

27
27

Name KEY

Visualizing Molecular Orbitals: A MacSpartan Pro Experience Advance Study Assignment

Read through the experiment carefully and then provide a 1-2 sentence synopsis of the objectives of the experiment in the box below.

The objective of this experiment is to generate molecular orbital surfaces using MacSpartan Pro. These surfaces will be examined to better ~~understand~~ understand the bonding in the substances of the lab experiment

+2

Please provide the answers to the following questions on a loose sheet of paper. Staple your answer sheet and this page together before turning in this assignment.

+4

1. The simplest diatomic molecule is H_2 . On the basis of the molecular orbital view of H_2 , predict the bond order and number of unpaired electrons of H_2 and H_2^+ .

+4

2. The diatomic oxygen molecule is paramagnetic. How can this be explained using molecular orbitals?

+4

3. Sketch the shapes of the π^*_{2p} and σ^*_{2p} orbitals of O_2 . [Note: you will discover during this experiment that the diagrams of these orbitals in the Silberberg text are oversimplified- can you guess what these orbitals might really look like?]

+7

4. Draw the important resonance (Lewis) structures of the following molecules:

- (a) ozone, O_3 (b) nitrate, NO_3^- (c) benzene, C_6H_6

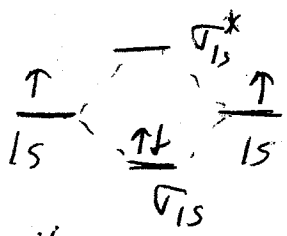
During this experiment you will see the molecular orbitals that account for delocalization of electrons in these molecules- a modern explanation of resonance.

+6

5. Indicate what types of hybrid orbitals are used by carbon in the following molecules.

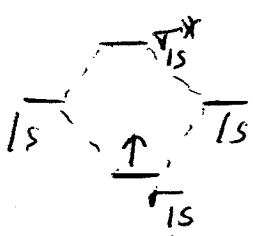
- (a) methane, CH_4 sp^3 (b) ethylene, C_2H_4 sp^2 (c) acetylene, C_2H_2 sp

1



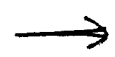
H_2

Bond Order = 1
Zero unpaired electrons



H_2^+

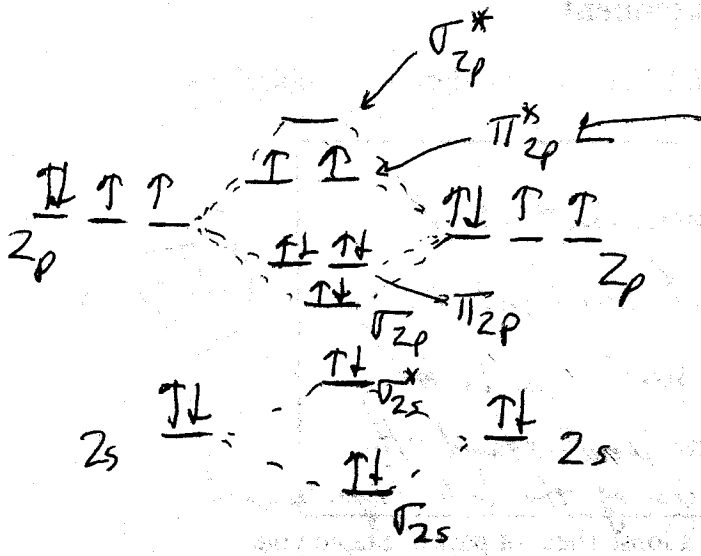
bond order = 0.5
one unpaired electron



#2 Paramagnetic \Rightarrow possesses unpaired electrons

Oxygen energy level diagram

(+4)

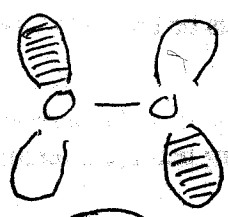


2 unpaired electrons in

π_{2p}^* molecular orbitals

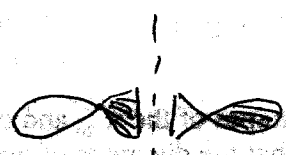
paramagnetic

#3 π_{2p}^*



(+2)

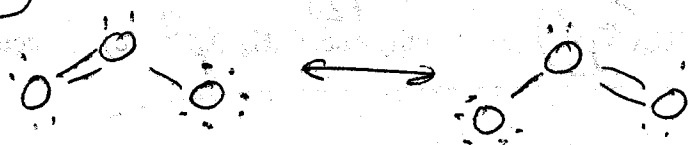
σ_{2p}^*



(+2)

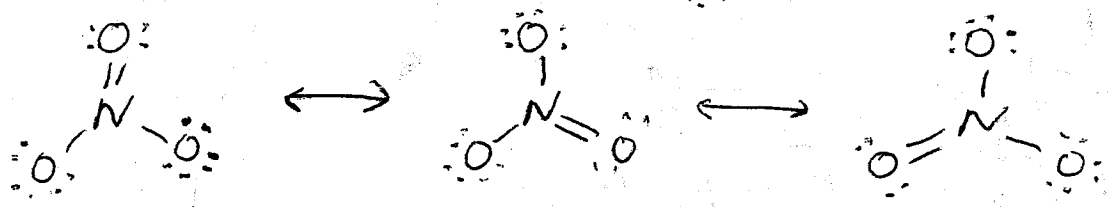
no point value for comment about actual orbital appearance.

4 (a) O_3



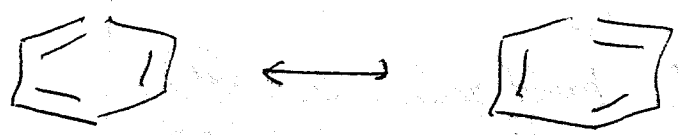
(+2)

(b)



(+3)

(c)



(+2)

doesn't have to be a line structure.