Creating and manipulating adf04 files

The chapter is concerned with the ab initio preparation of the basic atomic data required for the modelling the populations of ions in plasmas. The data collections called specific ion files, of format ADF04, are the starting point for population calculations in ADAS. It has been assumed up until now that a basis of such data sets is available from off-line calculations or from hand preparation from the open literature. The basis ADF04 datasets must include, at minimum, energy levels, A-values and electron impact excitation rate coefficient data between levels. Thereafter the earlier series in ADAS, especially series 2, series 4 and series 7, have provided the capability to amplify the base ADF04 dataset with state selective recombination data and projected data from higher, bundle-n levels so that complete collisional-radiative modelling can be performed. In practice, from independent calculations based on the Cowan/O'Mullane atomic structure code, a very large basis set of ADF04 files, under the sub-library name *copmm* have been supplied in the ADAS database. The new series allows the direct calculation of the basis *copmm* data and provides in addition supplementary utilities which assist in manouvering, checking and linking these data.

The chapter is centred on the code ADAS801 (Cowan/O'Mullane) which is a large intermediate coupling atomic structure code extended to provide plane-wave Born electron impact collisional rate ceofficient data. The code was originally designed for background calculation and generates extensive tables of energy levels, radiative rates, cross-sections and rates between all levels of designated configurations a multi-electron, configuration-interaction model. The collison data generated are comprehensive but of relatively low precision. It must be substituted by better data from improved calculations or measurements. It is intended to provide - also as an interactive ADAS utility - a more sophisticated cross-section calculation of the distorted wave type. It will be called ADAS802 and it will be ncessary to provide with it a post-processor, ADAS803. The latter will complete 'top-up' and the conversion to rate coefficients. Other data arrives as hand-assessed ADF04 files, usually over restricted level sets. Merging of such ADF04 datasets for the same ion is necessary. In this step, quite large data movements occur and aberrant data is easily missed. A fairly sophisticated merging code, ADAS806 is provided which seeks to clean-up the final ADF04 dataset and warn if any oddities are detected. It has become apparent that the linking of recombination data into the ADF04 file and the conduct of the supporting high level (bundle-n) supporting calculations - which require cross-referencing files and driver datasets - are difficult for the occasional user. In series 8, ADAS807 is provided to prepare these extra items automatically.

Finally series 8 includes some simple calculations which a number of users have indicated would be useful. These include at this time an impact parameter electron impact excitation

cross-section generator and a Gaunt factor generator. The latter handles bound-bound, bound-free and free-free cases in hydrogenic and non-hydrogenic approximations. It is of special value for integrated and spectrally-resolved bremsstrahlung and free-bound continua.

Figure 9.0