

General Guidelines to write Input Files for FAC calculations (by M. Gu)

Generally, the difference between different FAC calculations can be attributed to the choice of configurations and model potential used to determine the one electron radial wave functions. Below is a set of guidelines that one can generally follow for ions contain a few electrons (e.g., below Ne-like isoelectronic sequence). Following these guidelines one can eliminate a lot of variance observed in the FAC output.

- Include all configurations within the same n-complex, by that I mean all configurations within $n_1^*q_1 n_2^*q_2 n_3^*q_3$ should be included. Leaving something out would cause incomplete configuration interaction. Obviously for more complex ions, this may be impossible, as the number of atomic states within such a complex can be prohibitively large. In such cases, one must choose judiciously what to include and what to cut. And a good choice generally require a detailed understanding of the problem and know a priori to a certain degree what configurations interact strongly with the ones you are interested in.
- It is generally advised to use the ground configuration to derive the radial potential. This is the list of configurations included in the `fac.OptimizeRadial()` function. FAC constructs a fictitious average configuration by distributing fractional electron to the subshells included in this configuration list. Including highly excited configurations in this list can cause the electron screening to be too diffuse, and leads to inaccurate ground configuration energies. It's generally more important to get more accurate ground configuration energies than excited ones.
- The function call `fac.ConfigEnergy(0)` before the `fac.OptimizeRadial()` and `fac.ConfigEnergy(1)` after the `fac.OptimizeRadial()` are optional. Their purpose is to make some empirical energy corrections to the configurations not included in the `OptimizeRadial()` function. This can lead to some differences in the final level energies. My experience is these corrections improve the result for excited states overall, but this is not always guaranteed.
- When calling `fac.Structure()` to solve the level structure, the more configurations included in the call, the more configuration interaction is included, so generally leads to more accurate results. However, there is a limit how many configurations you can include in a single call, as the dimension of the Hamiltonian matrix can grow exponentially. I generally include all configurations within a single n-complex for excited configurations, and maybe put the ground n-complex and the next single excitation complex together. If one is particularly interested in getting a better result for certain energy levels, double excitation complexes can be included, as these represent some important pair correlations. In any case, these pair correlations are notoriously slow converging with respect to the principle quantum number of the excited electron, so a pure CI treatment may not be ideal anyway. A many-body perturbation theory treatment is more appropriate.