Experiment 17

Molecular Orbitals

Pre-Lab Assignment

Before coming to lab:

- Read the lab thoroughly.
- Answer the pre-lab questions that appear at the end of this lab exercise.

Purpose

Computer-generated diagrams of molecular orbitals will be used to visualize molecular orbital theory for diatomic molecules and analyzed to match predictions.

Background

Due to their wave-particle behavior, electrons in atoms and molecules are best described as densities. Each electron in an atom is assigned a set of four quantum numbers, (n, l, m_l, m_s) that describe its location, shape, and energy. The principal quantum number, n, describes an electron's energy level. The azimuthal, or angular momentum quantum number, l, describes the shape of an electron's orbital (s, p, d, or f). The magnetic quantum number, m_l, dictates the orientation in space of the orbital, and the spin quantum number, m_s, the direction of the electron's spin.

When atoms combine to form molecules, these atomic orbitals will average themselves into new shapes in order to match their three-dimensional VSEPR geometries. These new hybrid orbitals are formed on central atoms and are designated by the original atomic orbitals that made them. For example, a hybrid formed from an s-orbital and a p-orbital would make two sp-hybrids that are 180° apart, matching the linear VSEPR geometry.

To bond, atoms' electronic orbitals, either atomic or hybrid, must overlap by physically occupying the same space and form new molecular orbitals. The wave-like properties of electrons mean that this overlap can be either constructive, meaning that the phases of the waves match, or destructive, meaning that the phases of the waves are exactly opposite and cancel out. Constructive overlap forms bonding molecular orbitals which are lower in energy and more stable and destructive forms antibonding molecular orbitals which are higher in energy and less stable.

The direction of the overlap determines the type of bond that is formed. If the orbitals are facing one another, the overlap is said to be direct and called a σ-bond. If the orbitals are parallel to one another, it is called a π-bond. A molecular orbital diagram is a way to pictorially represent the types of molecular orbitals and bonds that a molecule can form and where the electrons in the molecule are placed. Bond order can be determined by Eqn. 1 and is a more powerful way than Lewis structures to define the bonding present in a molecule. Bond orders greater than 0 represent stable molecules, whereas bond orders with zero or negative values represent unstable molecules. It also explains why some respond to magnetic fields and others do not.

bond order = 1/2[(# of e^- in bonding orbitals) – (# of e^- in antibonding orbitals)] Eqn. 1

Diagmagnetic molecules have all electrons paired in their molecular orbitals and do not respond to magnetic fields. Paramagnetic molecules have at least one unpaired electron in their molecular orbitals and are attracted to magnetic fields.

Procedure

Part I: Valence Bond Theory

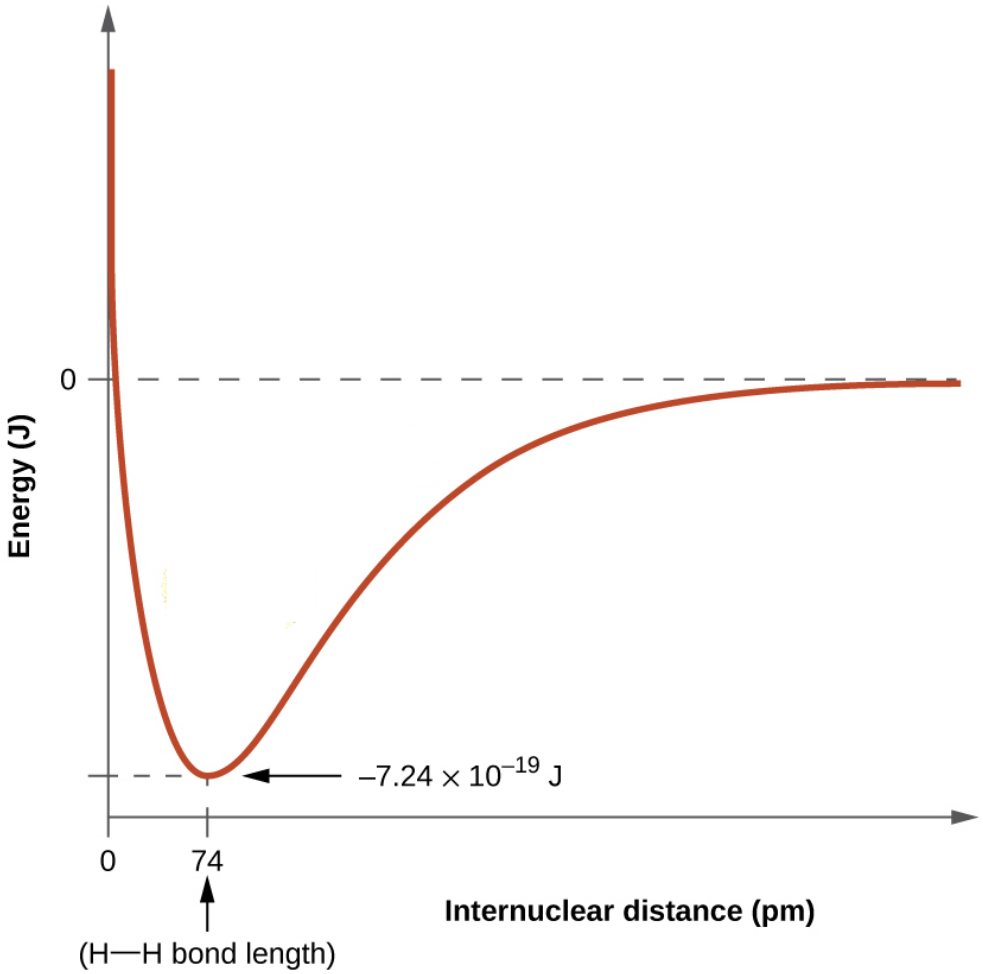


Fig. 1: The interaction of two hydrogen atoms as a function of distance

1. Fig. 1 represents the distance versus energy for two hydrogen atoms. When the distance is very large, the atoms are very far apart. The atoms are brought closer together until the nuclei are nearly touching. Note also the changes in energy. Answer the questions about this graph on your data sheet.

Part II: Molecular Orbitals

1. On a lab computer, go to the Chem1A folder and open the "orbitals animate" file with Internet Explorer. On the web page, click on the step-animations for either N_2, O_2, or F_2.

2. On each page, three images of one of the molecule's molecular orbitals are shown representing the x, y, and z axis point of view. There are ten images total representing ten total molecular orbitals. Red and blue indicate different phases. For some images, the nuclei are visible in the very center of the image colored either red or yellow. Answer the questions about these images on your data sheet.

Experiment 17—Data Sheet

Name: _____

Part I: Valence Bond Theory

1. When atoms that can bond approach one another, why does the energy decrease? Why does it reach a minimum? Why does it increase?

2. What is the minimum energy on the graph? What is happening in the molecule at this point?

3. What is the normal bond length for H_2, according to the graph?

4. Consider He_2. Does this molecule bond? Sketch a Valence Bond Theory graph of distance between the nuclei versus energy that you would expect for He_2.

Part II: Molecular Orbitals

1. Draw the complete molecular orbital diagram for whichever molecule you chose to analyze. Include labels on each atomic and molecular orbital, such as 1s, σ_{1s}, σ^*_{1s}, etc.

2. Next to each molecular orbital, label the image number that it matches.

3. Indicate whether the molecular orbital is bonding or antibonding.

4. Were the molecular orbitals in the expected order? Why or why not?

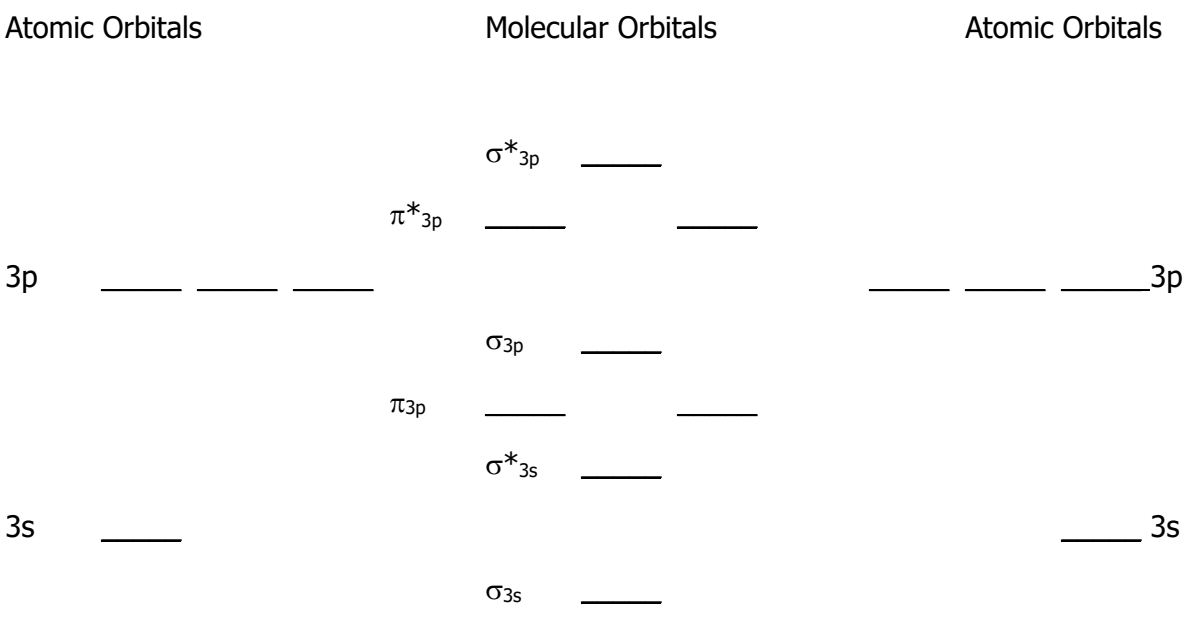
5. Why are the relative sizes of the σ_{1s} and σ_{2s} different?

6. How do bonding and antibonding orbitals differ?

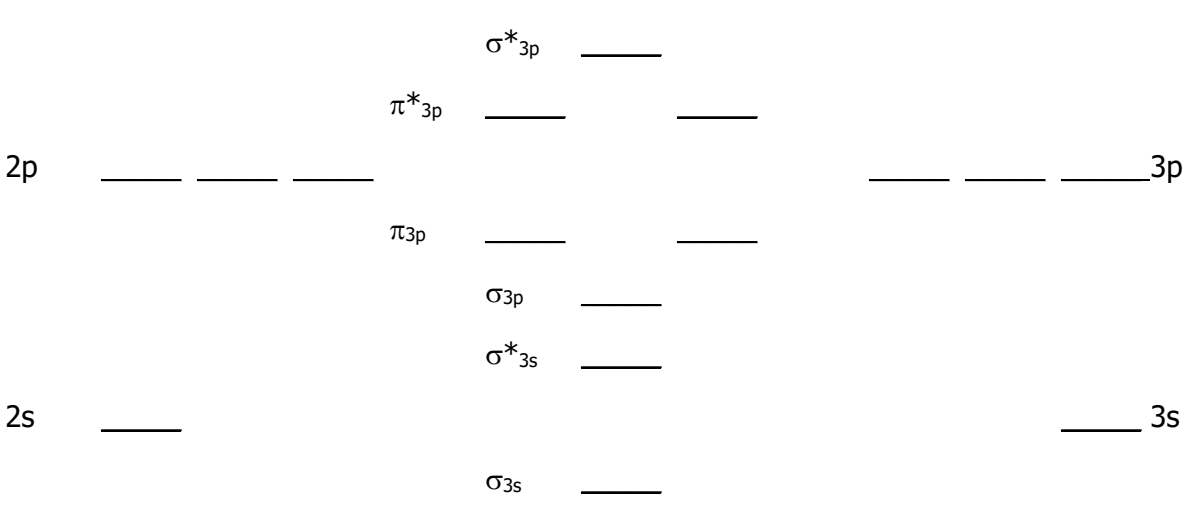
Experiment 17—Post-Lab Assignment

1. Complete the following molecular orbital diagrams by adding the correct electrons for Si_2 and SO^+. For each, determine the bond order and whether the molecule is paramagnetic or diamagnetic.

Si_2



SO^+



Experiment 17—Pre-Lab Assignment

Name: _____

1.For each of the following sets of quantum numbers (n, l, m_l, m_s), decide if the set is valid or invalid. For valid sets, identify the type of orbital (i.e., 2p) that the set describes. For invalid sets, explain why the set cannot exist.

a. n = 2, l = 1, m_l = 0, m_s = ½

b. n = 0, l = 0, m_l = 0, m_s = ½

c. n = 3, l = 2, m_l = -2, m_s = - ½

d. n = 3, l = -2, m_l = 3, m_s = ½

2. Explain the difference between Schrödinger's orbitals and Bohr's electron orbits.

3. For each quantum number, list the symbol and give a brief description.

a. Principal

b. Angular Momentum or Azimuthal

c. Magnetic

d. Spin

4. Complete the following table to indicate the total number of orbitals in each energy level (n). In the remaining columns, specify how many of those orbitals are s, p, d, and f.

Level n	**Total # of Orbitals**	**# of s-orbitals**	**# of p-orbitals**	**# of d-orbitals**	**# of f-orbitals**
1					
2					
3					
4					