The tight-binding parameters for the Bethe Lattice are read from files which are stored in the subdirectory BLDAT. The file names are *BLnnn.dat* where *nnn* specifies the atomic number of the electrode's material, i.e. 028 for Ni, 013 for Al etc. So far only parameter files for H, C, Al, Ni, Co, Fe, Mn, Cu, Pt, Pd, Au, and Pb exist, but feel free to add the ones you need.

Each file may contain several sets of parameters specified by a given name (see examples below) which you pass to the keyword BLPAR1(2) in the input file *<job_name>.ini*. The notation used is the standard Slater-Koster notation and the default units are Hartrees. When Rydbergs are used instead, one should add the word RYD in the parameters set. Parameters sets can be obtained, for instance, from http://cst-www.nrl.navy.mil/bind.

The number of orbitals and order of the shells used for the atoms belonging to the crystalline region in the electrodes, at least for those to be connected to branches of the Bethe lattice (see GAUSSIAN03/09 input file), should match that of the parameters set chosen. Typically a minimal basis set *s p d* is used, although larger basis sets can also be used if a larger set of parameters is defined). No need to say that a good match between these parameters and the functional used in the calculation is desirable. When a set of parameters is non-orthogonal, i.e., it contains overlap parameters, some care must be exercised (see keyword *OVERLAP* in *<job_name>.ini* input file).