

Assignment 13
Not to be turned in

Announcements: The final exam will be given Sunday, Dec. 19 at 9:00 am in Merrill Lecture Room 1. The exam will cover all course material through Wednesday's lecture (reading assigned below), focusing primarily (~67%) on material we have covered since the second exam (i.e. everything from Lewis structures to the end of the semester). No more than ~33% of the exam will be drawn from earlier material.

Sample exams will be posted by Tuesday 12/14. Review sessions to be held during reading period will be announced on Wednesday and posted on the course website.

All work must be handed in by the end of the day Wednesday 12/15 (the last day of classes). This particularly applies to laboratory reports. You must have completed and turned in a laboratory report for every lab experiment by Tuesday in order to receive a passing grade in this class.

Overview: The localized electron pair model (Lewis structures, VSEPR, and hybridization) is a useful description of covalent bonding. However, the need for the concept of resonance suggests that there are deficiencies in this very simple model. There are also some notable failures of the localized electron pair model to account for the experimentally-observable properties of some molecules, such as the paramagnetism of molecular oxygen (O_2). There is therefore a need to develop an alternate, more sophisticated model of covalent bonding. We will return to our wave function description of electrons within atoms, and we will use these atomic orbitals as the basis for construction of "molecular orbitals" that describe the wave functions of electrons within molecules. We will use MO theory to describe bonding in homonuclear and heteronuclear diatomic molecules in the second row of the periodic table and test its effectiveness at predicting the magnetic properties and bond orders of these molecules. Molecular orbital (MO) theory achieves success in some areas where the previous model failed, notably in explaining magnetic properties and in allowing for excited states of molecules. Although we are only able to explore the basic principles of molecular orbital theory in Chemistry 11, we are laying the foundation for future applications of this very powerful model for covalent bonding. We will consider polyatomic molecules, although we will see that the molecular orbitals of triatomic molecules are already rather complicated. Often a good compromise for polyatomic molecules, especially those that involve resonance structures, is to use hybrid orbitals from the localized electron pair model to describe the σ bonds and to use the molecular orbital model to describe the π bonds. This combined approach will also be used in organic chemistry.

Reading & Problems: Zumdahl, 6th edition
Solutions will be provided on Wednesday.

Date	Lecture	Reading	Assigned Problems
Wed., 12/8	MO Theory: H ₂ , and He ₂	Section 14.2 – 14.3	Ch. 14: #28, 30
Fri., 12/9	MO Theory: Homonuclear	Section 14.3	Ch. 14: #34, 60, 61, 72, 74

	diatomics		
Mon., 12/13	MO Theory: Heteronuclear Diatomics, Combined Model	Section 14.4 – 14.6	Ch. 14: #32, 36, 37, 38, 39, 40, 46, 48
Wed., 12/15	Semester Wrap-Up		

Challenge Problem:

1. Consider the diatomic molecules CO, NO, and O₂.
 - a. In the space below, draw MO diagrams (energy diagrams) for these three molecules. Make sure to draw energy levels in each diagram with the correct energies relative to the other diagrams (i.e. O should be the same in all three diagrams).
 - b. Add electrons to the MO diagrams to represent the ground state of each molecule.
 - c. For each molecule give the bond order and tell whether it is paramagnetic or diamagnetic.
 - d. Which molecule would you predict has the strongest bond? Which do you predict to have the weakest?
 - e. Using your MO diagrams, arrange the following species in order of increasing ionization energy: CO, NO, O₂, C, O, and N. If there are any for which you can't determine the relative IE based on the information you have, indicate these (hint: you should be able to order at least four of them).
 - f. Sketch the molecular orbitals (wavefunctions) for the molecule with the smallest dipole moment, and for the molecule with the largest dipole moment. What are the main differences?