

Chapter Summary and Review

Key Learning Outcomes

| CHAPTER OBJECTIVES | ASSESSMENT |
|---|--|
| Write Hybridization and Bonding Schemes Using Valence Bond Theory (6.3) | <ul style="list-style-type: none"> Examples 6.1, 6.2, 6.3 For Practice 6.1, 6.2, 6.3 For More Practice 6.3 Exercises 33, 34, 35, 36, 37, 38 |
| Draw Molecular Orbital Energy Diagrams and Predict Bond Order in a Homonuclear Diatomic Molecule (6.4) | <ul style="list-style-type: none"> Examples 6.4, 6.5 For Practice 6.4, 6.5 For More Practice 6.5 Exercises 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52 |
| Draw Molecular Orbital Energy Diagrams and Predict Magnetic Properties in a Heteronuclear Diatomic Molecule (6.4) | <ul style="list-style-type: none"> Example 6.6 For Practice 6.6 Exercises 53, 54 |

Key Terms

Section 6.2

valence bond theory

atomic orbitals (AO)

Section 6.3

hybridization

hybrid orbitals

pi (π) bond

sigma (σ) bond

isomer

Section 6.4

molecular orbital (MO)

molecular orbital (MO) theory

bonding orbital

antibonding orbital

molecular orbital (MO) diagram

bond order

nonbonding orbital

Key Concepts

Valence Bond Theory (6.2, 6.3)

- In contrast to the Lewis model, in which a covalent chemical bond is the sharing of electrons represented by dots, in valence bond theory a chemical bond is the overlap of half-filled atomic orbitals (or in some cases the overlap between a completely filled orbital and an empty one).
- The overlapping orbitals may be the standard atomic orbitals, such as $1s$ or $2p$, or they may be hybridized atomic orbitals, which are mathematical combinations of the standard orbitals on a single atom. The basic hybridized orbitals are sp , sp^2 , sp^3 , sp^3d , and sp^3d^2 .
- The geometry of the molecule is determined by the geometry of the overlapping orbitals.
- In valence bond theory, we distinguish between two types of bonds, σ (sigma) and π (pi). In a σ bond, the orbital overlap occurs in the region that lies directly between the two bonding atoms. In a π bond, formed from the side-by-side overlap of p orbitals, the overlap occurs above and below the region that lies directly between the two bonding atoms.
- Rotation about a σ bond is relatively free, while rotation about a π bond is restricted.
- In our treatment of valence bond theory, we use the molecular geometry determined by VSEPR theory to determine the correct hybridization scheme.

Molecular Orbital Theory (6.4, 6.5)

- The simplest molecular orbitals are linear combinations of atomic orbitals (LCAOs), weighted averages of the atomic orbitals of the different atoms in the molecule.
- When two atomic orbitals combine to form molecular orbitals, they form one molecular orbital of lower energy (the bonding orbital) and one of higher energy (the antibonding orbital).
- A set of molecular orbitals is filled in much the same way as a set of atomic orbitals.
- The stability of the molecule and the strength of the bond depend on the number of electrons in bonding orbitals compared to the number in antibonding orbitals.

Key Equations and Relationships

Bond Order of a Diatomic Molecule (6.4)

$$\text{Bond order} = \frac{(\text{number of electrons in bonding MOs}) - (\text{number of electrons in antibonding MOs})}{2}$$

Not for Distribution