Creating and using dielectronic data

The chapter is concerned with the preparation of dielectronic recombination data in the forms needed for analysing and modelling astrophysical and laboratory plasmas. Such needs are subject to re-definition and extension as time progresses. The capability which we seek to achieve here copes with the present front line of usage but anticipates what will be required in the medium future. Thus the treatment of very highly ionised, many electron systems in intermediate coupling is included, precision for low temperature dielectronic recombination is addressed and flexibility in the designation of metastables built in. Only modest extension will be required to address doubly excited state mixing and re-distribution under external fields and collisions.

The chapter is centred on the code ADAS701 (AUTOSTRUCTURE) which is a large atomic structure code extended to handle auto-ionising states. The code was designed for background calculation and generates extensive tables of energy levels, Auger rates and radiative rates between designated bound, resonant and free multi-electron atom configurations. The ADAS implementation is arranged to assist in the selection of the 'driver' data sets of type *adf27* which form the user input to the code. Also ADAS documentation provides detailed instructions on the preparation of such drivers. There are many output data sets from ADAS701. These were not designed or specifically organised for the present applications, nor are all required. ADAS701 assists in the sub-selection of these temporary output data sets according to present particular purposes and in the positioning of them for post-processing into the useful formats for archiving, modelling and analysis. The three main purposes are preparation of state selective dielectronic recombination coefficients for generalised collisional-radiative modelling of type *adf09*, preparation of specific ion files of type *adf04* including resonance capture and Auger rates for doubly excited population and satellite line modelling and finally creation of supplementary LS breakdown Auger rates for inclusion in the cross reference files of type *adf18/a04_p204* needed for bundle-nS population calculations of type ADAS204. ADAS702 performs the post-processing of temporary ADAS701 output files for the first purpose, ADAS703 for the second and ADAS704 for the third. A schematic is shown in figure 8.0 below.

None of the ADAS programs in this chapter generate graphical output and most are set up for execution as batch jobs. The calculations, especially of ADAS701, can be long and create substantial quantities of temporary output data. Also it is recommended that primary generation of dielectronic data for the ADAS data bases using these codes should be done in co-ordination with other members of the ADAS Project to avoid duplication and error. Such codes are a new development in ADAS in that they provide an *ab initio* fundamental atomic data calculation capability. Such calculations have up until now been carried out only in

background support of ADAS. In the future, it is planned to expand the *ab initio* aspect of ADAS further.

Figure 8.0