CHAPTER OVERVIEW

12: Group Theory - The Exploitation of Symmetry

Symmetry can help resolve many chemistry problems and usually the first step is to determine the symmetry. If we know how to determine the symmetry of small molecules, we can determine symmetry of other targets which we are interested in. Usually, it is not only the symmetry of molecule but also the symmetries of some local atoms, molecular orbitals, rotations and vibrations of bonds, etc. that are important. For example, if the symmetries of molecular orbital wave functions are known, we can find out information about the binding. Also, by the selection rules that are associated with symmetries, we can explain whether the transition is forbidden or not and also we can predict and interpret the bands we can observe in Infrared or Raman spectrum. The qualitative properties of molecular orbitals can be obtained using symmetry from group theory (whereas their precise energetics and ordering have to be determined by a quantum chemical method). Group Theory is a branch of the mathematical field of algebra. In quantum chemistry, group theory can applied to *ab initio* or semi-empirical calculations to significantly reduce the computational cost. Symmetry operations and symmetry elements are two basic and important concepts in group theory. When we perform an operation to a molecule, if we cannot tell any difference before and after we do the operation, we call this operation a *symmetry operation.* This means that the molecule seems unchanged before and after a symmetry operation. As Cotton defines it in his book, when we do a symmetry operation to a molecule, every points of the molecule will be in an equivalent position.