9.12: Learning Objectives

After mastering the material covered in this chapter, one will be able to:

1. Describe the Born-Oppenheimer Approximation and how it is used to construct potential energy surfaces describing the vibration of a diatomic molecule.
2. Construct a molecular orbital diagram for a diatomic molecule depicting both bonding and antibonding orbitals of s and p symmetries including inversion symmetry (g/u) as appropriate for homonuclear diatomic molecules. Utilize the diagram to
    a. Predict the ground state electronic configuration of a diatomic molecule, including
        i. Magnetic properties
        ii. Bond order
3. Describe the differences between Hund's Angular Momentum Cases (a) and (b) and how these cases manifest in the resulting energy levels in real molecules.
4. Determine molecular term symbols for diatomic molecules using the
    a. United Atom Method
    b. Separated Atom Method
    c. Molecular Orbital Method
5. Construct Herzberg Diagrams and use them to
    a. Determine the band structure of a spectroscopic transition, including the "first line" in each branch.
6. Derive the formulation for the Franck-Condon factor and explain how it determines relative intensity of vibrational bands in an electron transition.
7. Utilize the tools of Group Theory to predict the symmetries of the molecular orbitals that arise from linear combinations of atomic orbitals for a polyatomic molecule.