Reading guide and suggested problems for Chapter 5

Chapter 5: Molecular Orbitals. In molecular orbital (MO) theory, the symmetry of atomic orbitals and their relative energies, are used to determine how these orbitals interact with each other to form molecular orbitals. This is a more sophisticated take on how atoms interact with each other to form bonds. In this chapter we will learn the basics of molecular orbital theory and will apply this knowledge later on as well when discussing metal complexes.

Learning goals:
1) Understand how s, p, and d orbitals can interact to form molecular orbitals.
2) Be able to derive the molecular orbitals for simple diatomic molecules.
3) Understand the trends in atomic orbital energies.
4) Derive SALCs for multinuclear molecules using symmetry and the steps in 5.4.2.
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Suggested reading

5.1: Formation of Molecular Orbitals from Atomic Orbitals. This section introduces the basic concept of molecular orbitals. Molecular orbitals can be thought of as linear combinations of atomic orbitals (LCAOs) in which the sum of two orbitals corresponds to a bonding molecular orbitals and the difference of two orbitals corresponds to an antibonding orbital. In order to form a bond, two atomic orbitals must satisfy the following requirements: 1) the symmetry of the orbitals needs to be the same in the area of overlap; 2) the atomic orbital energies must be similar; 3) the distance between the two atoms must be short enough for the orbitals to overlap.

5.1.1, 5.1.2, 5.1.3, 5.1.4: Molecular orbitals from s, p, and d orbitals. The s, p, and d orbitals can interact in different ways to form molecular orbitals. These sections describe bonding, antibonding, and nonbonding orbitals, as well as sigma (σ), pi (π), and delta (δ) bonds.

5.2, 5.2.1, 5.2.2, 5.2.3: Molecular orbital diagrams for homonuclear diatomic molecules. These sections describe MOs for homonuclear diatomic molecules and the effects of orbital mixing on the energy levels in your MO diagram.. These sections also describe how diatomics can be diamagnetic or paramagnetic.

5.2.4: Photoelectron Spectroscopy. This section describes how PES can be used to support the existence of MO energy levels. ***You are NOT responsible for this material***, however it's good material for those who are interested.

5.3, 5.3.1: Heteronuclear diatomic molecules. These sections describe the energies of different orbitals. Figure 5.12 and Table 5.2 are informative, and demonstrate general trends in orbital energies as you go across a period and down a group. MOs resulting from heternuclear diatomics are less symmetric due to the differing energies of the atomic orbitals. CO is a very important example when thinking about metal-CO complexes! The concepts of HOMO and LUMO frontier orbitals are introduced, also important when thinking about metal complexes.

5.3.2: ***You are NOT responsible for this material***

5.4, 5.4.1: Molecular orbitals of larger molecules. This section describes how to build MO diagrams for molecules with more than 2 atoms, FHF is used as a simple first example.

5.4.2: MO of CO_2. This section describes all the basic steps you need to take in order to build MOs for molecules based on their point groups, character tables, and the generation or reducible representations similar to what was used for IR stretches. The 6 steps described in 5.4.2 are what we will apply to derive group orbitals (or Symmetry Adapted Linear Combinations of orbitals, SALCs) for multinuclear compounds.

5.4.3, 5.4.4, 5.4.5, 5.4.6. These sections describe the generation of MOs for H_2O, NH_3, and BF_3. ***NOTE: The projection operator method described and shown in sections 5.4.3-5.4.5 is beyond the scope of this course.*** We will simply apply the steps described in 5.4.2 to develop group orbitals/SALCs for MO diagrams..

5.4.7: ***You are NOT responsible for this material***

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Relevant homework problems:

5.1, 5.2, 5.3, 5.4, 5.5

5.7, 5.8, 5.9, 5.10

5.14, 5.15, 5.16, 5.17

5.18, 5.19, 5.20

5.28, 5.29: In these problems, apply the steps in 5.4.2 to determine the irreducible representations for the SALCs and predict what they will look like based on that. You are not expected to employ the projector operator method.

5.31