

Things You Should Know

Chapter 11: Quantum Mechanical Treatment of Simple Molecules

Be able to define the following terms (using words, equations, or figures):

valence bond theory
exchange integral
molecular-orbital theory
bonding orbital
bond order
Hückel theory

coulomb integral
overlap integral
molecular orbitals
antibonding orbital
hybrid orbitals
 π electron approximation

Concepts and Exercises:

1. Have a good qualitative understanding of the Heitler-London valence bond method for H_2 . Be able to interpret physically the various integrals that arise and know where the major contributions to the stability of the chemical bond come from.
2. Have an appreciation for the molecular orbital treatment of H_2^+ . Be able to predict the bonding properties of diatomic molecules by filling molecular orbitals with electrons and determining the resulting bond order.
3. Know the nomenclature for molecular orbitals of diatomic molecules.
4. Be able to predict trends in bond strengths and bond lengths.
5. Be able to determine molecular term symbols from the electronic configurations of diatomic molecules. Use Hund's rule to determine which is lowest in energy.
6. Be able to find sp , sp^2 and sp^3 hybrid orbitals.
7. Be able to apply Hückel theory for simple conjugated systems
8. Be able to do all the assigned exercises.