CHAPTER OVERVIEW

8: Electronic Configurations

One of the goals of quantum chemistry is to allow practicing chemists to use knowledge of the electronic states of fragments (atoms, radicals, ions, or molecules) to predict and understand the behavior (i.e., electronic energy levels, geometries, and reactivities) of larger molecules. In the preceding Section, orbital correlation diagrams were introduced to connect the orbitals of the fragments along a 'reaction path' leading to the orbitals of the products. In this Section, analogous connections are made among the fragment and product electronic states, again labeled by appropriate symmetries. To realize such connections, one must first write down N-electron wavefunctions that possess the appropriate symmetry; this task requires combining symmetries of the occupied orbitals to obtain the symmetries of the resulting states.