The primary excited state population calculation (ADAS205) provides extensive tabulations and graphs of the populations of a specific ion in a thermal plasma and prepares a passing data set for use by a diagnostic display routine (ADAS207). This routine allows spectral line intensity ratio and similar diagnostic displays. A variant of the population code (ADAS206) specifically provides total and specific line radiated power. An advanced version of the population code (ADAS208) is available for the most complete studies - principally production of generalised collisional-radiative coefficients and spectrum line emissivities. Several codes have been provided to manipulate specific ion files. Thus ADAS209 and ADAS210 allow the resolution level to be altered (eg. from LSJ to LS or *vice versa*) by bundling and un-bundling. ADAS215 changes the temperatures at which the specific ion file is tabulated. ADAS211, ADAS212 and ADAS213 add extra data lines for state selective dielectronic recombination, radiative recombination and electron impact ionisation respectively to the specific ion file. ADAS216 conducts a detailed sensitivity analysis of predicted excited state populations and emissivities to uncertainties of the fundamental data in the specific ion file. ADAS214 allows the examination of optical thickness of model plasmas and modifies specific ion files with associated escape factors.

ADAS3 is concerned with those situations in a plasma when charge transfer from neutral hydrogen (or its isotopes) or neutral helium in beams is a primary mechanism. There are five interrogation routines, displaying fundamental state selective charge transfer cross-section data (ADAS301), general ion/atom excitation, ionisation and charge transfer cross-section data (ADAS302), derived effective emission coefficients for charge exchange spectroscopy (ADAS303), effective beam stopping and beam emission coefficients (ADAS304). Analysis of charge exchange driven emission of hydrogen-like impurities in plasma, emission measure deduction and effective emission coefficient calculation are available in four routines designed for detailed display (ADAS308, ADAS306) and preparation of tabular scans over parameters (ADAS309, ADAS307) at two levels of refinement. Two further routines (ADAS310 and ADAS311) perform a similar role but for the calculation of beam emission and beam stopping respectively with hydrogen and helium beams. ADAS310 is a comprehensive bundle-n population model which provides complete tables of analysed populations as well as collisional-radiative coefficients. ADAS311 is an equivalent code but uses the more complex bundle-nl population model. ADAS312 and ADAS313 interrogate these tabulations for hydrogen and helium respectively to provide compact data sets of arbitrary beam stopping and emission coefficients for experiment analysis. ADAS314 performs beam/thermal, thermal/thermal and thermal/bundle-n averaging of the bundle-n and bundle-nl charge exchange cross-section tabulations. This improves the use of such data for charge exchange spectroscopy in fusion divertor (non-beam) environments.

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 iso-electronic sequence storage of data which is the preferred choice for atomic data preparation and manipulation to an iso-nuclear sequence storage preferred for applied studies in dynamical plasma models (ADAS404). The iso-electronic sequence data may be interrogated and displayed (ADAS401) as can the iso-nuclear data (ADAS402). Iso-electronic data exists in both generalised collisional dielectronic form and the simpler stage to stage form (see section 1.4). Merging of the generalised form to the stage to stage form may be carried out (ADAS404). Further programs allow computation of an equilibrium ionisation balance (ADAS405) or a time dependent model (ADAS406) by drawing on the iso-nuclear data. Historically in fusion, ionisation, recombination and radiated power have been obtained in large fusion codes by using simple approximate forms. Parameters of preferred approximate forms are also stored in the database and can be used to generate a baseline of modest quality iso-nuclear data (ADAS408). A capability for optimising parameters using best available numerical data is provided (ADAS407). An additional purpose of ADAS405 and ADAS406 is to provide emission functions for selected spectrum lines, that is taking into account the ionisation balance. The additional codes ADAS409 and ADAS412 execute a similar task but providing standard tabulations of  $G(T_e, N_e)$  and  $G(T_e)$  respectively. The latter is produced according to the solar astrophysical definition. ADAS410, ADAS411 and ADAS413 are interrogation codes on fundamental recombination and ionisation data collections.

ADAS5 provides a set of programs for interrogating data collections in the fundamental and derived database. The data classes addressed are those which have been found of particular importance for reduction of calibrated observed data and include 'ionisations per photon' (ADAS501), photon emissivity coefficients (ADAS502), zero density ionisation coefficients (ADAS503), zero density radiated power coefficients (ADAS504), thermal charge exchange rate coefficients (ADAS505),  $G(T_e)$  functions (ADAS506), generalised contribution functions (ADAS507),  $G(T_e, N_e)$  functions (ADAS508) and state selective charge exchange cross-sections for partially stripped species (ADAS509). ADAS506 also prepares a *collection file* for differential emission measure analysis (see ADAS series 6). ADAS509 additionally generates thermally averaged charge exchange rate coefficients.

ADAS6 series is concerned with analysis of spectral data. ADAS601 is a full implementation of the method of differential emission measure analysis. This technique is used extensively for determining the variation of temperature with density (and so height) in the solar upper atmosphere. ADAS602 is a Gaussian spectral line fitting program. It uses the maximum likelihood method and provides full statistical analysis of errors. The code is particularly tuned to the flow of data from solar observatory spacecraft. ADAS603 and ADAS604 are extensions of ADAS602 designed for dedicated fitting of particular types of spectral feature. These are respectively Zeeman multiplet features and dielectronic satellite line features. Both codes handle overlapping lines not associated with the special feature and provide feature analysis in terms of plasma parameters. ADAS605 will have a similar function for diatomic molecular band special features.

ADAS7 series is dedicated to the fundamental calculation of dielectronic recombination, ionisation and excitation/auto-ionisation data including their organisation for applications. ADAS701 is the primary code and is an implementation of the AUTOSTRUCTURE program (Badnell, 1993). ADAS702, ADAS703 and ADAS704 post-process the output from ADAS701 to produce three types of ADAS data (adf09, adf04, adf18) required in evaluating collisional-dielectronic recombination coefficients, analysing dielectronic satellite lines and population modelling. In practice, the adf04 file created by ADAS704 must be adjusted and completed by including best data for low-level transitions and by including higher level contributions. This is achieved by a merging and bundling code (ADAS705). The series also includes a population modelling code (ADAS706) and spectral line ratio prediction code (ADAS707) which are similar to series 2 codes but extended to treat the doubly excited populations and associated emissions occurring because of dielectronic recombination.

ADAS8 series is concerned with the *ab initio* calculation of atomic structure and associated collision data for arbitrary systems and their compilation into adf04 files for use by the ADAS machinery. Such calculations often must be carried out as very large, off-line computations. The ADAS interactive codes assist in setting up the drivers for these latter computations. ADAS801 is an implementation of the atomic structure program of Cowan, which is used in ADAS to provide *baseline* data. ADAS804 is used to calculate single transition cross-sections in an effective potential Born approximation. ADAS805, using a similar effective potential approach, is concerned with continuum emission and Gaunt factor calculation - both free-free and free-bound - in support of Bremsstrahlung measurements. ADAS806, ADAS807 and ADAS811 provide merging, cleaning and checking of adf04 files, setup of cross-referencing to assist in the assembly of adf04 files and finally comparison of adf04 files. Programs ADAS808, ADAS810 and ADAS802 are targeted on very heavy species. They allow the set up, regulation and preview of configurations for large scale structure, excitation, feature emissivity and ionisation cross-section calculations based on spectroscopic observational focus. These interactive ADAS programs provide complete sets of drivers ready for export of the substantive calculations to integrated background codes running on parallel machines.

<i>Series</i>	<i>Content</i>
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	General interrogation programs
ADAS6	Data analysis and spectral fitting programs
ADAS7	Creating and using dielectronic data
ADAS8	Structure and excitation calculations

ADAS atomic modelling codes generally create data sets as well as normal tabular output. These files are structured according to the requirement of the ADAS data base or for further ADAS programs. It is anticipated that the user will edit these files into standard ADAS naming convention files when establishing a personal database after being satisfied of their correctness. The ability to route text and graphical output after execution is a feature of ADAS.

## ADAS data formats

There are 45 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 A of this manual. These formats apply both to fundamental and derived data. They are as follow:

<i>adf01</i>	bundle-n and bundle-nl charge exchange cross-sections
<i>adf02</i>	ion impact cross-sections with named participant
<i>adf03</i>	recombination, ionisation and power parameter sets
<i>adf04</i>	resolved specific ion data collections
<i>adf05</i>	general z excitation data collections
<i>adf06</i>	general z recombination/ionisation data collections
<i>adf07</i>	direct resolved electron impact ionisation coefficients
<i>adf08</i>	direct resolved radiative recombination coefficients
<i>adf09</i>	direct resolved dielectronic recombination coefficients
<i>adf10</i>	iso-electronic master files
<i>adf11</i>	iso-nuclear master files
<i>adf12</i>	charge exchange effective emission coefficients
<i>adf13</i>	ionisation per photon coefficients
<i>adf14</i>	thermal charge exchange coefficients
<i>adf15</i>	photon emissivity coefficients
<i>adf16</i>	generalised contribution functions
<i>adf17</i>	condensed projection coefficients
<i>adf18</i>	cross-referencing data
<i>adf19</i>	zero-density radiative power data
<i>adf20</i>	G(Te) functions
<i>adf21</i>	effective beam stopping coefficients
<i>adf22</i>	effective beam emission coefficients
<i>adf23</i>	state selective electron impact ionisation coefficients
<i>adf24</i>	state selective charge transfer cross-sections
<i>adf25</i>	driver data-sets for ADAS204 calculation
<i>adf26</i>	bundle-n populations of excited states in beams
<i>adf27</i>	driver data-sets for ADAS701 calculations
<i>adf28</i>	driver data-sets for ADAS702 post-processing
<i>adf29</i>	driver data sets for ADAS707 calculation
<i>adf30</i>	driver data-sets for ADAS708 post-processing
<i>adf31</i>	feature files for satellite line spectral simulation
<i>adf32</i>	driver data-sets for ADAS802 calculations
<i>adf33</i>	driver data-sets for ADAS803 postprocessing
<i>adf34</i>	driver data-sets for ADAS801 calculations
<i>adf35</i>	spectral filter data
<i>adf36</i>	feature files for series limit spectral simulation
<i>adf37</i>	non-Maxwellian distribution function files
<i>adf38</i>	Seaton - opacity photo-excitation
<i>adf39</i>	Seaton - opacity - photo-ionisation
<i>adf40</i>	envelope feature photon emissivity coefficients
<i>adf41</i>	driver data-sets for offline ADAS8#1 calculations
<i>adf42</i>	driver data-sets for ADAS810 calculations
<i>adf43</i>	GTN photon emissivity functions
<i>adf44</i>	F_GTN envelope feature emissivity functions
<i>adf45</i>	feature files for continuum emission

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## 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 start-up

It is necessary to set up a number of sub-directories so that ADAS can work equally well on your personal data as well as on central ADAS data. Directories are also required for preserving a memory of your last use of an ADAS code and for holding ADAS created output.

```
cd ../<user identifier>
```

Change to your home directory

../ denotes the root path to user directories.

```
ls
```

Check file and directories present

If the directory /adas is not present create it.

```
mkdir adas
```

Make you personal adas database top directory

```
cd adas
```

Move into the directory adas

```
mkdir defaults
```

Make a defaults directory if it does not exist

```
mkdir pass
```

Make a passing file directory if it does not exist

```
mkdir scripts405
```

Make a script file directory for ADAS405 if it does not exist

```
mkdir arch101
```

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 sub-directory

Central ADAS data has the directory path ../adas/adas on most workstations. You can look at central ADAS datasets.

```
cd ../adas/adas/adf04/belike
```

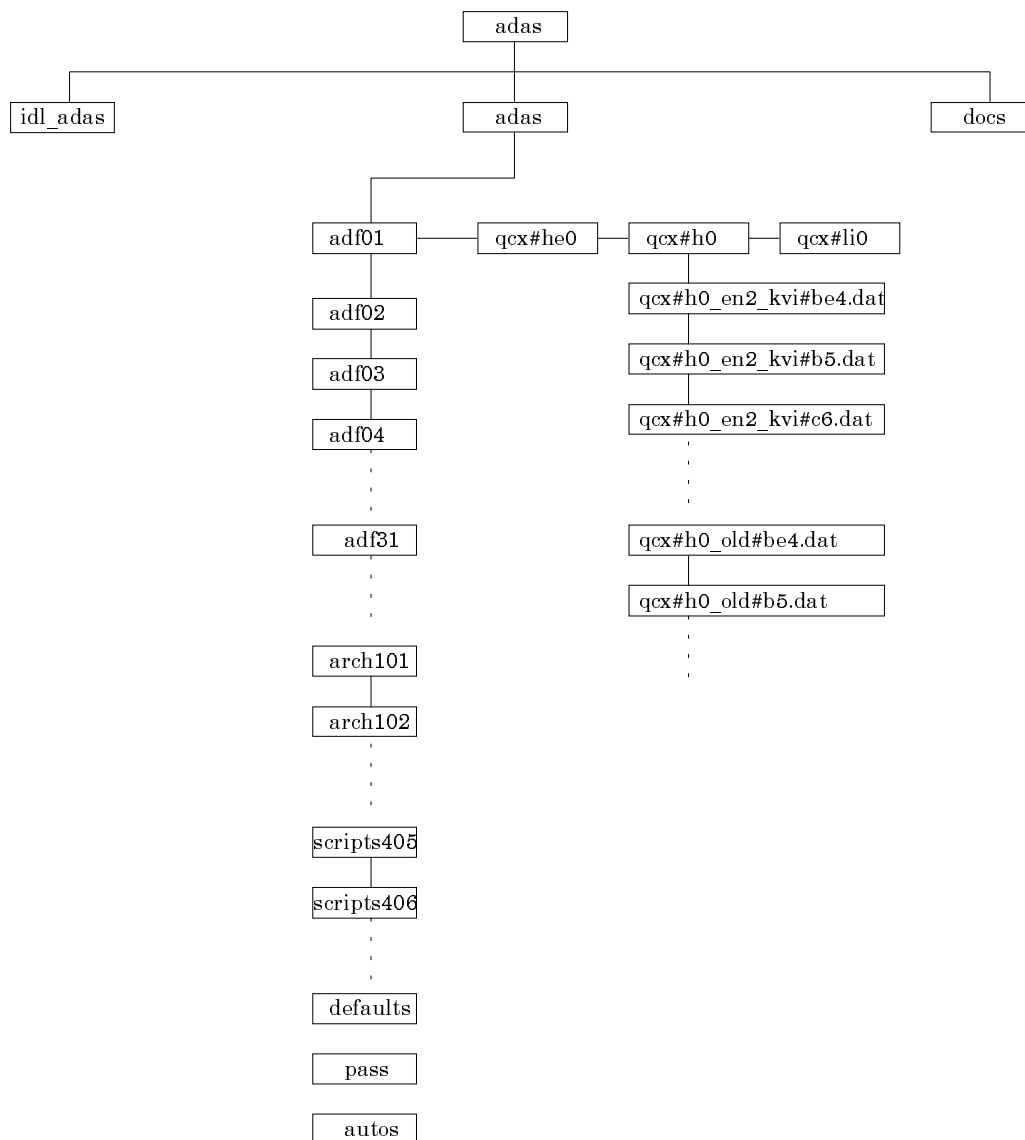
move to a Be-like specific ion file sub-directory

```
ls
```

list data files available

```
cat belike_jl1990o.dat
```

list a particular file for O<sup>+</sup> prepared by J. Lang



The figure above shows the full database directory structure in central ADAS. For central ADAS, sub-directories, *arch101*, ..., *scripts405*, ... contain only samples. Such data is normally personal to a user.

Copy the *NULL* and *test\_c* samples for your laboratory site from the central ADAS *scripts405* sub-directory

```

cd ~/adas/scripts405
cp ../../adas/adas/scripts405/NULL .
cp ../../adas/adas/scripts405/<site>_test_c .

```

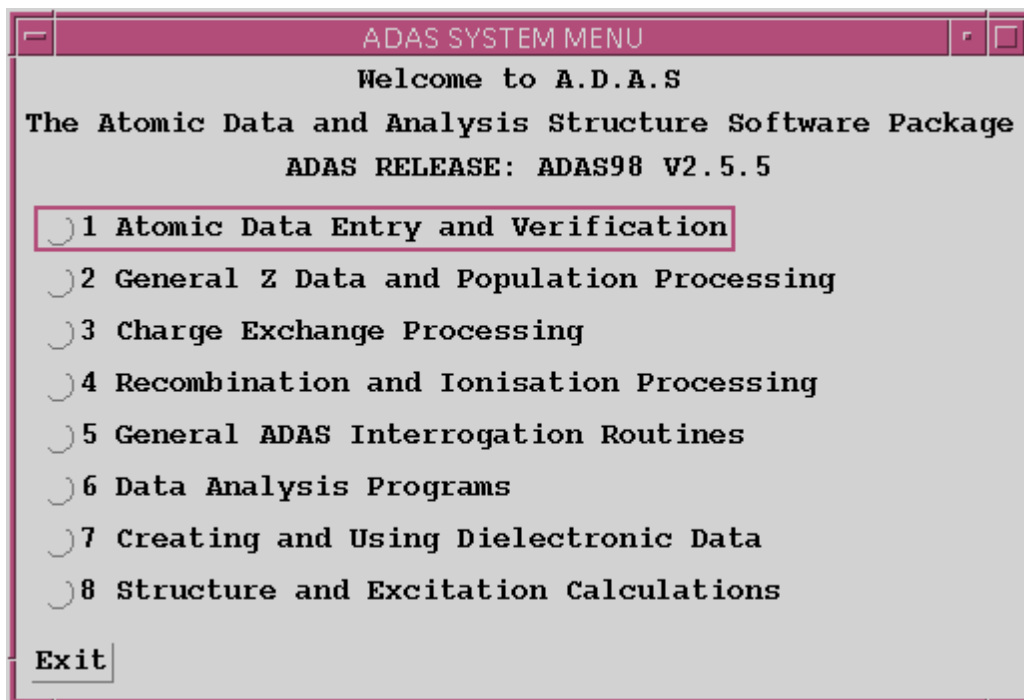
You are now ready to initiate ADAS. This can be done from any sub-directory position, but it is usual to move first to your *pass* directory. ADAS places its standard text and graphic output files, usually called *paper.txt* and *graph.ps* into the directory from which you launch ADAS.

```

cd ../../<user identifier>/adas/pass          return to your pass
directory
adas                                          start ADAS

```

The top level ADAS selection menu should be displayed as below



Select a series using the left mouse button. In the series sub-menu similarly select a particular ADAS program. The program will immediately execute showing firstly the *input options* widget. Details of using particular codes are given in the following chapters of this manual.

---

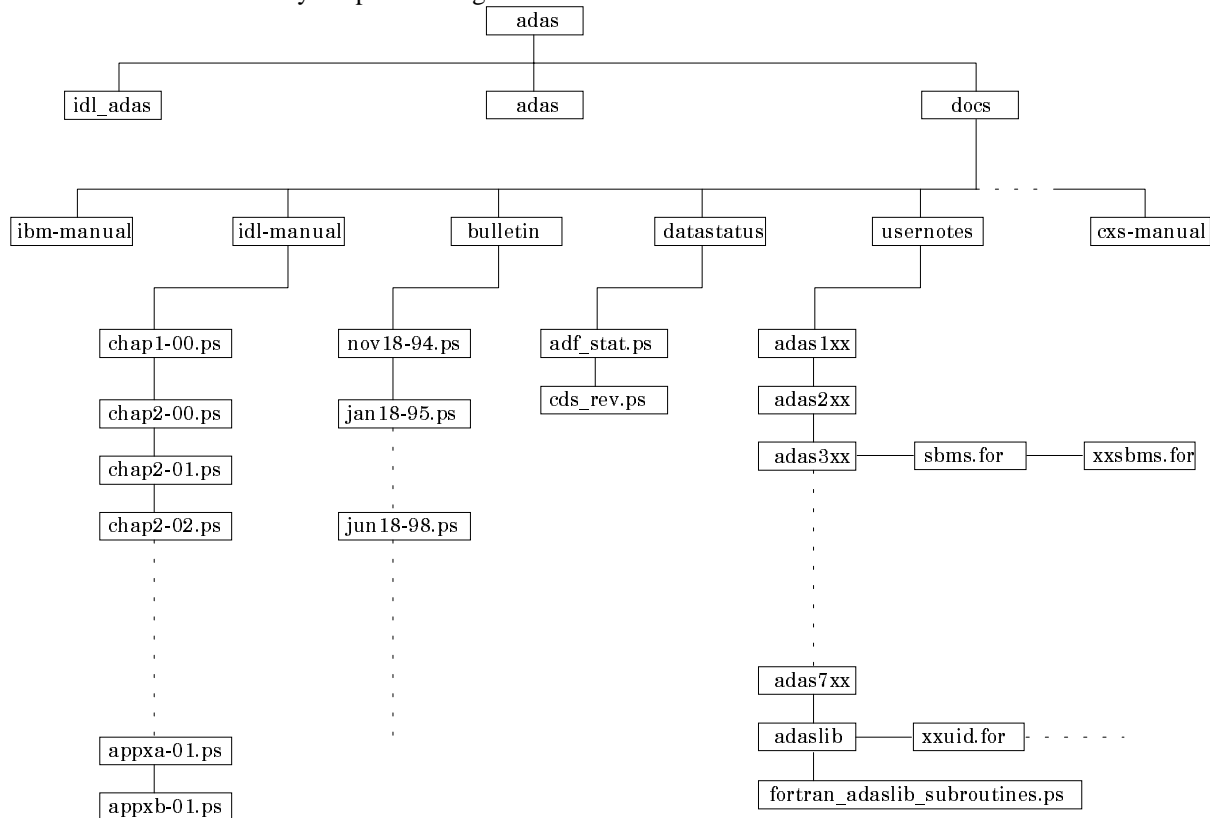
## ADAS documentation

Documentation is placed in the `../adas/docs` directory under several headings. A schematic is shown below.

1. *Bulletins*: files named as `../adas/docs/bulletin/<date>.ps` where `<date>` is of the form `<month><day>-<year>` [eg. **jun18-98**].
2. *Usernotes*: files named as `../adas/docs/usernote/chap<i>-<nn>.ps` where `<i>` denotes chapter number from the ADAS Usernotes Manual and `<nn>` denotes the sub-chapter. The document has been split into these sub-chapters for easy of interrogation. `<i-1>` is the associated library name [eg. **adastlib**, **adast<i>xx**, etc.]. There are separate Fortran and IDL sections. These provide the necessary descriptive header and parameters of each routine so that it can be used in personal applications.
3. *Manual*: files named as `../adas/docs/idl_manual/chap<i>-<nn>.ps` where `<i>` denotes chapter and `<nn>` denotes the sub-chapter number, gives the full ADAS Unix-Idl User Manual. The document has been split into these sub-chapters for ease of interrogation. The ADAS code ADAS<i><jk> description is to be found in chap `<i+1>-<jk>.ps`.
4. *Special manuals*: There are a number of shorter special manuals which describe particular types of activity within ADAS, such as charge exchange spectroscopy or influx spectroscopy. The files are named as `../adas/docs/<name>-manual/chap<i>.ps`. These include:
  - *flx-manual*                      influx spectroscopy
  - *bms-manual*                      beam emission spectroscopy
  - *cxs-manual*                      charge exchange spectroscopy
  - *ion1-manual*                     basic ionisation balance studies
  - *ion2-manual*                     advanced ionisation balance studies
  - *opac-manual*                    opacity studies
  - *spec-manual*                    spectral analysis
  - *cds-manual*                     atomic modelling for solar analysis
4. *Datastatus*: file named as `../adas/docs/datastatus/adf<nn>.ps` where `<nn>` is an ADAS data format number. These give the specification of each *adf* number together with a summary of the data of this type available in the database at the

file date stamp. There may be additional files such as data reviews conducted by ADAS participants.

5. *Tutorial notes:* files named as `../../adas/docs/<lab><yr>-tut/<section>.ps` where `<lab>` is a mnemonic for a laboratory and `<yr>` is a two digit year number. These are tutorial presentations originating from taught courses given at particular laboratories. They are divided into sections in which a sub-area is summarised with viewgraphs followed by simple learning exercises with ADAS.



All these files are 'postscript' files.

To look at the files, activate Ghostview in a terminal window outside ADAS:

```
ghostview &
Button select media A4
Double click on directory names to move to required sub-directory
Click on required file to select it
Button select OK
```

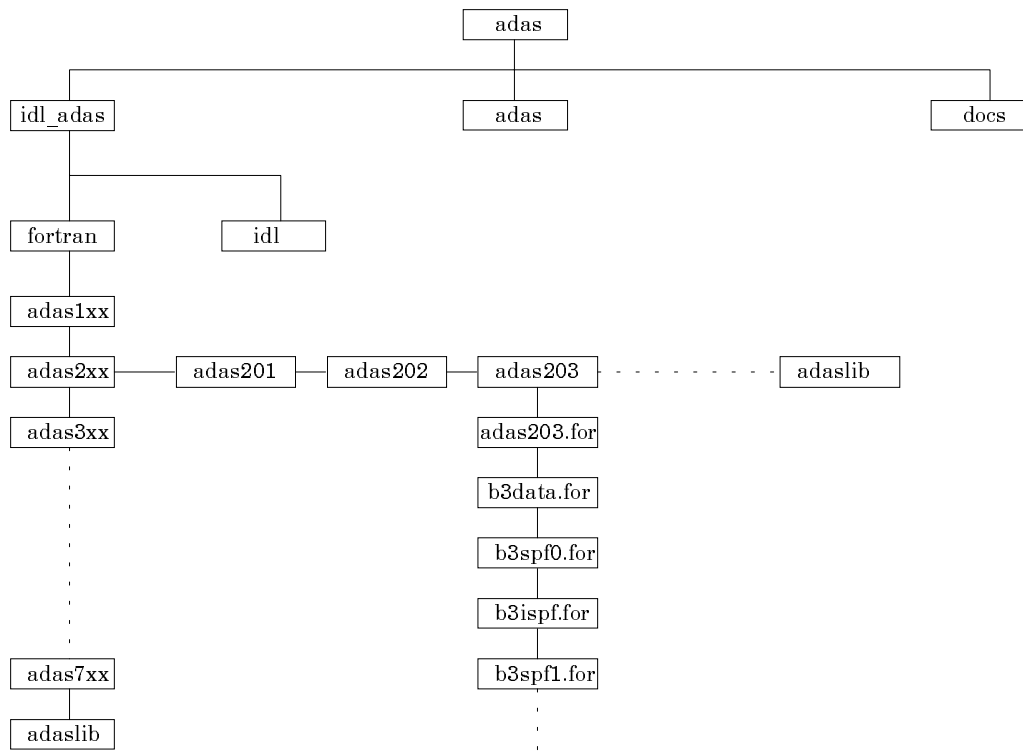
To terminate Ghostview

```
Button select FILE at top left of window
Button select EXIT on drop down menu.
```

## The ADAS library

### *Non-interactive library routines*

An objective of ADAS is to provide a capability for embedding fundamental and derived atomic data from the database into a user's own measurement reduction and analysis codes. The complete ADAS object module fortran library is available but not the source code. The organisation of the programs is as shown below. Some extra subroutines are provided to draw data of the important ADAS types directly into applications with little overhead. Access is obtained by searching an ADAS load module library. These independent extraction routines open appropriate files and are consistent with the related interactive interrogation programs. In most cases, they form primitive kernels at the heart of the interactive programs. Besides the extraction subroutines, there are additional subroutines providing equilibrium populations, equilibrium ionisation balance and so on. They are described in appendix B.




---

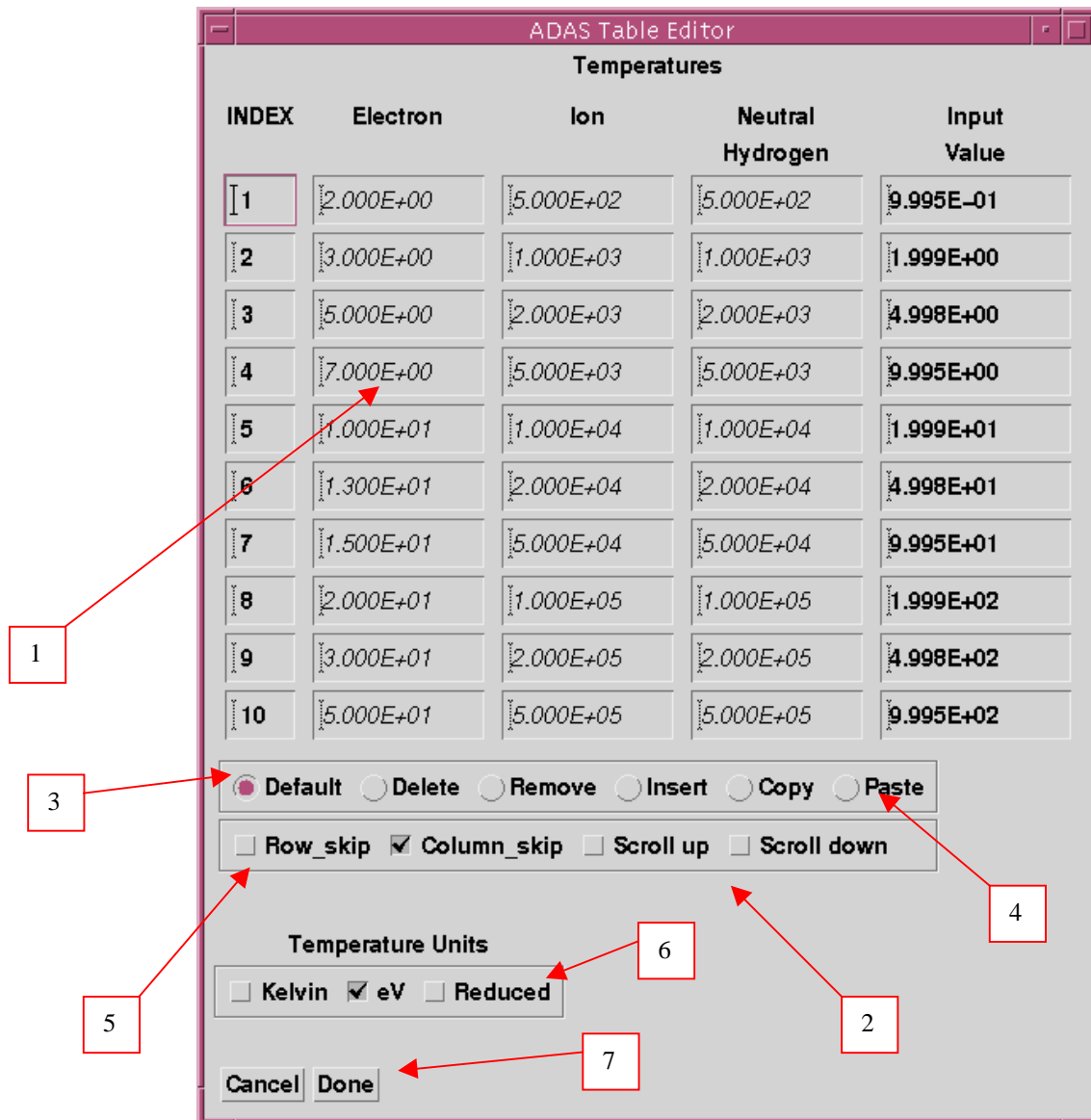
## Supplementary windows

### Table Editor

A necessary operation in interactive ADAS is entry of user values into a table. Since this is common to many ADAS programs, a special window has been developed to assist in this task. A typical appearance of the **Table Editor** window is shown below

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. This is the normal editing mode.
2. The set of round 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.
3. The *Default* round button is the reset to normal editing mode. 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. These buttons stay active until you click *Default*.
4. The *Copy* and *Paste* round buttons operate for the next immediate action only.
5. Square buttons have a continuing effect until an alternative is pressed. 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 than this.
6. 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 not** change any Output values already typed in. It merely interprets Output values in the selected units.

- 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.

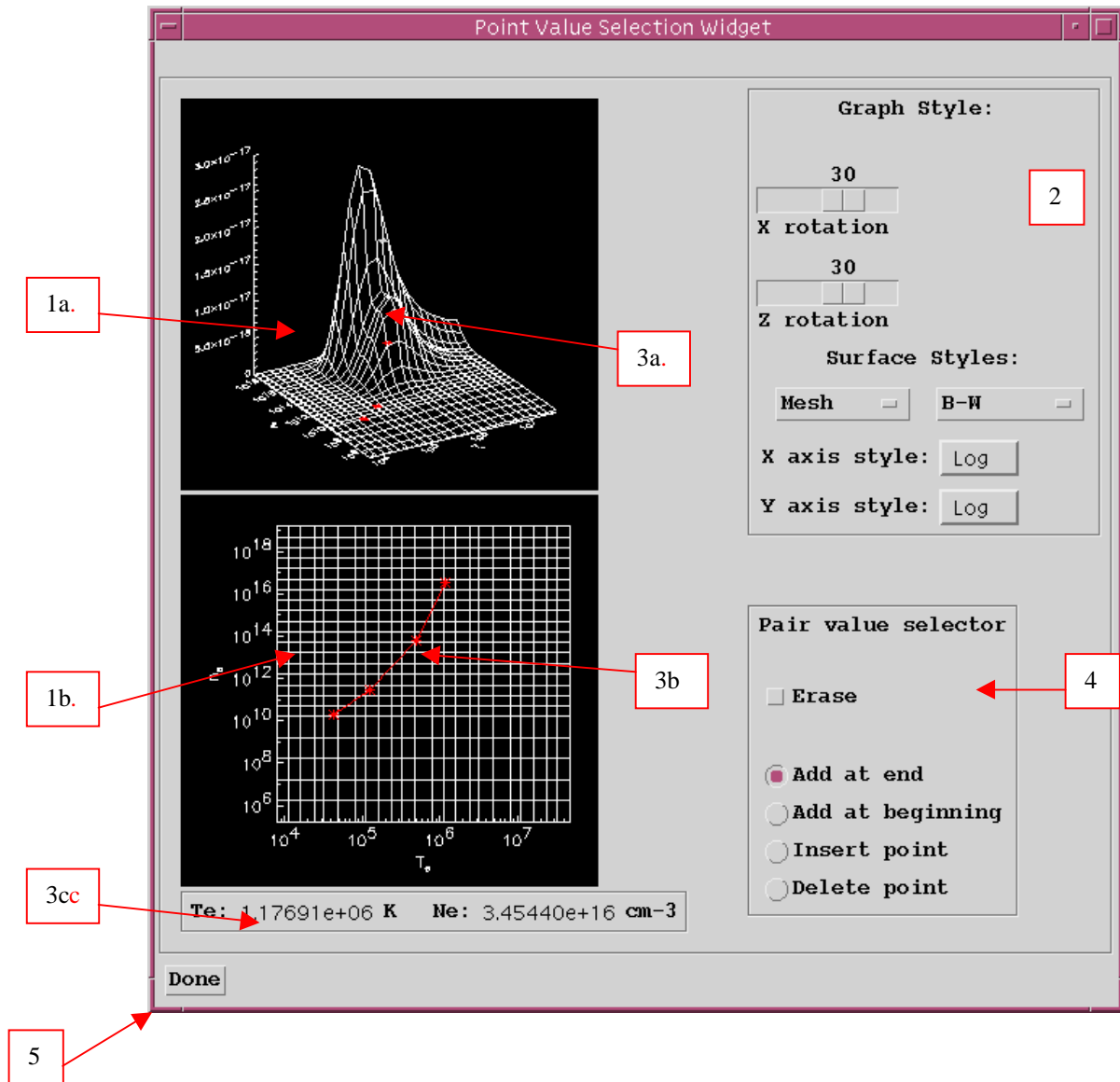


## Graphical pair selection window

The **point value selection** window is designed for model pair selection from 2-D data such as PECs. The window provides a sophisticated method for selecting pairs, for example Te/Ne pairs, by mouse click, which allows the user to track over interesting parts of the surface. The appearance shown below

- The surface is shown at 1a). At 1b), the two dimensional Te/Ne plane is displayed. Note that the grid lines are those of the actual data in the source file.
- Controls are provided to orientate and alter the appearance of the display. Sliders allow rotation about the X-axis and about the Y-axis so that the whole surface can be examined. The surface styles can be altered by selecting from drop-down menus. The styles include continuous or mesh surfaces and the colour of the surface. Finally the form of the axes, that is logarithmic or linear can be chosen from drop-down menus.
- Move the mouse cursor over the lower Te/Ne grid. A tracking pointer moves over the surface in the upper display as at 3a). Click the left mouse button to select a Te/Ne pair. A symbol marks the selection on the Te/Ne grid in the

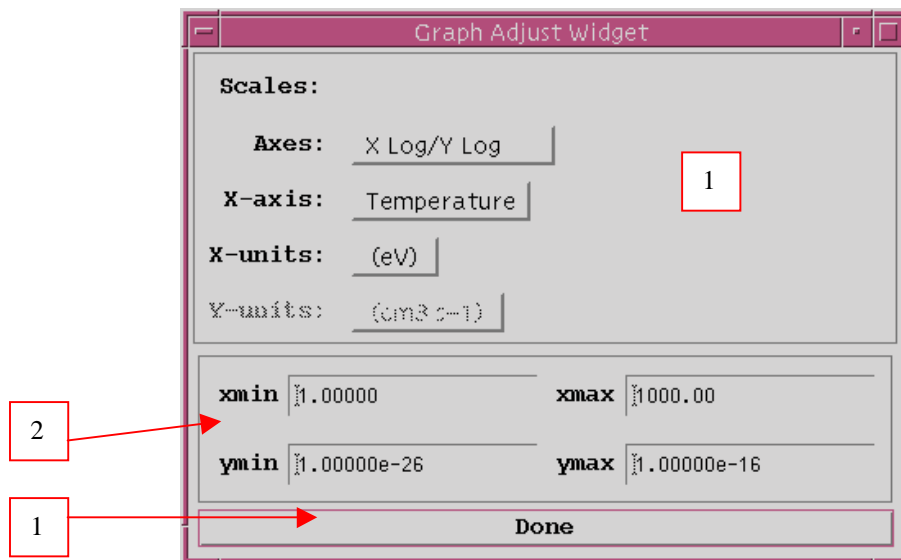
- lower display as at 3b) and a marker also appears on the surface in the upper display. Continue to select point pairs as required. Note that the position of the cursor in Te/Ne space is shown numerically at 3c) for precise positioning
- Control buttons allow adjustments to your selection set. Pairs can be added at the beginning or end of the set or inserted between pairs. Also a pair can be deleted. Finally the whole set of pairs can be erased.
  - Click *Done* on completion to return to the processing options window. The pairs selected will be present in the editable table. Note that conventional entry or modification of user data with Table Editor remains an option as before.
  - Note that when *Value Selection by display* is activated, the *Fit Polynomial* button is de-activated. It is clearly easy in pair selection over a surface to produce pair orderings, which are inappropriate for fitting a polynomial.



## Graph Adjust window

The **graph adjust** window has the appearance shown below

- Full control is provided to alter the axes styles, the independent variable and the units for the independent variable. These choices are provided by drop-down menus.
- Manual entry of minima and maxima for the axis scales is supported.
- Click *Done* to return to the graphical window.



## Multiplot window

The *Retain* button on selected graph windows allows the graph to be displayed with other retained graphs. A new window appears, called the **multiplot window**, which has the appearance shown below

1. The retained curves appear in the list. The current curve is placed at the end of the list and up to seven curves are allowed.
2. The editable box in the *Key* column of each row is a numerical selector for the line style used for that curve. This is followed by a brief descriptor for the curve which will also appear on the whole graph when printed. The button in the *Dis* column is activated to display that retained curve and the *Del* button is used to delete a curve from the retained list.
3. Note that the *Adjust* button is again present. At this point, only the axis maxima and minima are allowed to be modified.
4. Click *Done* to return to the ordinary graphical window or *Print* to print the multiplot graph.





## Graph Editor window

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 window has been developed to assist in this task. A summary of how to use **Graph Editor** is given here. A typical appearance (in fact from ADAS108) is shown below.

1. Input values are displayed as diamonds as at 1a). The points can be modified by using the buttons beneath the graph in association with the mouse. In the table editor for ADAS108, a least squares spline fit is made to these tabular points. The spline passes through nine special knot points, which are distinguished in the Graph Editor as crosses. The knots have fixed x-co-ordinates displayed as grid lines.
2. To **move a point**, click the *Move 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 forced by the editor. Each point has a small active zone around it for picking by the mouse. **Terminate** point moving operations by pressing the *right* mouse button.
3. An extra button is present *Move Knot* to allow the knot points to be moved vertically.
4. To delete a point, click the *Delete Pt.* button. Then click the *left* mouse button with the pointer over the point to be deleted. Terminate point deletion operations by pressing the *right* mouse button.
5. To add a new point in the x-ordered position between two existing points, click the *Add X-Pt.* button. Then click the *left* 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.
6. For completeness, the capability for adding a point anywhere is given although physically unreasonable. The operation is slightly different. Click the *Add Any Pt.* 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.
7. To insert a point by value use the special sub-window.
8. Buttons 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. Further actions depend on the particular ADAS program which launched Graph Editor. Thus for ADAS108 with the ADAS analysis option, if any points are modified, the program cycles back for reanalysis. With the Burgess analysis option, movement of the spline knots alone does not force re-analysis.
9. The graph editor for ADAS108 also includes two sliders to adjust the parameters 'B' and 'C' which affect the plot.

