What is Molecular Orbital Theory?

Worksheet

Molecular orbital (MO) theory describes molecules using delocalized orbitals formed by combining atomic orbitals. Bonding MOs stabilise molecules; antibonding MOs destabilise them. The HOMO-LUMO gap predicts reactivity.

Questions

1. In molecular orbital theory, bonding orbitals

A) have high energy and destabilise molecules
B) have low energy and stabilise molecules
C) are always empty
D) don't interact with atomic orbitals

2. What does HOMO stand for?

A) High Occupied Molecular Orbital
B) Highest Occupied Molecular Orbital
C) Homogeneous Orbital Matrix
D) Home Orbital

3. Antibonding orbitals form from

A) constructive wave overlap
B) destructive wave overlap
C) only s orbitals
D) only electrons

4. Which factor increases chemical reactivity in MO theory?

A) large HOMO-LUMO gap
B) small HOMO-LUMO gap
C) all bonding orbitals empty
D) no antibonding orbitals

5. In H, how many electrons occupy bonding orbitals?

6. Explain why O is paramagnetic using molecular orbital theory.

7. Define the HOMO-LUMO gap.

8. Define: What does molecular orbital theory assume?

9. Define: Bonding vs. antibonding orbital?

10. Define: What is the HOMO-LUMO gap?

Answer Key

1. B) have low energy and stabilise molecules - Bonding orbitals form from constructive overlap of atomic orbitals and lower molecular energy.

2. B) Highest Occupied Molecular Orbital - HOMO = highest occupied molecular orbital, the topmost electron-filled orbital.

3. B) destructive wave overlap - Destructive overlap of atomic orbitals creates antibonding MOs with a node between nuclei.

4. B) small HOMO-LUMO gap - A small gap means electrons can easily jump to LUMO, making the molecule more reactive.

5. H has 2 valence electrons (1 from each H) Both electrons pair in the bonding orbital (lower energy) Result: 2 electrons in bonding orbital

6. O has 12 valence electrons After filling bonding and orbitals, two * antibonding orbitals have unpaired electrons Unpaired electrons = paramagnetic (attracts magnetic field)

7. HOMO = highest occupied molecular orbital (where top electrons sit) LUMO = lowest unoccupied molecular orbital (empty orbital above) Gap = energy difference between them; smaller gap = more reactive

8. Electrons occupy orbitals that span the entire molecule, not just single atoms.

9. Bonding orbitals have lower energy and stabilise molecules; antibonding orbitals have higher energy and destabilise them.

10. The energy gap between the highest occupied and lowest unoccupied molecular orbitals; determines chemical reactivity.