

Principles of Chemical Bonding

Introduction

- Atoms are rarely found floating alone in nature; they prefer to stick together.
- Chemical bonding is the process where atoms combine to form compounds, driven by the desire to reach a lower, more stable energy state.
- This stability is usually achieved by obtaining a full outer shell of electrons, similar to noble gases.
- In this module, we will explore how these bonds form, how they shape molecules in 3D space, and the theories that explain their behavior.

Learning Objectives

By the end of this module, you will be able to:

- Recognize the principles and theories behind the formation of chemical bonds.
- Apply the **Octet Rule** to draw **Lewis Structures** for ionic and covalent compounds.
- Predict the **Molecular Geometry** of molecules using the **VSEPR model**.
- Distinguish between **Valence Bond Theory** (hybridization) and basic **Molecular Orbital Theory**.

Key Concepts and Definitions

Term	Definition
Ionic Bond	A chemical bond formed through the electrostatic attraction between oppositely charged ions (cation and anion), typically involving the transfer of electrons.
Covalent Bond	A bond formed by the sharing of electron pairs between atoms.

Octet Rule	The tendency of atoms to prefer to have eight electrons in their valence shell.
Lewis Structure	A diagram that shows the bonding between atoms of a molecule and the lone pairs of electrons that may exist.
VSEPR Theory	(Valence Shell Electron Pair Repulsion) A model used to predict the geometry of individual molecules based on the number of electron pairs surrounding their central atoms.
Hybridization	The concept of mixing atomic orbitals into new "hybrid" orbitals (like sp^3 , sp^2) suitable for the pairing of electrons to form chemical bonds.

Detailed Discussion

Ionic Bonds and Lewis Structures

1. The Octet Rule Atoms are most stable when they have 8 valence electrons (a "full octet").

- **Metals** tend to lose electrons to reveal a full inner shell.
- **Nonmetals** tend to gain or share electrons to fill their current shell.
- *Exception:* Hydrogen and Helium are happy with just 2 electrons (the "Duet Rule").

2. Ionic vs. Covalent

- **Ionic Bonding:** Complete transfer of electrons. Occurs between a Metal and a Nonmetal (e.g., NaCl). The bond is non-directional; it's a crystal lattice held together by charge attraction.
- **Covalent Bonding:** Sharing of electrons. Occurs between two Nonmetals (e.g., H₂O). The bond is directional and forms specific shapes.

3. Drawing Lewis Structures

1. Count total valence electrons.
2. Place the least electronegative atom in the center (Hydrogen is always on the outside).

3. Connect atoms with single bonds (2 electrons each).
4. Fill outer atoms' octets with remaining electrons.
5. If electrons are left, put them on the central atom. If the central atom lacks an octet, move lone pairs to form double or triple bonds.

Molecular Geometry and VSEPR

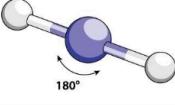
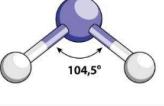
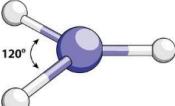
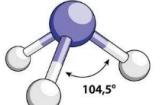
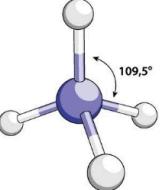
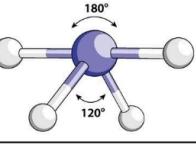
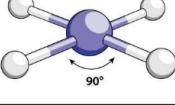
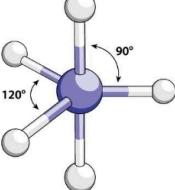
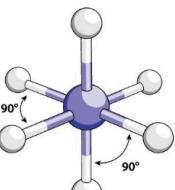
We can predict the 3D shape of a molecule by counting "electron domains" (bonding pairs + lone pairs) around the central atom. Electron pairs repel each other and want to be as far apart as possible.

Common Geometries:

- **2 Domains (Linear):**
 - Angle: 180 degrees
 - Example: CO₂
 - Shape: A straight line.
- **3 Domains (Trigonal Planar):**
 - Angle: 120 degrees
 - Example: BF₃
 - Shape: A flat triangle.
- **4 Domains (Tetrahedral):**
 - Angle: 109.5 degrees
 - Example: CH₄ (Methane)
 - Shape: A pyramid with a triangular base.

Effect of Lone Pairs: Lone pairs take up more space than bonding pairs, pushing the bonds closer together.

- *Example (Water - H₂O):* Oxygen has 4 domains (2 bonds + 2 lone pairs). The electron geometry is tetrahedral, but the *molecular shape* is **Bent** (or V-shaped), with an angle of approx. 104.5 degrees.

Molecular Formula	VSEPR Notation	Molecular Geometry	Geometric Shape	Example
AX_2	AX_2		Linear	CO_2
	AX_2E_2		Bent(V-shaped)	$\text{H}_2\text{O}, \text{OF}_2$
AX_3	AX_3		Trigonal Planar	BH_3, SO_3
	AX_3E		Trigonal Pyramidal	$\text{NH}_3, \text{PCl}_3$
AX_4	AX_4		Tetrahedral	CH_4
	AX_4E		Seesaw	SF_4
	AX_4E_2		Square Planar	XeF_4
AX_5	AX_5		Trigonal Bipyramidal	PCl_5
AX_6	AX_6		Octahedral	SF_6

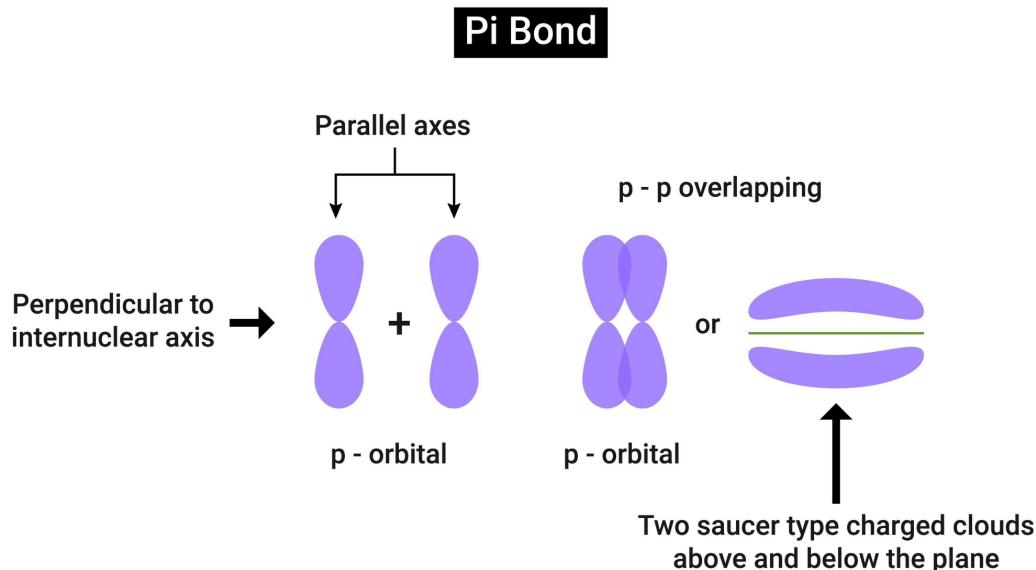
Valence Bond Theory & MO Theory

1. Valence Bond Theory (VBT) This theory describes bonds as the **overlap** of atomic orbitals.

- **Sigma Bond (head-on):** The first bond formed between two atoms. Strong and allows rotation.
- **Pi Bond (side-on):** Formed by parallel p-orbitals. Only found in double (1 sigma + 1 pi) and triple bonds (1 sigma + 2 pi). Weaker and prevents rotation.
- **Hybridization:** To fit VSEPR shapes, orbitals mix.
 - 4 domains = **sp³** hybridization (Tetrahedral)
 - 3 domains = **sp²** hybridization (Trigonal Planar)
 - 2 domains = **sp** hybridization (Linear)

2. Basic Molecular Orbital (MO) Theory While VBT treats bonds as localized (stuck between two atoms), MO theory says electrons spread over the *entire* molecule.

- When orbitals combine, they create **Bonding Orbitals** (lower energy, stable) and **Antibonding Orbitals** (higher energy, unstable).
- This theory is essential for explaining why Oxygen (O₂) is magnetic (paramagnetic), which Lewis structures cannot explain.



References

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2. Zumdahl, S. S., & Zumdahl, S. A. (2014). *Chemistry* (9th ed.). Belmont, CA: Brooks/Cole, Cengage Learning.
3. Brown, T. L., LeMay, H. E., Bursten, B. E., Murphy, C. J., & Woodward, P. M. (2017). *Chemistry: The Central Science* (14th ed.). Pearson.