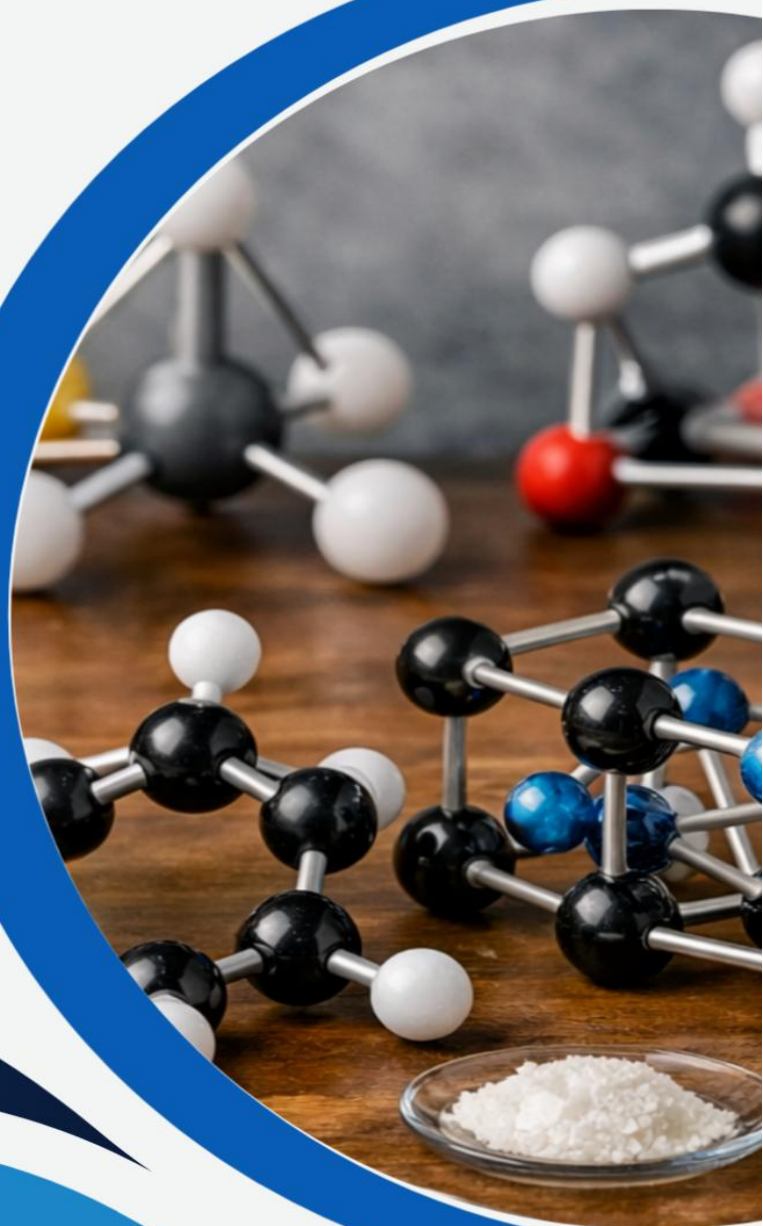
CHM214

STRUCTURE AND BONDING



- **Course code:** CHM 214
- **Course title:** Structure and Bonding
- **Course credit load:** 2 Units (C: LH 30)
- **Series titles:**

  Quantum States, Orbitals, Shape and Energy
  Valence Theory, Electron Repulsion and Atomic Spectra
  Symmetry, Molecular Geometry and Molecular Orbital Theory
  Methods of Determining Molecular Shape, Bond Lengths and Angles
  Structure and Chemistry of Representative Main Group Compound

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Suggested Outline

Part 1: Concept of Quantum States

Sub-Part 1.1: Definition of quantum states
Sub-Part 1.2: Energy levels and quantisation
Sub-Part 1.3: Significance in atomic structure

Part 2: Atomic Orbitals

Sub-Part 2.1: Definition and shapes of orbitals
Sub-Part 2.2: Types of orbitals (s, p, d, f)
Sub-Part 2.3: Orbital energy ordering

Part 3: Orbital Shapes and Orientation

Sub-Part 3.1: Visualising orbital shapes
Sub-Part 3.2: Spatial orientation and nodal planes
Sub-Part 3.3: Implications for bonding

Part 4: Energy Considerations in Orbitals

Sub-Part 4.1: Relative energies of orbitals
Sub-Part 4.2: Factors affecting orbital energy (n, l values)
Sub-Part 4.3: Applications in predicting chemical behaviour

Series Learning Outcomes

Upon completing this Series, you should be able to:

SLO 1.1 define quantum states and explain their significance in atomic structure,
SLO 1.2 describe the shapes and characteristics of atomic orbitals,
SLO 1.3 illustrate orbital orientation and nodal planes with examples,
SLO 1.4 analyse the relative energies of orbitals and the factors that influence them, and
SLO 1.5 apply knowledge of orbital energy considerations to predict chemical behaviour.

Introduction

The study of quantum states and orbitals forms the foundation of modern chemistry. Atoms and molecules behave in ways that cannot be explained by classical physics alone, and it is through quantum theory that we understand their structure, energy, and bonding. This Series introduces you to the essential concepts of quantum states, orbitals, their shapes, and the energy considerations that govern chemical behaviour. By engaging with these ideas, you will gain a deeper appreciation of how atomic structure underpins the entire discipline of chemistry.

The aim of this Series is to equip you with the knowledge and skills to define quantum states, describe orbital shapes and orientations, and analyse how energy levels influence chemical bonding and reactivity.

We shall commence this Series by examining the concept of quantum states, focusing on their definition, energy levels, and significance in atomic structure. Next, we will explore atomic orbitals, considering their shapes, types, and energy ordering. Following that, we will move on to orbital shapes and orientation, where you will learn how spatial features and nodal planes affect bonding. Finally, we will conclude with energy considerations in orbitals, analysing relative energies and the factors that influence them, while also highlighting their applications in predicting chemical behaviour.

1.1 Concept of Quantum States

1.1.1 Definition of quantum states

A **quantum state** is a description of the condition of an electron in an atom, defined by a set of quantum numbers that specify its energy, position, and spin. These quantum numbers include the principal quantum number (n), the azimuthal quantum number (l), the magnetic quantum number (m), and the spin quantum number (s). Together, they provide a complete picture of the electron's behaviour within the atom.

Fill in the blank: The quantum number that defines the main energy level of an electron is called the ___________________ quantum number.

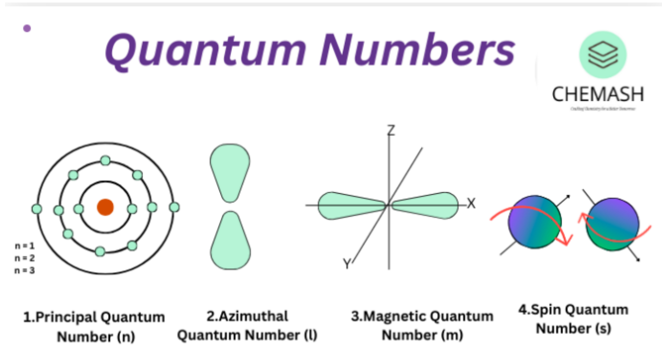

Figure 1.1: Quantum numbers defining an electron's quantum state

1.1.2 Energy levels and quantisation

Quantisation means that electrons can only occupy specific energy levels, not values in between. These levels are determined by the principal quantum number (n). When electrons absorb or release energy, they move between these discrete levels, producing phenomena such as atomic spectra. This explains why atoms emit or absorb light at characteristic wavelengths.

Fill in the blank: The idea that electrons can only occupy specific energy levels is known as __________________.

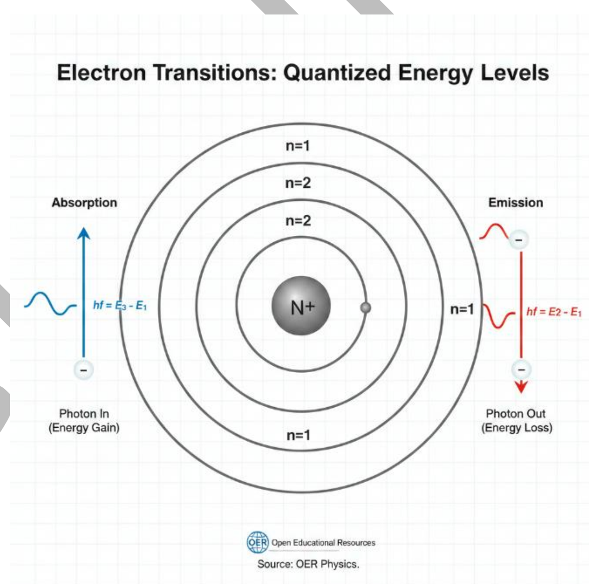

Plate 1.1: Electron transitions in quantised energy levels

1.1.3 Significance in atomic structure

Quantum states explain why electrons are arranged in shells and subshells, which in turn determine the chemical properties of elements. The arrangement of electrons, known as the **electronic configuration**, dictates how atoms bond and interact with one another. This makes quantum states fundamental to understanding **atomic structure** and chemical behaviour.

Fill in the blank: The arrangement of electrons in shells and subshells within an atom is called the __________________ configuration.

The Importance of Quantum States in Chemistry

Aspect	Role of Quantum States	Impact on Chemical Behavior
Electron Arrangement	Defines the "filling order" of electrons (Aufbau Principle and Hund's Rule) based on energy levels (n) and subshells (l).	Determines the ground state stability of an atom and identifies which electrons are "valence" (outermost).
Chemical Bonding	Governs how orbitals (m^1) overlap or hybridize (e.g., sp^3) to share or transfer electrons.	Dictates molecular geometry (VSEPR), bond strength, and whether a bond is ionic, covalent, or metallic.
Periodic Trends	Explains the repeating patterns of properties based on the completion of electron shells.	Directly influences Atomic Radius, Electronegativity, and Ionization Energy as shells are added or filled.
Magnetism	Relies on the spin quantum number (m_s) and whether electrons are paired or unpaired in orbitals.	Determines if a substance is Paramagnetic (attracted to magnets) or Diamagnetic (repelled by magnets).
Spectroscopy	Involves electrons jumping between discrete quantum energy levels (n).	Allows for the identification of elements via Atomic Emission Spectra (the "fingerprint" of an atom).
Reactivity	Determined by the presence of "vacant" quantum states in the valence shell.	Explains why noble gases are inert (full states) while alkali metals are highly reactive (one electron in a new state).

Box 1.1: Importance of quantum states in chemistry

Determine electron arrangement in atoms
Explain chemical bonding and reactivity
Predict magnetic and optical properties
Provide basis for periodic trends

Pilot questions 1.1

The quantum number that defines the main energy level of an electron is called the:
A. Spin quantum number
B. Principal quantum number
C. Magnetic quantum number
D. Azimuthal quantum number
(Linked to SLO 1.1)

The idea that electrons can only occupy specific energy levels is known as:
A. Quantisation
B. Magnetisation
C. Ionisation

D. Excitation
(Linked to SLO 1.1)

The arrangement of electrons in shells and subshells within an atom is called the:
A. Orbital diagram
B. Electronic configuration
C. Quantum state
D. Energy distribution
(Linked to SLO 1.1)

Which quantum number specifies the orientation of an orbital in space?
A. Principal quantum number
B. Azimuthal quantum number
C. Magnetic quantum number
D. Spin quantum number
(Linked to SLO 1.1)

State one reason why quantum states are important in chemistry.
(Linked to SLO 1.1)

1.2 Atomic Orbitals

1.2.1 Definition and shapes of orbitals

An **atomic orbital** is a region around the nucleus of an atom where there is a high probability of finding an electron. Orbitals are solutions to the Schrödinger equation and describe both the energy and spatial distribution of electrons. Each orbital has a characteristic shape that reflects how electrons are distributed in space.

Fill in the blank: The simplest orbital, which is spherical in shape, is called the ___________________ orbital.

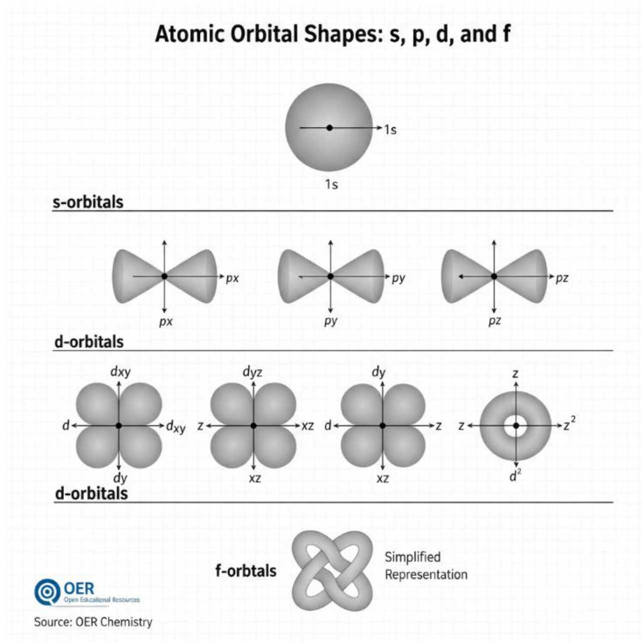

Figure 1.2: Shapes of atomic orbitals

1.2.2 Types of orbitals (s, p, d, f)

Orbitals are classified into types based on the azimuthal quantum number (l). The **s-orbital** (l = 0) is spherical, the **p-orbital** (l = 1) has three orientations (px, py, pz), the **d-orbital** (l = 2) has five orientations with more complex shapes, and the **f-orbital** (l = 3) has seven orientations with intricate structures. These orbitals combine to form subshells, which determine the electronic configuration of atoms.

Fill in the blank: The orbital type with three orientations (px, py, pz) is the ___________________ orbital.

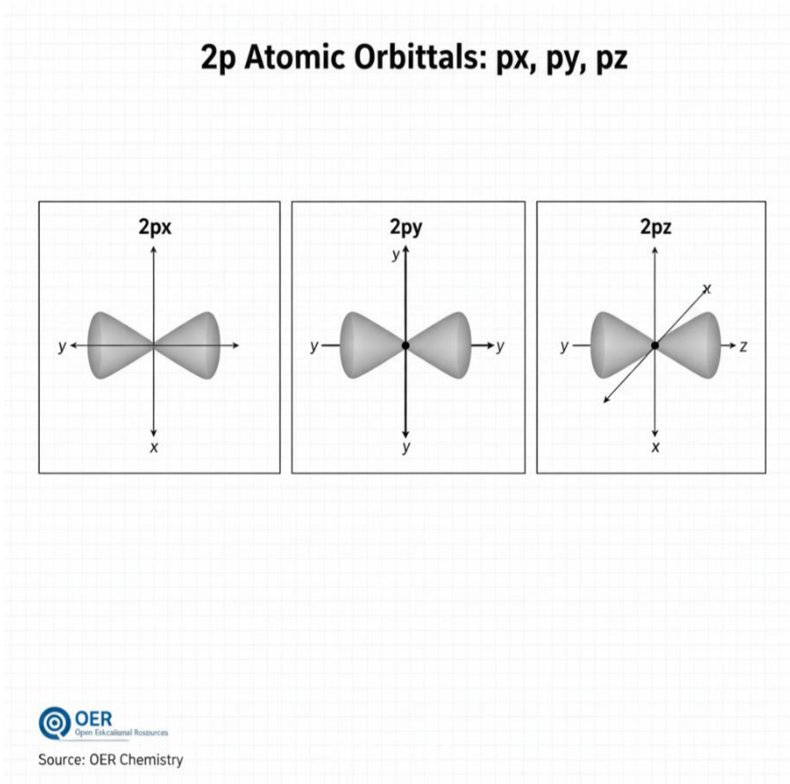

Plate 1.2: Orientations of p-orbitals

1.2.3 Orbital energy ordering

The energy of orbitals increases with both the principal quantum number (n) and the azimuthal quantum number (l). The general order of filling orbitals is given by the **Aufbau principle**, which states that electrons occupy the lowest energy orbitals first. This order is typically 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, and so on. Exceptions occur in transition metals due to stability considerations.

Fill in the blank: The principle that states electrons occupy the lowest energy orbitals first is called the ___________________ principle.

The **Aufbau Principle** (from the German *Aufbau*, meaning "building up") describes the process by which electrons fill subshells in order of increasing energy. This sequence is generally governed by the **Madelung Rule** (or $n + l$ rule), which states that orbitals with a lower $n + l$ value are filled first.

Orbital Energy Ordering (The Aufbau Sequence)

The standard filling order is as follows:
1s → 2s → 2p → 3s → 3p → 4s → 3d → 4p → 5s → 4d → 5p → 6s → 4f → 5d → 6p → 7s

Energy Level (n)	Subshells Available (l)	Filling Order	Max Electron Capacity
$n = 1$	1s	1st	2
$n = 2$	2s, 2p	2nd, 3rd	8
$n = 3$	3s, 3p, (3d*)	4th, 5th, 7th	18
$n = 4$	4s, 4p, 4d, 4f	6th, 8th, 10th, 13th	32
$n = 5$	5s, 5p, 5d, 5f	9th, 11th, 14th, 16th	32

Exceptions in Transition Metals

Nature often favors **symmetry** and **lower energy states**. In certain transition metals (specifically the d-block and f-block), an electron will "jump" from an s orbital to a d orbital to create a half-filled or fully-filled subshell, which provides extra electronic stability.

Element	Symbol	Expected (Aufbau)	Actual (Observed)	Reason for Exception
Chromium	Cr	$[Ar]4s^2 3d^4$	$[Ar]4s^1 3d^5$	Two **half-filled** subshells ($4s^1$ and $3d^5$) are more stable.
Copper	Cu	$[Ar]4s^2 3d^9$	$[Ar]4s^1 3d^{10}$	A **fully-filled** $3d^{10}$ subshell is significantly more stable.
Molybdenum	Mo	$[Kr]5s^2 4d^4$	$[Kr]5s^1 4d^5$	Similar to Chromium; favors half-filled stability.
Silver	Ag	$[Kr]5s^2 4d^9$	$[Kr]5s^1 4d^{10}$	Similar to Copper; favors fully-filled stability.

Box 1.2: Orbital energy ordering (Aufbau principle)

1s → 2s → 2p → 3s → 3p → 4s → 3d → 4p → 5s → 4d → 5p → 6s → 4f → 5d → 6p → 7s
Electrons fill orbitals in order of increasing energy
Exceptions occur in transition metals due to stability factors

Pilot questions 1.2

The simplest orbital, which is spherical in shape, is called the:
A. p-orbital
B. s-orbital
C. d-orbital
D. f-orbital
(Linked to SLO 1.2)

The orbital type with three orientations (px, py, pz) is the:
A. s-orbital
B. p-orbital
C. d-orbital
D. f-orbital
(Linked to SLO 1.2)

The principle that states electrons occupy the lowest energy orbitals first is called the:
A. Hund's rule
B. Pauli exclusion principle
C. Aufbau principle
D. Octet rule
(Linked to SLO 1.2)

How many orientations does a d-orbital have?
A. Three
B. Five
C. Seven
D. Nine
(Linked to SLO 1.2)

1.3 Orbital Shapes and Orientation

1.3.1 Visualising orbital shapes

Orbital shapes describe the regions in space where electrons are most likely to be found. Each type of orbital has a distinct shape: the **s orbital** is spherical, the **p orbital** is dumbbell-shaped, while **d** and **f orbitals** have more complex geometries. These shapes are not arbitrary; they are solutions to the Schrödinger equation and reflect the probability distribution of electrons.

Fill in the blank: The orbital type that is spherical in shape is the __________________ orbital.

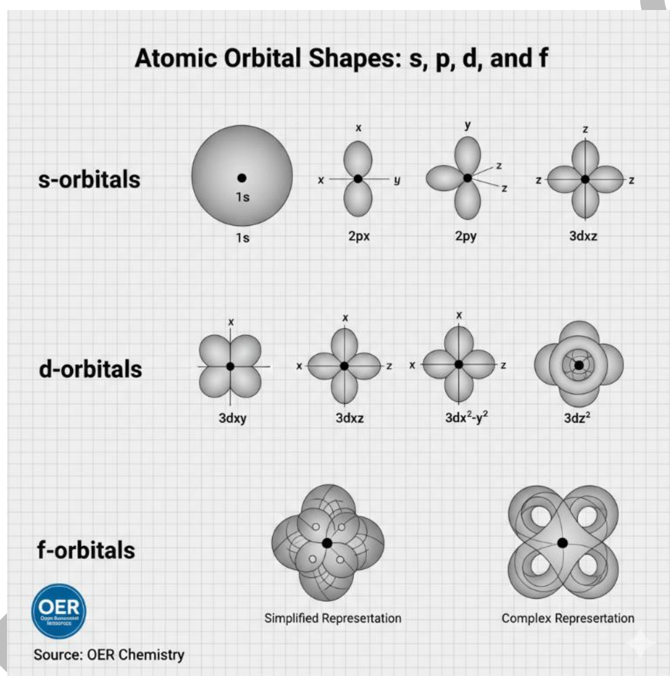

Figure 1.3: Visualization of orbital shapes

1.3.2 Spatial orientation and nodal planes

Spatial orientation refers to the direction in which orbitals are aligned in three-dimensional space. For example, the three p orbitals (px, py, pz) are oriented along the x, y, and z axes. **Nodal planes** are regions where the probability of finding an electron is zero. These planes help explain why orbitals have specific orientations and how they interact with each other.

Fill in the blank: A region where the probability of finding an electron is zero is called a __________________ plane.

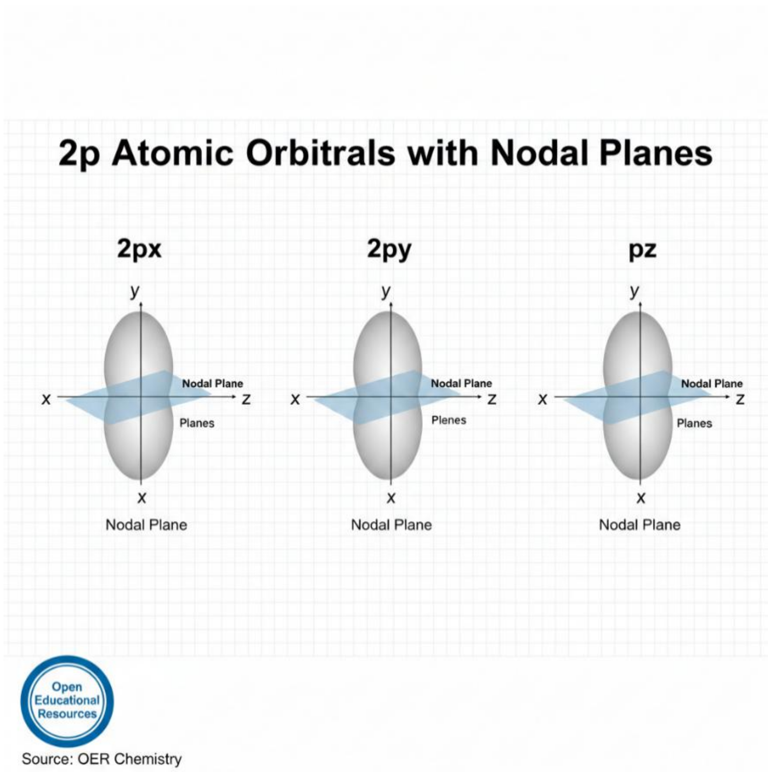

Plate 1.3: Orientation of p-orbitals and nodal planes

1.3.3 Implications for bonding

The shapes and orientations of orbitals have direct implications for **chemical bonding**. For instance, the overlap of s orbitals forms sigma bonds, while the sideways overlap of p orbitals forms pi bonds. The orientation of d orbitals explains bonding in transition metals, influencing properties such as magnetism and colour. Understanding orbital orientation is therefore essential for predicting molecular geometry and reactivity.

Fill in the blank: The overlap of two s-orbitals produces a __________________ bond.

Summary of Orbital Overlaps and Bond Types

Overlap Type	Orbital Combination	Bond Type	Description & Geometry	Bond Strength
Head-on	s + s	σ (Sigma)	Overlap occurs directly along the internuclear axis.	Strongest
Head-on	s + p	σ (Sigma)	Overlap between a spherical s-orbital and one lobe of a p-orbital.	Strong
Head-on	p + p	σ (Sigma)	Two p-orbitals pointing toward each other overlap end-to-end.	Strong
Side-by-side	p + p	π (Pi)	Parallel p-orbitals overlap above and below the internuclear axis.	Weaker
Side-by-side	d + p / d + d	π (Pi)	Overlap between parallel d and p orbitals or two d orbitals.	Weak

Box 1.3: Orbital orientation and bonding implications

- s-orbital overlap → sigma bond

- p-orbital side-by-side overlap → pi bond

- Orbital orientation influences molecular geometry

- Bond strength depends on type and extent of overlap

Pilot questions 1.3

1. The orbital type that is spherical in shape is the:

A. p-orbital

B. s-orbital

C. d-orbital

D. f-orbital

(Linked to SLO 1.3)

2. A region where the probability of finding an electron is zero is called a:

A. Nodal plane

B. Energy level

C. Subshell

D. Quantum state

(Linked to SLO 1.3)

3. The overlap of two s-orbitals produces a:

A. Pi bond

B. Sigma bond

C. Double bond

D. Ionic bond

(Linked to SLO 1.3)

4. How many orientations do p-orbitals have?

A. One

B. Two

C. Three

D. Four

(Linked to SLO 1.3)

5. State one reason why orbital orientation is important in bonding.

(Linked to SLO 1.3)

1.4 Energy Considerations in Orbitals

1.4.1 Relative energies of orbitals

The **relative energy of orbitals** refers to the order in which electrons occupy different orbitals. Orbitals with lower principal quantum numbers (n) generally have lower energy, but the azimuthal quantum number (l) also plays a role. For example, the 4s orbital is filled before the 3d orbital because it is lower in energy. This ordering is essential for predicting the electronic configuration of atoms.

Fill in the blank: The orbital that is filled before the 3d orbital due to lower energy is the __________________ orbital.

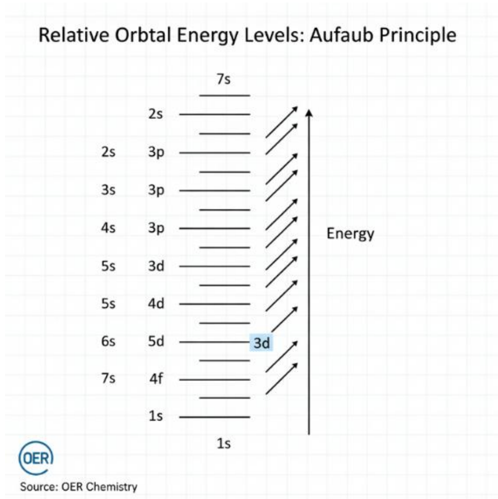

Figure 1.4: Relative energies of orbitals

1.4.2 Factors affecting orbital energy (n, l values)

The energy of an orbital depends on both the **principal quantum number (n)**, which indicates the main energy level, and the **azimuthal quantum number (l)**, which defines the shape of the orbital. Orbitals with higher n values are generally higher in energy, while orbitals with higher l values within the same n level also have higher energy. This explains why p-orbitals are higher in energy than s-orbitals in the same shell.

Fill in the blank: Within the same shell, orbitals with higher __________________ quantum numbers have higher energy.

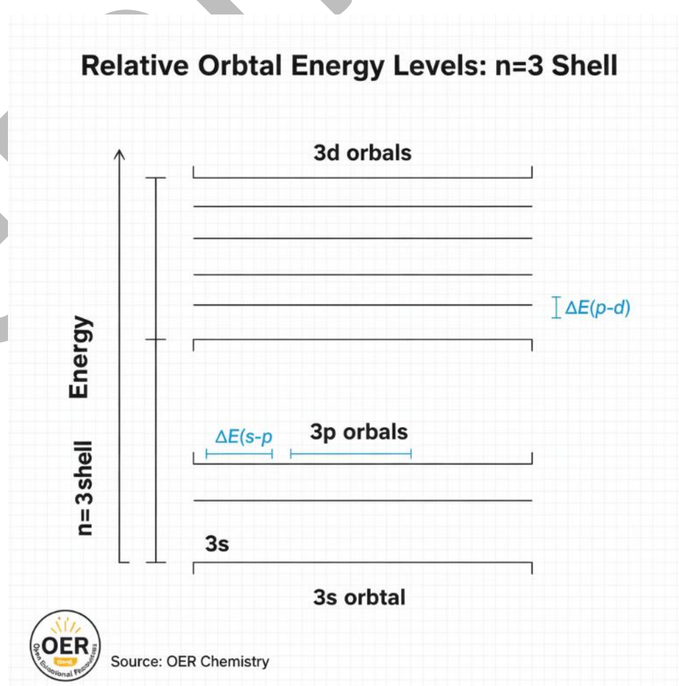

Plate 1.4: Energy differences among orbitals in the same shell

1.4.3 Applications in predicting chemical behaviour

Understanding orbital energies allows chemists to **predict chemical behaviour**. For example, the relative energy of orbitals explains why transition metals can form multiple oxidation states, or why elements in the same group of the periodic table exhibit similar reactivity. Orbital energy considerations also help in predicting molecular geometry, bonding patterns, and the likelihood of chemical reactions.

Fill in the blank: The periodic trend that describes the energy required to remove an electron from an atom is called __________________ energy.

Application	Role of Orbital Energy	Practical Chemical Outcome
Electronic Configurations	Electrons occupy the lowest energy states available (Aufbau Principle).	Predicts the ground-state arrangement and identifies valence electrons available for reactions.
Oxidation States	Energy proximity between subshells (like 4s and 3d) allows for the loss of different numbers of electrons.	Explains why transition metals like Iron (Fe) can exist as both +2 and +3ions.
Periodic Trends	Increasing nuclear charge lowers orbital energy, while increasing raises it.	Explains why Ionization Energy increases across a period and why atoms get smaller.
Chemical Reactivity	Energy "gaps" between occupied and empty orbitals determine how easily an atom gains or loses electrons.	Predicts that Alkali Metals are highly reactive because their ns^1 electron is at a high, unstable energy level.
Bonding Patterns	Atoms seek to achieve a "closed shell" (minimum energy) configuration.	Explains the Octet Rule and why molecules like H_2O or CH_4 form specific stable structures.
Color & Spectroscopy	The specific energy difference (ΔE) between orbitals corresponds to light frequencies.	Explains the vibrant colors of transition metal complexes (d-d transitions) and flame tests.

Box 1.4: Applications of orbital energy considerations

Predicting electronic configurations
Explaining oxidation states
Understanding periodic trends (ionisation energy, electronegativity)
Interpreting chemical reactivity and bonding patterns

Pilot questions 1.4

The orbital that is filled before the 3d orbital due to lower energy is the:

A. 2p orbital
B. 3p orbital
C. 4s orbital
D. 5s orbital
(Linked to SLO 1.4)

Within the same shell, orbitals with higher __________ quantum numbers have higher energy.

A. Principal
B. Azimuthal
C. Magnetic

D. Spin
(Linked to SLO 1.4)

The periodic trend that describes the energy required to remove an electron from an atom is called:
A. Electronegativity
B. Ionisation energy
C. Electron affinity
D. Atomic radius
(Linked to SLO 1.5)

Which principle explains why the 4s orbital is filled before the 3d orbital?
A. Hund's rule
B. Pauli exclusion principle
C. Aufbau principle
D. Octet rule
(Linked to SLO 1.4)

State one application of orbital energy considerations in predicting chemical behaviour.
(Linked to SLO 1.5)

Series Summary

This Series on **Quantum States, Orbitals, Shape and Energy** was designed to help you understand how electrons are organised within atoms and how their behaviour shapes chemical properties. Beginning with the concept of quantum states, you explored their definition, energy levels, and significance in atomic structure. You then examined atomic orbitals, learning about their shapes, types, and energy ordering. Building on this, you visualised orbital shapes and orientations, including nodal planes, and considered their implications for bonding. Finally, you studied energy considerations in orbitals, focusing on relative energies, the influence of quantum numbers, and applications in predicting chemical behaviour.

By completing this Series, you should now be able to **define quantum states and explain their role in atomic structure (SLO 1.1)**, **describe the shapes and characteristics of orbitals (SLO 1.2)**, **illustrate orbital orientation and nodal planes with examples (SLO 1.3)**, **analyse the relative energies of orbitals and the factors influencing them (SLO 1.4)**, and **apply orbital energy concepts to predict chemical behaviour (SLO 1.5)**. These outcomes ensure you can connect theoretical principles of quantum mechanics with practical insights into atomic and molecular chemistry.

Glossary of Terms

Atomic orbital: A region around the nucleus of an atom where there is a high probability of finding an electron.

Aufbau principle: The rule stating that electrons fill orbitals in order of increasing energy, beginning with the lowest energy orbital.

Chemical bonding: The interaction between atoms that involves the overlap of orbitals, leading to the formation of molecules.

Energy levels: Specific, quantised states that electrons can occupy within an atom, determined by the principal quantum number.

Nodal planes: Regions within an orbital where the probability of finding an electron is zero.

Orbital orientation: The spatial direction in which an orbital is aligned in three-dimensional space, such as px, py, and pz orbitals.

Orbital shapes: The geometric forms of orbitals, such as spherical (s), dumbbell-shaped (p), cloverleaf (d), and complex (f).

Principal quantum number (n): A quantum number that indicates the main energy level of an electron in an atom.

Quantum numbers: A set of values (n, l, m, s) that define the state of an electron, including its energy, shape, orientation, and spin.

Quantum state: The condition of an electron in an atom, defined by its quantum numbers and describing its energy and position.

Sigma bond: A type of chemical bond formed by the direct overlap of orbitals along the axis connecting two nuclei.

Pi bond: A type of chemical bond formed by the sideways overlap of p orbitals, usually accompanying a sigma bond in double or triple bonds.

Spin quantum number (s): A quantum number that describes the intrinsic spin of an electron, which can be either +½ or −½.

Concept Check Questions [Series 1]

Objective Questions

Which set of values defines the condition of an electron in an atom?
A. Atomic numbers
B. Quantum numbers
C. Energy levels
D. Orbital indices
(Linked to SLO 1.1)

The orbital that has a spherical shape is the:
A. p orbital
B. d orbital
C. s orbital
D. f orbital
(Linked to SLO 1.2)

The regions within an orbital where the probability of finding an electron is zero are called:
A. Energy levels
B. Nodal planes
C. Shells
D. Orbitals
(Linked to SLO 1.3)

The principle that states orbitals are filled in order of increasing energy is called the:

A. Hund's rule
B. Pauli exclusion principle
C. Aufbau principle
D. Heisenberg uncertainty principle
(Linked to SLO 1.4)

The sideways overlap of p orbitals leads to the formation of:

A. Sigma bonds
B. Pi bonds
C. Ionic bonds
D. Metallic bonds
(Linked to SLO 1.3)

Short-Answer Questions

Define a quantum state and explain its significance in atomic structure.
(Linked to SLO 1.1)

Describe the shapes of s and p orbitals.
(Linked to SLO 1.2)

Explain the concept of nodal planes with an example.
(Linked to SLO 1.3)

State one factor that influences orbital energy and explain its effect.
(Linked to SLO 1.4)

Give one example of how orbital energy considerations help predict chemical behaviour.
(Linked to SLO 1.5)

Long-Answer Questions

Analyse the importance of quantum numbers in defining the state of an electron.
(Linked to SLO 1.1)

Evaluate how orbital shapes and orientations influence chemical bonding.
(Linked to SLO 1.3)

Assess the role of orbital energy considerations in predicting the chemical behaviour of elements, with examples from transition metals.
(Linked to SLO 1.5)

Answers to Concept Check Questions [Series 1]

Objective Questions

B. Quantum numbers
C. s orbital

B. Nodal planes
C. Aufbau principle
B. Pi bonds

Short-Answer Questions

A quantum state is defined by quantum numbers and describes the energy and position of an electron. It is significant because it explains atomic structure and electron arrangement.
The s orbital is spherical, while the p orbital is dumbbell-shaped.
Nodal planes are regions where the probability of finding an electron is zero, such as the plane between the lobes of a p orbital.
The principal quantum number (n) influences orbital energy, with higher values corresponding to orbitals further from the nucleus.
Orbital energy considerations explain why transition metals can form multiple oxidation states.

Long-Answer Questions

Question 1

Basic response: Quantum numbers (n, l, m, s) define the energy, shape, orientation, and spin of electrons, making each electron state unique.
Value-added response: Outstanding learners may explain how quantum numbers underpin electron configurations, periodic trends, and spectroscopic properties.

Question 2

Basic response: Orbital shapes and orientations determine how orbitals overlap, leading to sigma and pi bonds.
Value-added response: Learners may expand by discussing molecular geometry, hybridisation, and how orbital orientation influences bond strength and reactivity.

Question 3

Basic response: Orbital energy considerations explain electron configurations and chemical behaviour, such as oxidation states in transition metals.
Value-added response: Learners may elaborate with examples like the variable oxidation states of iron or copper, and how orbital energies influence catalytic activity and colour in compounds.

Answers to Pilot Questions [Series 1]

Part 1: Concept of Quantum States

Principal quantum number
Quantisation
Electronic configuration
Magnetic quantum number

Quantum states are important because they determine electron arrangement, bonding, and chemical properties.

Part 2: Atomic Orbitals

s-orbital
p-orbital
Aufbau principle
Five
Exceptions occur due to stability factors in transition metals.

Part 3: Orbital Shapes and Orientation

s-orbital
Nodal plane
Sigma bond
Three
Orbital orientation is important because it influences bonding and molecular geometry.

Part 4: Energy Considerations in Orbitals

4s orbital
Azimuthal quantum number
Ionisation energy
Aufbau principle
Orbital energy considerations help predict electronic configurations, oxidation states, and chemical reactivity.

References and Attributions [Series 1]

Textual Sources

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Levine, I. N. (2014). *Quantum Chemistry* (7th ed.). Pearson.
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IUPAC. (1997). *Compendium of Chemical Terminology (the "Gold Book")*.

Illustrations (Figures, Plates, Tables, Boxes)

Figure 1.1 Quantum numbers defining a quantum state
AI prompt: "Generate a labelled diagram showing the four quantum numbers (n, l, m, s) that define a quantum state."
Search string: "quantum numbers electron state diagram OER"

Plate 1.1 Discrete energy levels in an atom
AI prompt: "Create an image showing discrete energy levels in an atom with electron transitions."
Search string: "atomic energy levels quantisation diagram OER"

Box 1.1 Significance of quantum states in atomic structure
AI prompt: "Generate a text box summarising the significance of quantum states in atomic structure and chemical behaviour."
Search string: "quantum states atomic structure summary OER"

Figure 2.1 Representation of atomic orbitals around the nucleus
AI prompt: "Generate a labelled diagram showing atomic orbitals as regions of high electron probability around the nucleus."
Search string: "atomic orbitals electron probability diagram OER"

Table 2.1 Types of orbitals and their shapes
AI prompt: "Generate a table listing s, p, d, and f orbitals with their characteristic shapes."
Search string: "types of orbitals shapes table OER"

Figure 2.2 Orbital energy ordering
AI prompt: "Generate a labelled diagram showing orbital energy ordering according to the Aufbau principle."
Search string: "orbital energy ordering Aufbau principle diagram OER"

Figure 3.1 Visualisation of orbital shapes
AI prompt: "Generate a labelled diagram showing s, p, d, and f orbital shapes."
Search string: "atomic orbital shapes s p d f diagram OER"

Plate 3.1 Spatial orientation of p orbitals and nodal planes
AI prompt: "Create an image showing p orbitals oriented along x, y, and z axes with nodal planes."
Search string: "p orbitals orientation nodal planes diagram OER"

Box 3.1 Implications of orbital orientation for bonding
AI prompt: "Generate a text box summarising sigma and pi bond formation based on orbital overlap."
Search string: "sigma pi bond orbital overlap summary OER"

Figure 4.1 Relative energies of orbitals
AI prompt: "Generate a labelled diagram showing relative energies of orbitals (1s, 2s, 2p, 3s, 3p, 3d)."
Search string: "relative energies of orbitals diagram OER"

Table 4.1 Factors affecting orbital energy
AI prompt: "Generate a table listing principal quantum number (n) and azimuthal quantum number (l) with their effects on orbital energy."
Search string: "quantum numbers orbital energy table OER"

Box 4.1 Applications of orbital energy considerations
AI prompt: "Generate a text box summarising applications of orbital energy considerations in predicting chemical behaviour."
Search string: "orbital energy considerations chemical behaviour summary OER"

Notes on Attribution

AI-generated illustrations are documented with prompts and should be noted with the generation date and platform used.
Where OERs are used, attribution must comply with the licence terms of the source.
References are presented in APA style for consistency.

- **Course code:** CHM 214
- **Course title:** Structure and Bonding
- **Course credit load:** 2 Units (C: LH 30)
- **Series titles:**

  Quantum States, Orbitals, Shape and Energy
  Valence Theory, Electron Repulsion and Atomic Spectra
  Symmetry, Molecular Geometry and Molecular Orbital Theory
  Methods of Determining Molecular Shape, Bond Lengths and Angles
  Structure and Chemistry of Representative Main Group Compound

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Suggested Outline

Part 2.1: Fundamentals of Valence Theory

Sub-Part 2.1.1: Definition and principles of valence theory
Sub-Part 2.1.2: Application of valence theory in predicting bonding
Sub-Part 2.1.3: Limitations of valence theory

Part 2.2: Electron Repulsion Theory

Sub-Part 2.2.1: Concept of electron pair repulsion
Sub-Part 2.2.2: Valence Shell Electron Pair Repulsion (VSEPR) model
Sub-Part 2.2.3: Predicting molecular shapes using VSEPR

Part 2.3: Atomic Spectra

Sub-Part 2.3.1: Definition and types of atomic spectra
Sub-Part 2.3.2: Line spectra and their significance
Sub-Part 2.3.3: Applications of atomic spectra in chemistry

Part 2.4: Linking Theories to Chemical Behaviour

Sub-Part 2.4.1: Relationship between valence theory and molecular geometry
Sub-Part 2.4.2: Role of electron repulsion in determining stability

Sub-Part 2.4.3: Spectroscopic evidence supporting bonding theories

Introduction

Chemical bonding and atomic behaviour cannot be fully explained without considering how electrons interact and how their energies are revealed through spectra. While the previous Series introduced you to quantum states and orbitals, this Series builds on that foundation by examining valence theory, electron repulsion, and atomic spectra. These concepts are central to predicting molecular shapes, understanding bonding patterns, and interpreting the light emitted or absorbed by atoms.

The aim of this Series is to enable you to explain valence theory, apply electron repulsion concepts to predict molecular geometry, and analyse atomic spectra as evidence for electronic structure.

We shall commence this Series by exploring the fundamentals of valence theory, focusing on its principles, applications, and limitations. Next, we will move on to electron repulsion theory, where you will learn how the Valence Shell Electron Pair Repulsion (VSEPR) model predicts molecular shapes. Following that, we will examine atomic spectra, considering their types, significance, and applications in chemistry. Finally, we will bring this Series to a close by linking these theories together, showing how valence theory, electron repulsion, and spectroscopic evidence collectively explain chemical behaviour and bonding.

Series Learning Outcomes

Upon completing this Series, you should be able to:

SLO 2.1 define the principles of valence theory and explain how they are applied to predict bonding patterns,
SLO 2.2 analyse the concept of electron pair repulsion and demonstrate how the Valence Shell Electron Pair Repulsion (VSEPR) model predicts molecular shapes,
SLO 2.3 describe the types of atomic spectra and explain their significance in understanding electronic structure,
SLO 2.4 evaluate the relationship between valence theory, electron repulsion, and molecular geometry, and
SLO 2.5 apply spectroscopic evidence to support bonding theories and interpret chemical behaviour.

2.1 Fundamentals of Valence Theory

2.1.1 Definition and principles of valence theory

Valence theory is a model in chemistry that explains how atoms bond by considering the number of electrons in their outermost shell, known as valence electrons. These electrons are responsible for chemical bonding, as atoms tend to achieve stable configurations similar to noble gases. The theory is based on the principle that atoms combine to complete their valence shells, often following the **octet rule**, which states that atoms are most stable when they have eight electrons in their outer shell.

Fill in the blank: The electrons in the outermost shell of an atom that determine bonding capacity are called __________________ electrons.

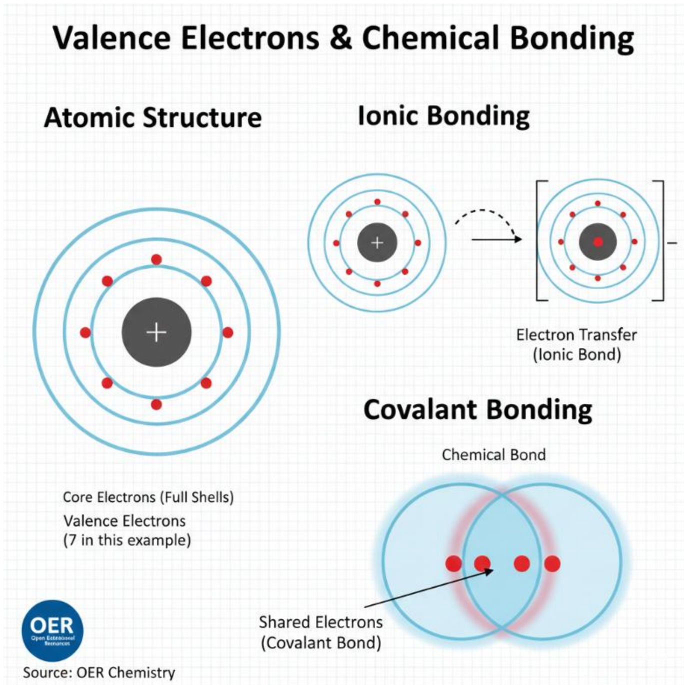

Figure 2.1: Representation of valence electrons in bonding

2.1.2 Application of valence theory in predicting bonding

Valence theory helps predict how atoms will bond to form molecules. For example, hydrogen with one valence electron bonds with oxygen, which has six valence electrons, to form water (H_2O). By sharing electrons, both atoms achieve stable configurations. This sharing of electrons leads to **covalent bonds**, while the transfer of electrons results in **ionic bonds**. Valence theory therefore provides a simple way to understand bonding patterns and molecular structures.

Fill in the blank: When atoms share electrons to achieve stability, they form __________________ bonds.

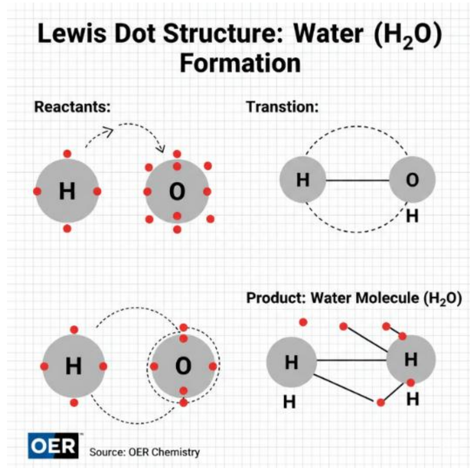

Plate 2.1: Application of valence theory in water formation

2.1.3 Limitations of valence theory

Although valence theory is useful, it has limitations. It does not fully explain the shapes of molecules or the complexities of bonding in transition metals. For example, while it predicts that carbon forms four bonds, it does not explain why these bonds are arranged tetrahedrally. To address these gaps, more advanced theories such as **Valence Shell Electron Pair Repulsion (VSEPR)** and **Molecular Orbital Theory** are used.

Fill in the blank: Valence theory cannot explain why oxygen is __________________ in nature.

Limitation	Description of Failure	Consequences in Chemistry
Molecular Shapes	Struggles to explain exact bond angles (e.g., why CH_4 is a perfect tetrahedron) using simple s and p orbitals.	Led to the "fix" of **Hybridization**, which is an extension rather than a natural part of basic VB theory.
Magnetic Properties	Predicts all electrons in molecules like O_2 are paired, suggesting they should be diamagnetic.	Fails to explain why **Liquid Oxygen** is paramagnetic (attracted to magnets), which requires unpaired electrons.
Delocalized Bonding	Views bonds as strictly between two atoms; cannot easily describe "resonance" or shared electron clouds.	Cannot accurately represent molecules like **Benzene (C_6H_6)** or the nitrate ion (NO_3^-) without complex resonance structures.
Spectroscopic Data	Cannot predict the specific energy levels needed to explain electronic absorption and emission spectra.	Makes it impossible to explain why transition metal complexes have specific **colors**.
Bond Order	Primarily deals with integer bonds (1, 2, or 3).	Cannot easily account for fractional bond orders (e.g., 1.5) found in many stable ions and molecules.

Box 2.1: Limitations of valence theory

Cannot explain molecular shapes accurately
Fails to account for magnetic properties
Does not describe delocalised bonding in complex molecules
Requires supplementation by advanced bonding theories

Pilot questions 2.1

The electrons in the outermost shell of an atom that determine bonding capacity are called:

A. Core electrons
B. Valence electrons
C. Free electrons
D. Bonding orbitals
(Linked to SLO 2.1)

When atoms share electrons to achieve stability, they form:

A. Ionic bonds
B. Covalent bonds
C. Metallic bonds
D. Hydrogen bonds
(Linked to SLO 2.1)

Which of the following is a limitation of valence theory?

A. It explains molecular shapes accurately
B. It accounts for delocalised bonding
C. It fails to explain magnetic properties
D. It predicts paramagnetism correctly
(Linked to SLO 2.1)

Give one example of a molecule where valence theory successfully explains bonding.
(Linked to SLO 2.1)

State one reason why valence theory needed to be supplemented by molecular orbital theory.
(Linked to SLO 2.1)

2.2 Electron Repulsion Theory

2.2.1 Concept of electron pair repulsion

Electron pair repulsion refers to the tendency of electron pairs around a central atom to repel each other because they carry negative charges. This repulsion influences the spatial arrangement of atoms in a molecule, as the electron pairs try to stay as far apart as possible. The concept is fundamental to understanding molecular geometry, since the positions of atoms are determined by the distribution of electron pairs around the central atom.

Fill in the blank: The tendency of electron pairs to arrange themselves as far apart as possible is called __________________.

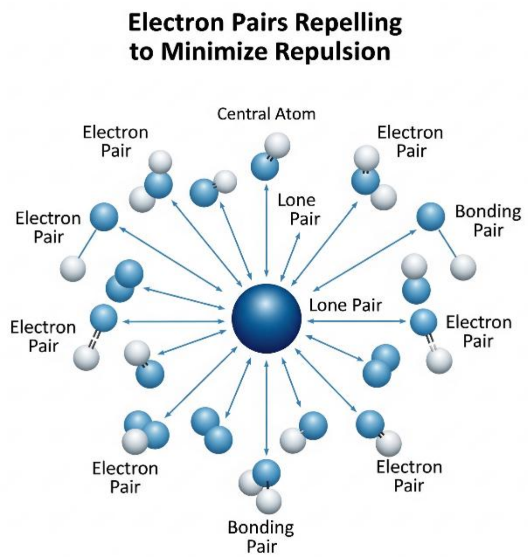

Figure 2.2: Electron pair repulsion around a central atom

2.2.2 Valence Shell Electron Pair Repulsion (VSEPR) model

The **Valence Shell Electron Pair Repulsion (VSEPR) model** is a theory used to predict the shape of molecules based on electron pair repulsion. According to this model, both bonding pairs and lone pairs of electrons around the central atom arrange themselves to minimise repulsion. For example, methane (CH_4) adopts a tetrahedral shape because its four bonding pairs are positioned as far apart as possible.

Fill in the blank: The model that predicts molecular shapes based on electron pair repulsion is called the ___________________ model.

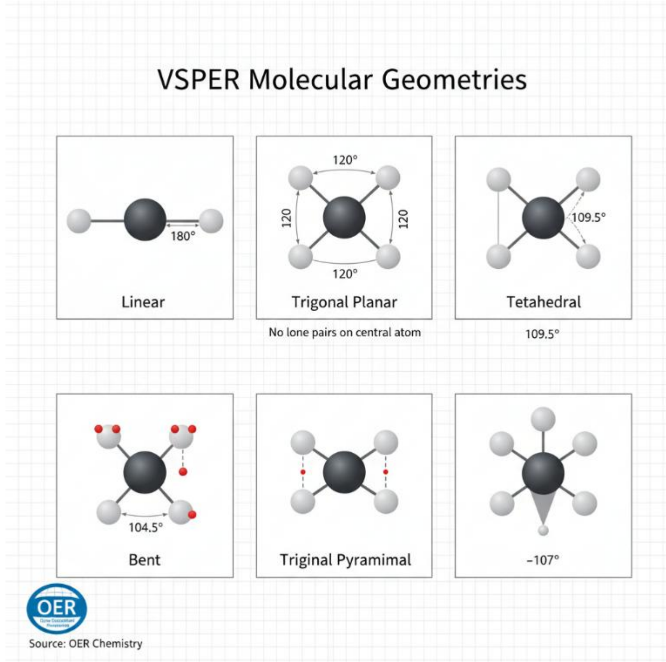

Plate 2.2: Common molecular geometries predicted by VSEPR

2.2.3 Predicting molecular shapes using VSEPR

The VSEPR model allows chemists to predict molecular shapes by counting the number of electron pairs around the central atom. For instance, two bonding pairs result in a linear shape (e.g., $BeCl_2$), three bonding pairs form a trigonal planar shape (e.g., BF_3), and four bonding pairs form a tetrahedral shape (e.g., CH_4). Lone pairs also affect geometry, as seen in water (H_2O), where two bonding pairs and two lone pairs create a bent shape.

Fill in the blank: The molecule CH_4 adopts a __________________ geometry according to the VSEPR model.

Molecular Shapes Predicted by VSEPR

Molecule	Central Atom	Electron Groups (Bonding + Lone)	Electron Geometry	Molecular Shape	Bond Angle (Approx.)
CO_2	C	2 (2 double bonds)	Linear	**Linear**	180°
CH_4	C	4 (4 single bonds)	Tetrahedral	**Tetrahedral**	109.5°
NH_3	N	4 (3 bonds + 1 lone pair)	Tetrahedral	**Trigonal Pyramidal**	107°
H_2O	O	4 (2 bonds + 2 lone pairs)	Tetrahedral	**Bent (V-shaped)**	104.5°

Box 2.2: Examples of molecular shapes predicted by VSEPR

CH_4 → tetrahedral
NH_3 → trigonal pyramidal

H_2O → bent
CO_2 → linear

Pilot questions 2.2

The tendency of electron pairs to arrange themselves as far apart as possible is called:

A. Electron affinity
B. Electron pair repulsion
C. Ionisation energy
D. Bond polarity
(Linked to SLO 2.2)

The model that predicts molecular shapes based on electron pair repulsion is called the:

A. Molecular orbital model
B. VSEPR model
C. Valence bond model
D. Hybridisation model
(Linked to SLO 2.2)

According to the VSEPR model, the geometry of methane (CH_4) is:

A. Linear
B. Bent
C. Tetrahedral
D. Trigonal planar
(Linked to SLO 2.2)

Which type of electron pair exerts stronger repulsion in the VSEPR model?

A. Bonding pair
B. Lone pair
C. Shared pair
D. Delocalised pair
(Linked to SLO 2.2)

State one reason why water (H_2O) has a bent shape according to the VSEPR model.
(Linked to SLO 2.2)

2.3 Atomic Spectra

2.3.1 Definition and types of atomic spectra

Atomic spectra are the patterns of light emitted or absorbed by atoms when their electrons move between energy levels. Each element has a unique atomic spectrum, acting like a fingerprint that identifies it. There are three main types: **emission spectra**, where atoms release light; **absorption spectra**, where atoms absorb specific wavelengths; and **continuous spectra**, which show all wavelengths without gaps.

Fill in the blank: The type of spectrum produced when electrons absorb energy to move to higher levels is called an __________________ spectrum.

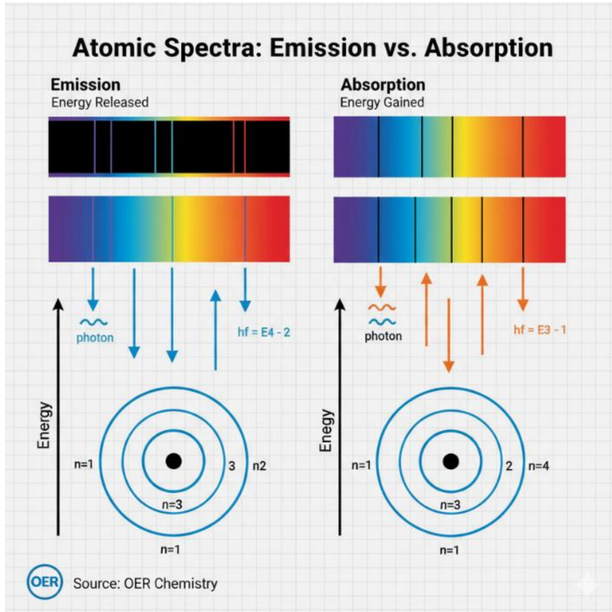

Figure 2.3: Comparison of emission and absorption spectra

2.3.2 Line spectra and their significance

A **line spectrum** is a series of distinct lines representing specific wavelengths of light emitted or absorbed by electrons transitioning between quantised energy levels. Unlike continuous spectra, line spectra are discrete and unique to each element. They are significant because they provide direct evidence of quantisation in atoms and are used to identify elements in stars and laboratory samples.

Fill in the blank: The hydrogen spectrum that shows visible lines corresponding to electron transitions is called the ____________________ series.

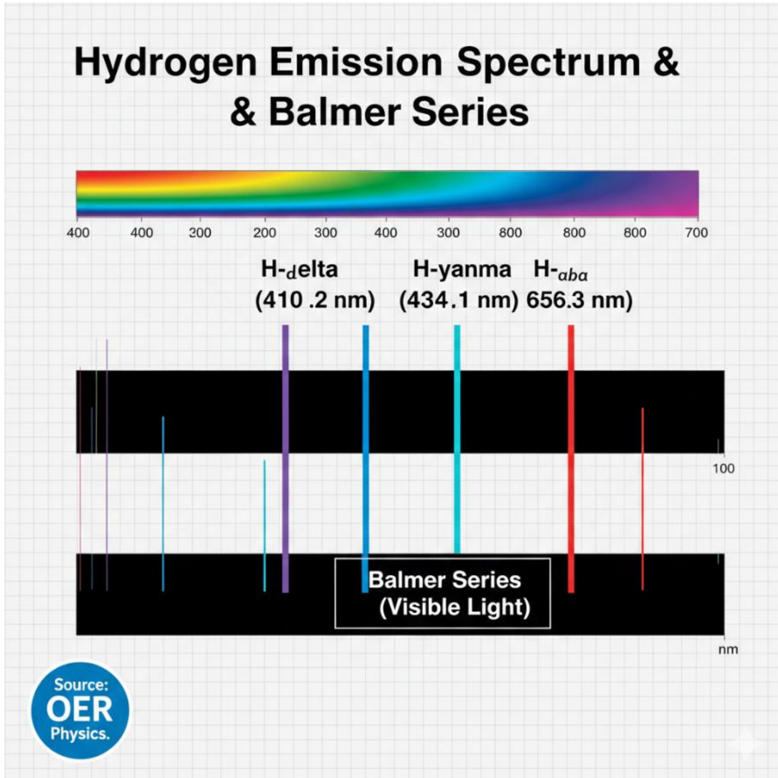

Plate 2.3: Hydrogen line spectrum (Balmer series)

2.3.3 Applications of atomic spectra in chemistry

Atomic spectra have many applications in chemistry and related sciences. They are used in **spectroscopy** to identify elements in unknown samples, in **astronomy** to determine the composition of stars, and in **quantum mechanics** to confirm theories of electron transitions. For example, the hydrogen spectrum provided crucial evidence for Bohr's model of the atom.

Fill in the blank: The study of atomic spectra to detect and measure substances is called ________________.

Applications of Atomic Spectra in Chemistry and Physics

Application	Field	Mechanism	Importance
Elemental Identification	Analytical Chemistry	Each element emits a unique set of spectral lines (Emission Spectrum).	Used in Flame Tests and ICP-OES to detect metals in soil, water, or blood.
Astrophysics/Astronomy	Physics	Analyzing light from distant stars and galaxies (Absorption Spectra).	Identified Helium in the sun before it was found on Earth; determines the composition and temperature of stars.
Validating Quantum Theory	Theoretical Physics	Discrete lines prove that energy levels in atoms are quantized.	Provided the experimental proof for the Bohr Model and later the Quantum Mechanical Model.
Chemical Bonding	Physical Chemistry	Shift in spectral lines when atoms form bonds (e.g., UV-Vis spectroscopy).	Helps determine the strength of bonds and the electronic structure of molecules.
Cosmological Redshift	Cosmology	Spectral lines of distant galaxies shifting toward longer wavelengths.	Provides evidence for the Expanding Universe and the Big Bang theory.
Forensic Science	Applied Chemistry	Trace evidence analysis (Atomic Absorption Spectroscopy).	Detects minute amounts of poisons (like arsenic) or gunshot residue.

Box 2.3: Applications of atomic spectra

Identifying elements in stars and galaxies
Supporting quantum theory and atomic models
Detecting substances in analytical chemistry
Explaining periodic trends and bonding behaviour

Pilot questions 2.3

The type of spectrum produced when electrons absorb energy to move to higher levels is called an:
A. Emission spectrum
B. Absorption spectrum
C. Continuous spectrum
D. Line spectrum
(Linked to SLO 2.3)

The hydrogen spectrum that shows visible lines corresponding to electron transitions is called the:
A. Lyman series
B. Balmer series
C. Paschen series
D. Brackett series
(Linked to SLO 2.3)

Which of the following is unique to each element and acts like a fingerprint?
A. Continuous spectrum
B. Line spectrum
C. Absorption spectrum
D. Infrared spectrum
(Linked to SLO 2.3)

The study of atomic spectra to detect and measure substances is called:

A. Chromatography
B. Spectroscopy
C. Photometry
D. Calorimetry
(Linked to SLO 2.3)

State one application of atomic spectra in chemistry or physics.
(Linked to SLO 2.3)

2.4 Linking Theories to Chemical Behaviour

2.4.1 Relationship between valence theory and molecular geometry

Valence theory explains how atoms bond by considering their valence electrons, but it also connects to **molecular geometry**, which describes the three-dimensional arrangement of atoms in a molecule. For example, valence theory predicts that carbon forms four bonds, while molecular geometry shows that these bonds are arranged tetrahedrally. This link helps chemists understand not only how atoms bond but also the spatial arrangement that influences reactivity and physical properties.

Fill in the blank: The three-dimensional arrangement of atoms in a molecule is called __________________.

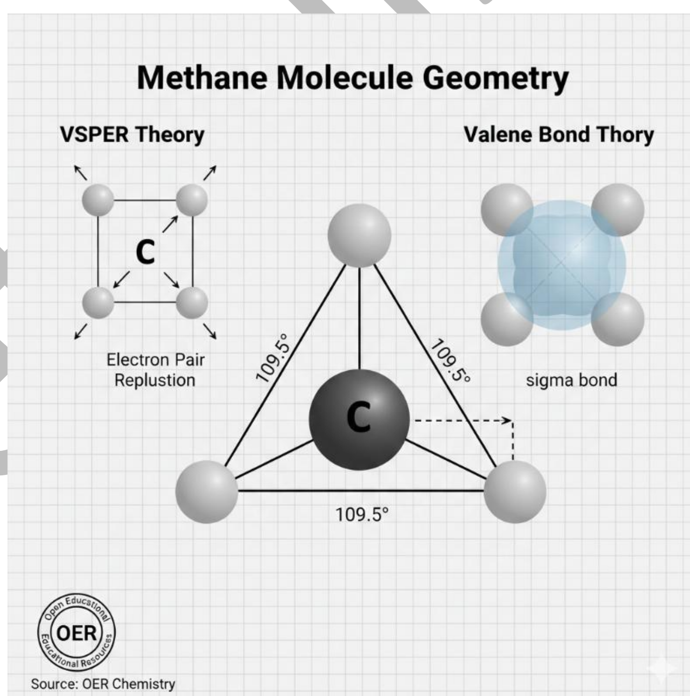

Figure 2.4: Tetrahedral geometry of methane

2.4.2 Role of electron repulsion in determining stability

Electron repulsion plays a key role in determining the stability of molecules. According to the VSEPR model, electron pairs arrange themselves to minimise repulsion, which leads to stable molecular shapes. For instance, water adopts a bent shape because its two lone pairs push the bonding pairs closer together. This repulsion not only influences geometry but also affects bond angles, polarity, and intermolecular interactions.

Fill in the blank: Lone pairs exert stronger __________________ than bonding pairs, leading to distortions in molecular shape.

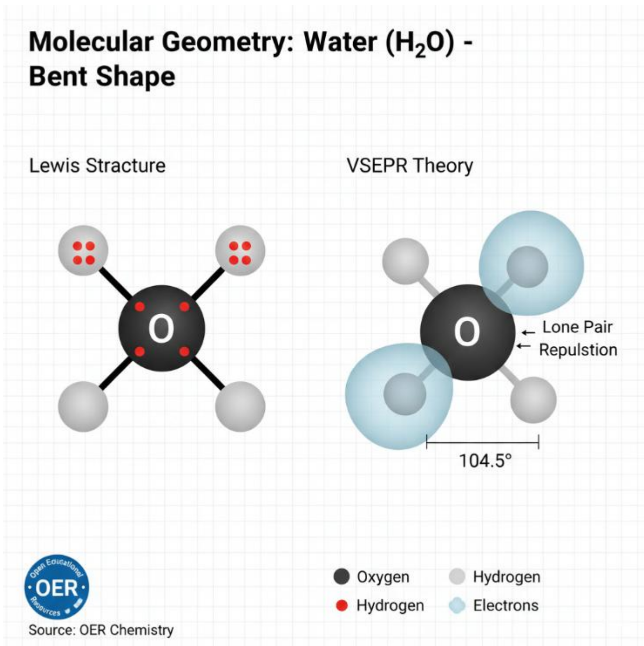

Plate 2.4: Bent geometry of water molecule explained by electron repulsion

2.4.3 Spectroscopic evidence supporting bonding theories

Spectroscopic evidence provides experimental support for bonding theories. Atomic spectra, particularly line spectra, confirm that electrons occupy quantised energy levels, which underpins valence theory and molecular orbital theory. For example, the hydrogen emission spectrum validated Bohr's model, while modern spectroscopy continues to support quantum mechanical descriptions of bonding. Spectroscopy therefore bridges theoretical predictions with observable data, strengthening our understanding of chemical behaviour.

Fill in the blank: Experimental evidence for quantised energy levels and bonding theories is provided by __________________.

Spectroscopic Evidence Supporting Bonding Theories

Evidence Type	Bonding Theory Supported	Observed Phenomenon	Conclusion
Hydrogen Line Spectrum	Bohr / Quantum Model	Discrete, sharp lines of light rather than a continuous rainbow.	Confirms that electrons exist in quantized energy levels (n); they cannot exist "between" states.
Photoelectron Spectroscopy (PES)	Shell Model / Aufbau	Kinetic energy of ejected electrons shows distinct "peaks" of binding energy.	Validates the existence of subshells (s, p, d, f) and their relative energy ordering.
Infrared (IR) Spectroscopy	Valence Bond Theory	Specific frequencies of light cause bonds to stretch and bend.	Confirms that bonds have specific strengths and stiffness (force constants), behaving like quantized springs.
Microwave Spectroscopy	VSEPR / Molecular Geometry	Rotational transitions depend on the molecule's moment of inertia.	Provides precise measurements of bond lengths and bond angles, validating VSEPR shape predictions.
UV-Visible Spectroscopy	Molecular Orbital (MO) Theory	Absorption of light during transitions between HOMO and LUMO.	Confirms the existence of delocalized orbitals and the energy gap between bonding and antibonding states.
X-ray Crystallography	Lattice/Crystal Theory	Diffraction patterns produced by X-rays hitting a solid crystal.	Directly maps the 3D position of atoms and electron density in a crystal lattice.

Box 2.4: Spectroscopic evidence supporting bonding theories

Hydrogen line spectrum confirms quantised energy levels
Spectroscopy validates predictions of valence theory
Spectroscopic data support molecular geometry models
Bond strengths and periodic trends explained through spectra

Pilot questions 2.4

The three-dimensional arrangement of atoms in a molecule is called:
- A. Molecular geometry
- B. Bond angle
- C. Orbital orientation
- D. Electron configuration

(Linked to SLO 2.4)

Lone pairs exert stronger __________ than bonding pairs, leading to distortions in molecular shape.
- A. Attraction
- B. Repulsion
- C. Bonding
- D. Stability

(Linked to SLO 2.4)

Experimental evidence for quantised energy levels and bonding theories is provided by:
- A. Chromatography
- B. Spectroscopy
- C. Calorimetry
- D. Photometry

(Linked to SLO 2.5)

Why does water have a bent shape according to electron repulsion theory?
(Linked to SLO 2.4)

State one way spectroscopy supports bonding theories.
(Linked to SLO 2.5)

Series Summary

Series Summary

This Series on **Valence Theory, Electron Repulsion and Atomic Spectra** was designed to show how fundamental bonding theories connect with molecular geometry and observable chemical behaviour. You began by exploring the principles of valence theory, learning how valence electrons determine bonding patterns and why the theory has certain limitations. Building on this, you studied electron repulsion and the VSEPR model, which explains how electron pairs arrange themselves to minimise repulsion and thereby predict molecular shapes. You then examined atomic spectra, focusing on line spectra as evidence of quantised energy levels, before finally linking these theories together to understand how bonding, geometry, and spectroscopic data reinforce one another.

By completing this Series, you should now be able to **define valence theory and apply it to predict bonding (SLO 2.1)**, **analyse electron pair repulsion and use the VSEPR model to predict molecular shapes (SLO 2.2)**, **describe atomic spectra and explain their significance (SLO 2.3)**, **evaluate the relationship between valence theory, electron repulsion, and molecular geometry (SLO 2.4)**, and **apply spectroscopic evidence to support bonding theories and interpret chemical behaviour (SLO 2.5)**. These outcomes ensure you can connect theoretical models with experimental evidence, strengthening your understanding of how atomic and molecular structures shape chemical properties.

Glossary of Terms

Absorption spectrum: A type of atomic spectrum where atoms absorb specific wavelengths of light, leaving dark lines in the spectrum.

Atomic spectra: The unique patterns of light emitted or absorbed by atoms when electrons move between energy levels.

Bonding pairs: Pairs of electrons shared between atoms that form covalent bonds.

Covalent bond: A type of chemical bond formed when atoms share electrons to achieve stability.

Electron pair repulsion: The tendency of electron pairs around a central atom to repel each other due to their negative charges.

Emission spectrum: A type of atomic spectrum where atoms release light at specific wavelengths, producing bright lines.

Line spectrum: A series of distinct lines representing specific wavelengths of light emitted or absorbed by electrons transitioning between quantised energy levels.

Lone pairs: Pairs of electrons that are not involved in bonding but still influence molecular geometry by repelling bonding pairs.

Molecular geometry: The three-dimensional arrangement of atoms in a molecule, determined by bonding and lone pairs of electrons.

Spectroscopy: A technique used to study atomic spectra and identify elements based on the light they emit or absorb.

Spectroscopic evidence: Experimental data from atomic spectra that supports bonding theories and confirms quantised energy levels.

Valence electrons: Electrons in the outermost shell of an atom that determine how it bonds with other atoms.

Valence Shell Electron Pair Repulsion (VSEPR) model: A model used to predict molecular shapes based on the repulsion between electron pairs around a central atom.

Valence theory: A theory that explains how atoms bond by considering the number of valence electrons and their tendency to achieve stable configurations.

Concept Check Questions [Series 2]

Objective Questions

Which electrons determine how atoms bond with one another?
A. Core electrons
B. Valence electrons
C. Free electrons
D. Inner shell electrons
(Linked to SLO 2.1)

The model used to predict molecular shapes based on electron pair repulsion is called the:
A. Valence Bond model
B. VSEPR model
C. Hybridisation model
D. Molecular Orbital model
(Linked to SLO 2.2)

A series of distinct lines representing specific wavelengths of light emitted or absorbed by atoms is called a:
A. Continuous spectrum
B. Line spectrum
C. Absorption spectrum
D. Emission spectrum
(Linked to SLO 2.3)

The hydrogen emission spectrum provided crucial evidence for which model of the atom?
A. Dalton model
B. Rutherford model
C. Bohr model

D. Quantum mechanical model
(Linked to SLO 2.5)

Lone pairs of electrons influence molecular geometry by increasing:
A. Attraction between bonding pairs
B. Repulsion between bonding pairs
C. Bond strength
D. Bond length
(Linked to SLO 2.2)

Short-Answer Questions

Define valence theory and explain its importance in predicting bonding patterns.
(Linked to SLO 2.1)

Describe how the VSEPR model predicts the shape of a water molecule.
(Linked to SLO 2.2)

Explain the difference between emission spectra and absorption spectra.
(Linked to SLO 2.3)

State one limitation of valence theory in explaining molecular geometry.
(Linked to SLO 2.4)

Give one example of how spectroscopic evidence supports bonding theories.
(Linked to SLO 2.5)

Long-Answer Questions

Analyse how valence theory and molecular geometry are connected in predicting chemical behaviour.
(Linked to SLO 2.4)

Evaluate the role of electron pair repulsion in determining molecular stability, using examples.
(Linked to SLO 2.2)

Assess the significance of atomic spectra in confirming quantised energy levels and supporting bonding theories.
(Linked to SLO 2.3 & 2.5)

Answers to Concept Check Questions [Series 2]

Objective Questions

B. Valence electrons
B. VSEPR model
B. Line spectrum
C. Bohr model
B. Repulsion between bonding pairs

Short-Answer Questions

Valence theory explains bonding by considering valence electrons. It is important because it predicts how atoms combine to achieve stable configurations.

The VSEPR model predicts that water has a bent shape because two lone pairs push the two bonding pairs closer together.

Emission spectra show bright lines where atoms release light, while absorption spectra show dark lines where atoms absorb specific wavelengths.

Valence theory does not explain the three-dimensional arrangement of bonds, such as the tetrahedral shape of carbon compounds.

The hydrogen emission spectrum supports Bohr's model by showing electrons occupy quantised energy levels.

Long-Answer Questions

Question 1

Basic response: Valence theory predicts bonding patterns, while molecular geometry explains the spatial arrangement of atoms. Together, they show how atoms bond and how molecules are shaped.

Value-added response: Outstanding learners may expand by discussing hybridisation, bond angles, and how geometry influences reactivity and physical properties such as polarity.

Question 2

Basic response: Electron pair repulsion determines molecular stability by arranging electron pairs to minimise repulsion, as seen in linear, trigonal planar, and tetrahedral shapes.

Value-added response: Learners may elaborate with examples such as ammonia (NH_3), where lone pairs reduce bond angles, and explain how this affects polarity and intermolecular forces.

Question 3

Basic response: Atomic spectra confirm quantised energy levels, supporting bonding theories and models like Bohr's.

Value-added response: Learners may extend by discussing spectroscopy in astronomy to identify elements in stars, or modern quantum mechanical models that refine our understanding of electron transitions.

Answers to Pilot Questions [Series 2]

Part 2.1: Fundamentals of Valence Theory

Valence electrons
Covalent bonds
It fails to explain magnetic properties
Water (H_2O)
Because valence theory cannot explain molecular shapes or magnetic behaviour

Part 2.2: Electron Repulsion Theory

Electron pair repulsion
VSEPR model
Tetrahedral
Lone pair
Water has a bent shape because lone pairs on oxygen exert stronger repulsion than bonding pairs, pushing hydrogen atoms closer together

Part 2.3: Atomic Spectra

Absorption spectrum
Balmer series
Line spectrum
Spectroscopy
Identifying elements in stars and galaxies

Part 2.4: Linking Theories to Chemical Behaviour

Molecular geometry
Repulsion
Spectroscopy
Because lone pairs on oxygen exert stronger repulsion than bonding pairs, distorting the bond angle and giving water a bent shape
Spectroscopy confirms quantised energy levels and validates bonding theories, such as the hydrogen line spectrum supporting discrete transitions

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References and Attributions [Series 2]

Textual Sources

Atkins, P., & Friedman, R. (2011). *Molecular Quantum Mechanics* (5th ed.). Oxford University Press.
Levine, I. N. (2014). *Quantum Chemistry* (7th ed.). Pearson.
McQuarrie, D. A. (2008). *Quantum Chemistry*. University Science Books.
IUPAC. (1997). *Compendium of Chemical Terminology (the "Gold Book")*.

Illustrations (Figures, Plates, Tables, Boxes)

Figure 2.1 Representation of valence electrons in bonding
AI prompt: "Generate a labelled diagram showing valence electrons in the outermost shell of an atom and their role in bonding."
Search string: "valence electrons bonding diagram OER"

Plate 2.1 Application of valence theory in water formation
AI prompt: "Create an image showing hydrogen atoms bonding with oxygen through valence electrons to form water molecules."
Search string: "valence theory water molecule bonding OER"

Box 2.1 Limitations of valence theory
AI prompt: "Generate a table summarising the limitations of valence theory, including molecular shapes, magnetic properties, and delocalised bonding."
Search string: "limitations of valence theory chemistry OER"

Figure 2.2 Electron pair repulsion around a central atom
AI prompt: "Generate a labelled diagram showing electron pairs around a central atom repelling each other to minimise repulsion."
Search string: "electron pair repulsion diagram chemistry OER"

Plate 2.2 Common molecular geometries predicted by VSEPR
AI prompt: "Create an image showing common molecular geometries predicted by VSEPR, including linear, trigonal planar, and tetrahedral."
Search string: "VSEPR molecular geometries diagram OER"

Box 2.2 Examples of molecular shapes predicted by VSEPR
AI prompt: "Generate a table listing examples of molecules and their shapes predicted by the VSEPR model, including CH_4, NH_3, H_2O, and CO_2."
Search string: "examples of VSEPR molecular shapes OER"

Figure 2.3 Comparison of emission and absorption spectra
AI prompt: "Generate a labelled diagram comparing emission and absorption spectra with electron transitions."
Search string: "emission vs absorption spectra diagram OER"

Plate 2.3 Hydrogen line spectrum (Balmer series)
AI prompt: "Create an image showing the hydrogen line spectrum with Balmer series lines labelled."
Search string: "hydrogen line spectrum Balmer series OER"

Box 2.3 Applications of atomic spectra
AI prompt: "Generate a table summarising applications of atomic spectra in chemistry and physics, including identification of elements and spectroscopy."
Search string: "applications of atomic spectra chemistry OER"

Figure 2.4 Tetrahedral geometry of methane
AI prompt: "Generate a labelled diagram showing methane molecule with tetrahedral geometry explained by valence theory and electron repulsion."
Search string: "methane tetrahedral geometry valence VSEPR OER"

Plate 2.4 Bent geometry of water molecule explained by electron repulsion
AI prompt: "Create an image showing water molecule with bent geometry due to lone pair repulsion."
Search string: "water molecule bent geometry lone pair repulsion OER"

Box 2.4 Spectroscopic evidence supporting bonding theories
AI prompt: "Generate a table summarising spectroscopic evidence supporting bonding theories, including hydrogen line spectrum and molecular geometry validation."
Search string: "spectroscopic evidence bonding theories chemistry OER"

Notes on Attribution

AI-generated illustrations are documented with prompts and should be noted with the generation date and platform used.
Where OERs are used, attribution must comply with the licence terms of the source.
References are presented in APA style for consistency.

Course code: CHM 214

- **Course title:** Structure and Bonding
- **Course credit load:** 2 Units (C: LH 30)
- **Series titles:**

Quantum States, Orbitals, Shape and Energy
Valence Theory, Electron Repulsion and Atomic Spectra
Symmetry, Molecular Geometry and Molecular Orbital Theory
Methods of Determining Molecular Shape, Bond Lengths and Angles
Structure and Chemistry of Representative Main Group Compound

---

Suggested Outline

Part 3.1: Fundamentals of Symmetry in Chemistry

Sub-Part 3.1.1: Definition and importance of symmetry
Sub-Part 3.1.2: Symmetry elements and operations
Sub-Part 3.1.3: Applications of symmetry in molecular classification

Part 3.2: Molecular Geometry and Bonding

Sub-Part 3.2.1: Relationship between symmetry and molecular geometry
Sub-Part 3.2.2: Common molecular shapes and their symmetry properties
Sub-Part 3.2.3: Influence of geometry on chemical behaviour

Part 3.3: Introduction to Molecular Orbital Theory

Sub-Part 3.3.1: Principles of molecular orbital formation
Sub-Part 3.3.2: Bonding and antibonding orbitals
Sub-Part 3.3.3: Molecular orbital diagrams for simple diatomic molecules

Part 3.4: Linking Symmetry, Geometry, and Molecular Orbital Theory

---

Introduction

In the last Series, we explored valence theory, electron repulsion, and atomic spectra, which together provided a strong foundation for understanding how atoms bond and how their behaviour can be observed experimentally. Building on that knowledge, this Series takes you further into the structural and theoretical aspects of molecules by examining symmetry, molecular geometry, and molecular orbital theory. These concepts are central to modern chemistry, as they explain not only how molecules are shaped but also why they are stable or reactive.

The aim of this Series is to equip you with the ability to identify symmetry elements, analyse molecular geometry, and apply molecular orbital theory to explain bonding and stability. By the end, you will be able to connect these ideas to predict chemical behaviour with greater accuracy.

We shall commence this Series by introducing the fundamentals of symmetry in chemistry, including symmetry elements and operations. Next, we will move on to molecular geometry, considering how symmetry relates to common molecular shapes and their influence on bonding. Following that, we will explore molecular orbital theory, focusing on the formation of molecular orbitals, bonding and antibonding interactions, and diagrams for simple diatomic molecules. Finally, we will bring the Series to a close by linking symmetry, geometry, and molecular orbital theory together, showing how these concepts collectively explain molecular stability and reactivity.

Series Learning Outcomes

Upon completing this Series, you should be able to:

SLO 3.1 define the principles of symmetry in chemistry and identify common symmetry elements and operations,
SLO 3.2 explain how symmetry relates to molecular geometry and analyse its influence on molecular shapes,
SLO 3.3 describe the principles of molecular orbital formation and distinguish between bonding and antibonding orbitals,
SLO 3.4 construct molecular orbital diagrams for simple diatomic molecules, and
SLO 3.5 evaluate how symmetry, molecular geometry, and molecular orbital theory collectively explain molecular stability and reactivity.

3.1 Fundamentals of Symmetry in Chemistry

3.1.1 Definition and importance of symmetry

Symmetry in chemistry refers to the balanced arrangement of parts of a molecule in space. A molecule is said to possess symmetry when certain operations, such as rotation or reflection, leave it looking unchanged. Symmetry is important because it helps classify molecules, predict their physical properties, and understand how they interact in chemical reactions. For example, symmetrical molecules often have lower polarity, which influences solubility and boiling points.

Fill in the blank: The balanced arrangement of atoms or parts of a molecule in space is called __________________.

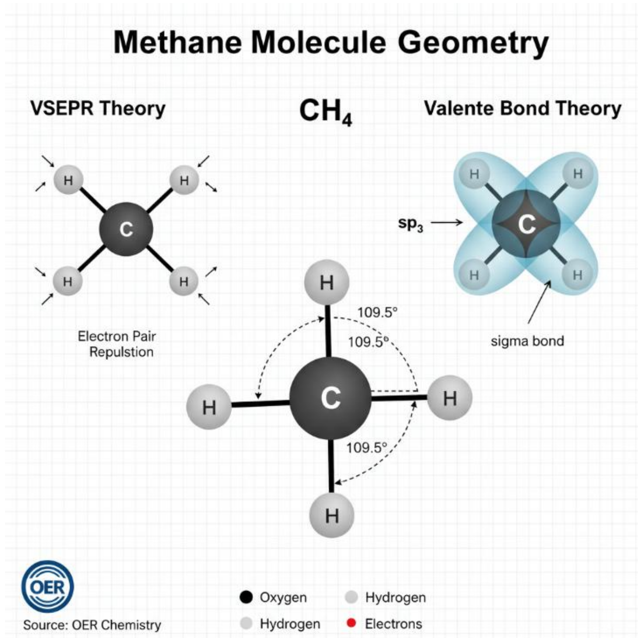

Figure 3.1: Symmetry in methane molecule

3.1.2 Symmetry elements and operations

Symmetry elements are specific features of a molecule, such as an axis, plane, or point, about which symmetry operations can be performed. **Symmetry operations** are the actions carried out, such as rotation, reflection, or inversion, that leave the molecule unchanged. Common symmetry elements include:

Axis of rotation (Cn)

Plane of symmetry (σ)

Centre of inversion (i)

Identity operation (E)

These elements and operations form the basis for classifying molecules into point groups, which are used in advanced studies of spectroscopy and molecular orbital theory.

Fill in the blank: The movement of a molecule that results in a configuration indistinguishable from the original is called a symmetry __________________.

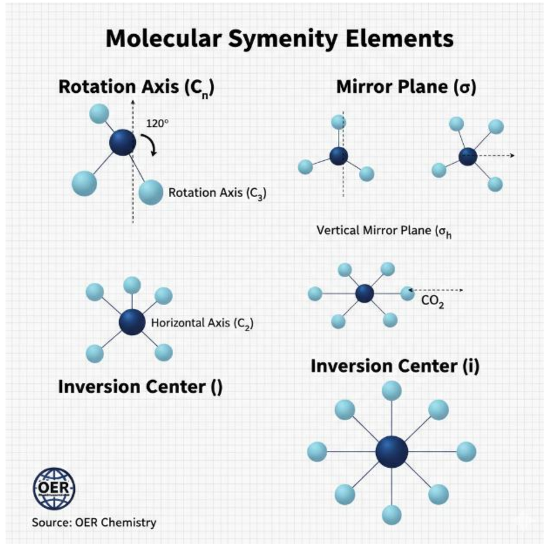

Plate 3.1: Common symmetry elements in molecules

3.1.3 Applications of symmetry in molecular classification

Symmetry is widely applied in chemistry to classify molecules into **point groups**, which are sets of symmetry elements that describe the overall symmetry of a molecule. This classification is essential in predicting molecular behaviour, such as vibrational modes in spectroscopy or orbital overlap in bonding. For instance, water belongs to the C_2v point group, while methane belongs to the Td point group. These classifications help chemists understand why molecules absorb light differently or why they adopt certain geometries.

Fill in the blank: Molecules are classified into __________________ groups based on their symmetry elements.

Molecular Point Groups for Common Molecules

Molecule	Molecular Shape	Symmetry Elements Present	Point Group
Water (H_2O)	Bent	E, one C_2 axis, two σ_v planes	C_{2v}
Ammonia (NH_3)	Trigonal Pyramidal	E, one C_3 axis, three σ_v planes	C_{3v}
Methane (CH_4)	Tetrahedral	E, eight C_3, three C_2, six S_4, six σ_d	T_d
Carbon Dioxide (CO_2)	Linear	E, C_∞, ∞ C_2, i, ∞ σ_v, σ_h	$D_{\infty h}$

Box 3.1: Examples of point groups

Water (H_2O) → C_2v
Ammonia (NH_3) → C_3v
Methane (CH_4) → Td
Carbon dioxide (CO_2) → D∞h

Pilot questions 3.1

The balanced arrangement of atoms or parts of a molecule in space is called:

A. Geometry
B. Symmetry
C. Bonding
D. Polarity
(Linked to SLO 3.1)

The movement of a molecule that results in a configuration indistinguishable from the original is called a symmetry:

A. Element
B. Operation
C. Group
D. Plane
(Linked to SLO 3.1)

Molecules are classified into __________ groups based on their symmetry elements.

A. Bond
B. Point
C. Orbital
D. Energy
(Linked to SLO 3.1)

Give one example of a molecule and its point group classification.
(Linked to SLO 3.1)

State one reason why symmetry is important in chemistry.
(Linked to SLO 3.1)

3.2 Molecular Geometry and Bonding

3.2.1 Relationship between symmetry and molecular geometry

Molecular geometry refers to the three-dimensional arrangement of atoms in a molecule. It is closely linked to **symmetry**, which describes how the molecule can be transformed without changing its overall appearance. For example, a linear molecule such as carbon dioxide (CO_2) has high symmetry because it looks the same when rotated around its axis. In contrast, water (H_2O) has a bent geometry with lower symmetry. Understanding this relationship helps chemists predict physical properties such as polarity and reactivity.

Fill in the blank: The three-dimensional arrangement of atoms in a molecule is called _________________.

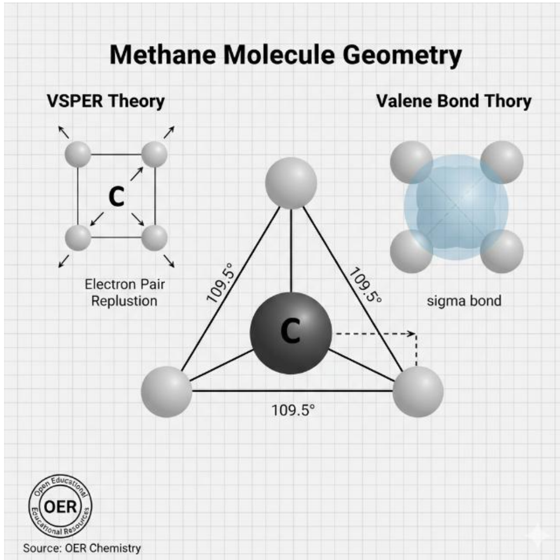

Figure 3.2: Relationship between symmetry and molecular geometry

3.2.2 Common molecular shapes and their symmetry properties

Molecules adopt common shapes such as **linear**, **trigonal planar**, **tetrahedral**, **trigonal bipyramidal**, and **octahedral**. Each shape has characteristic symmetry elements. For instance, carbon dioxide is linear and belongs to the $D_{\infty}h$ point group, while ammonia is trigonal pyramidal and belongs to the C_3v point group. Recognising these shapes and their symmetry properties helps predict molecular polarity and reactivity.

Fill in the blank: Carbon dioxide (CO_2) has a __________ geometry and belongs to the $D_{\infty}h$ point group.

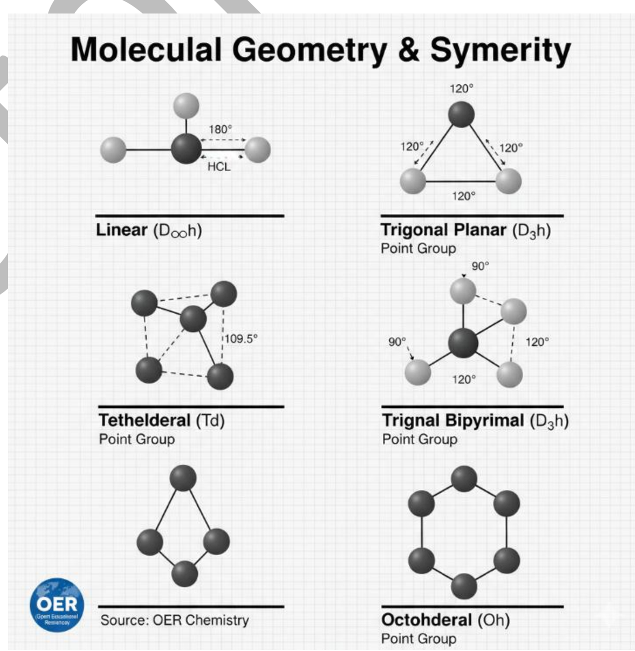

Plate 3.2: Common molecular geometries and their symmetry properties

3.2.3 Influence of geometry on chemical behaviour

The geometry of a molecule strongly influences its **chemical behaviour**. For example, the bent geometry of water makes it polar, allowing it to form hydrogen bonds and act as a universal solvent. In contrast, the linear geometry of CO_2 makes it non-polar, affecting its solubility and reactivity. Geometry also determines bond angles, which influence reaction mechanisms and stability. By linking geometry to chemical behaviour, chemists can predict how molecules will interact in different environments.

Fill in the blank: The bent geometry of water makes it ___________________, enabling hydrogen bonding.

Molecule	Molecular Geometry	Bond Polarity	Molecular Polarity	Dominant Intermolecular Force	Impact on Chemical Behavior
Water (H_2O)	**Bent** (104.5°)	Polar ($O-H$)	**Highly Polar**	Hydrogen Bonding	High boiling point; excellent solvent for ionic salts.
Carbon Dioxide (CO_2)	**Linear** (180°)	Polar ($C=O$)	**Non-Polar**	London Dispersion	Gas at room temperature; sublimes at $-78°C$.
Ammonia (NH_3)	**Trigonal Pyramidal**	Polar ($N-H$)	**Polar**	Hydrogen Bonding	Highly soluble in water; acts as a weak base.
Methane (CH_4)	**Tetrahedral**	Weakly Polar ($C-H$)	**Non-Polar**	London Dispersion	Highly flammable gas; insoluble in water.

Box 3.2: Influence of geometry on chemical behaviour

Water (H_2O): bent geometry → polar → hydrogen bonding
Carbon dioxide (CO_2): linear geometry → non-polar → weak intermolecular forces
Ammonia (NH_3): trigonal pyramidal geometry → polar → strong intermolecular interactions

Pilot questions 3.2

The three-dimensional arrangement of atoms in a molecule is called:
A. Symmetry
B. Molecular geometry
C. Bonding
D. Polarity
(Linked to SLO 3.2)

Carbon dioxide (CO_2) has a ___________ geometry and belongs to the $D_{\infty h}$ point group.
A. Bent
B. Linear
C. Tetrahedral
D. Trigonal planar
(Linked to SLO 3.2)

The bent geometry of water makes it ___________, enabling hydrogen bonding.
A. Non-polar

B. Polar
C. Symmetrical
D. Linear
(Linked to SLO 3.2, SLO 3.4)

Give one example of a molecule with tetrahedral geometry and state its symmetry classification.
(Linked to SLO 3.2)

Explain how molecular geometry influences chemical behaviour, using water or carbon dioxide as an example.
(Linked to SLO 3.2, SLO 3.4)

3.3 Introduction to Molecular Orbital Theory

3.3.1 Principles of molecular orbital formation

Molecular orbital theory (MOT) explains bonding by considering how atomic orbitals combine to form molecular orbitals that extend over the entire molecule. When atoms approach each other, their atomic orbitals overlap, producing new orbitals that can accommodate electrons. These molecular orbitals are classified as either **bonding orbitals**, which stabilise the molecule, or **antibonding orbitals**, which destabilise it. MOT provides a more accurate description of bonding than valence bond theory, especially for molecules with delocalised electrons.

Fill in the blank: When two atomic orbitals overlap constructively, they form a __________________ orbital.

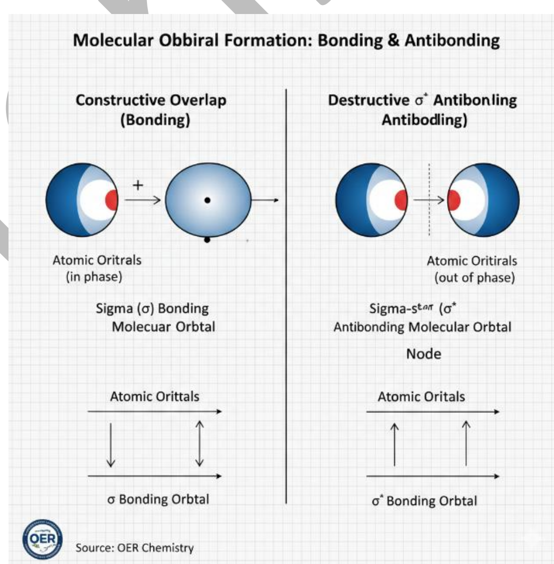

Figure 3.3: Formation of bonding and antibonding molecular orbitals

3.3.2 Bonding and antibonding orbitals

Bonding orbitals are molecular orbitals formed when atomic orbitals overlap constructively, leading to increased electron density between the nuclei. This stabilises the molecule and lowers its energy. In contrast, **antibonding orbitals** result from destructive overlap, where electron density is reduced between the nuclei, raising the energy and destabilising the molecule. The relative occupancy of bonding and antibonding orbitals determines whether a molecule is stable.

Fill in the blank: The relative number of electrons in bonding and antibonding orbitals determines the ___________________ of a molecule.

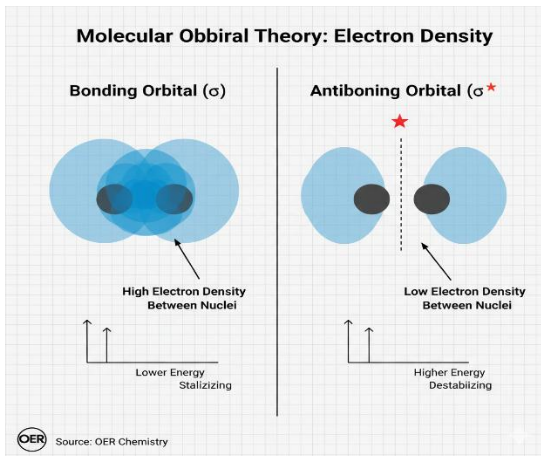

Plate 3.3: Bonding and antibonding orbital electron density

3.3.3 Molecular orbital diagrams for simple diatomic molecules

Molecular orbital diagrams are visual representations that show the relative energy levels of molecular orbitals formed from atomic orbitals. For simple diatomic molecules such as H_2, O_2, and N_2, these diagrams help explain bond order, stability, and magnetic properties. For example, oxygen's molecular orbital diagram shows unpaired electrons in antibonding orbitals, explaining why O_2 is paramagnetic. Bond order is calculated as half the difference between the number of electrons in bonding and antibonding orbitals.

Fill in the blank: The molecular orbital diagram of oxygen explains its ___________________ property.

Molecular Orbital Comparison for H_2, N_2, and O_2

Molecule	Valence Electron Config.	Bond Order	Magnetic Property	Chemical Characteristic
H_2	$(\sigma_{1s})^2$	1	**Diamagnetic** (all paired)	Simple single bond; stable under standard conditions.
N_2	$(\sigma_{2s})^2(\sigma^*_{2s})^2(\pi_{2p})^4(\sigma_{2p})^2$	3	**Diamagnetic** (all paired)	Extremely strong triple bond; very inert and stable.
O_2	$(\sigma_{2s})^2(\sigma^*_{2s})^2(\sigma_{2p})^2(\pi_{2p})^4(\pi^*_{2p})^2$	2	**Paramagnetic** (2 unpaired)	Double bond; highly reactive; attracted to magnetic fields.

Box 3.3: Examples of molecular orbital diagrams

H_2 → bond order = 1 → stable molecule
N_2 → bond order = 3 → strong triple bond
O_2 → bond order = 2 → paramagnetic behaviour

Pilot questions 3.3

When two atomic orbitals overlap constructively, they form a __________ orbital.

A. Antibonding
B. Bonding
C. Hybrid
D. Lone pair
(Linked to SLO 3.3)

The relative number of electrons in bonding and antibonding orbitals determines the __________ of a molecule.

A. Bond order
B. Bond length
C. Bond angle
D. Bond polarity
(Linked to SLO 3.3)

The molecular orbital diagram of oxygen explains its __________ property.

A. Non-polarity
B. Paramagnetism
C. Symmetry
D. Polarity
(Linked to SLO 3.4)

Give one example of a molecule and its bond order as predicted by molecular orbital theory.

(Linked to SLO 3.4)

Explain the difference between bonding and antibonding orbitals in terms of electron density. (Linked to SLO 3.3)

3.4 Linking Symmetry, Geometry, and Molecular Orbital Theory

3.4.1 How symmetry influences orbital overlap

Orbital overlap refers to the way atomic orbitals combine to form molecular orbitals. **Symmetry** plays a crucial role because only orbitals with compatible symmetry can overlap effectively. For example, in diatomic molecules, the overlap of s-orbitals is always symmetrical, while p-orbitals must align along the same axis to form strong bonds. If symmetry does not match, overlap is weak or forbidden, which influences bond strength and molecular stability.

Fill in the blank: Only orbitals with compatible ___________________ can overlap effectively to form strong bonds.

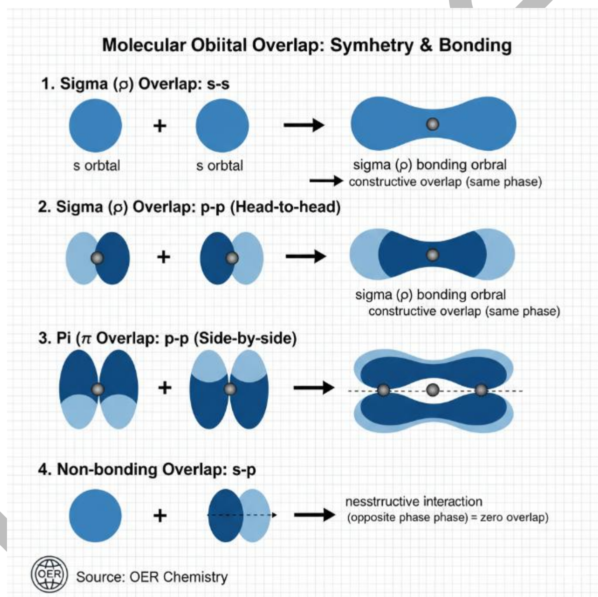

Figure 3.4: Symmetry and orbital overlap

3.4.2 Predicting stability and reactivity using molecular orbital theory

Molecular orbital theory (MOT) allows chemists to predict the stability and reactivity of molecules by examining the distribution of electrons in bonding and antibonding orbitals. The **bond order**, calculated as half the difference between bonding and antibonding electrons, indicates stability. A higher bond order means stronger and more stable bonds, while a bond order of zero suggests instability. MOT also explains reactivity, as molecules with electrons in antibonding orbitals are more reactive.

Fill in the blank: A higher ___________________ indicates greater stability in molecular orbital theory.

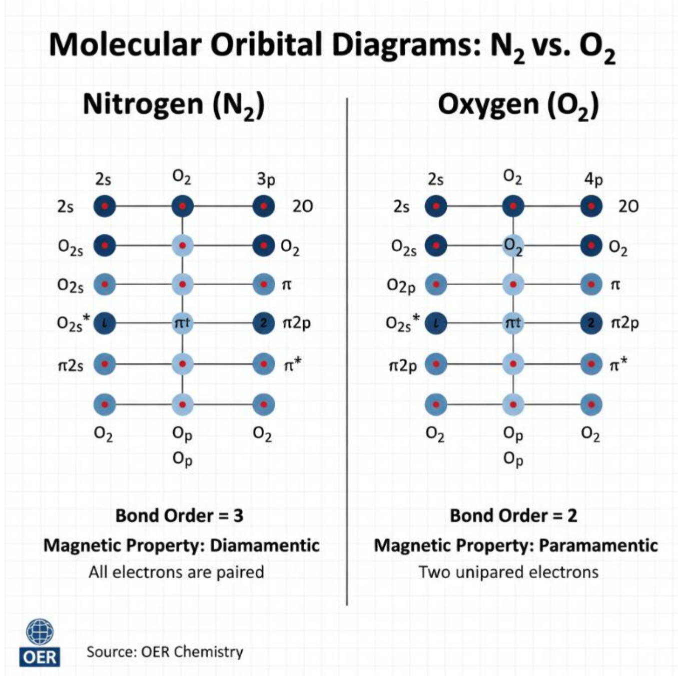

Plate 3.4: Predicting stability and reactivity using molecular orbital theory

3.4.3 Case studies connecting symmetry, geometry, and orbital theory

Case studies highlight how symmetry, geometry, and molecular orbital theory work together to explain chemical behaviour. For example:

Water (H_2O): Its bent geometry and C_2v symmetry influence orbital overlap, leading to polar bonds and hydrogen bonding.

Methane (CH_4): Its tetrahedral geometry and Td symmetry allow effective overlap of sp^3 hybrid orbitals, explaining its stability.

Oxygen (O_2): MOT shows unpaired electrons in antibonding orbitals, explaining its paramagnetism, while its linear geometry and symmetry elements support orbital overlap.

These examples demonstrate how combining symmetry, geometry, and MOT provides a complete picture of molecular properties.

Fill in the blank: The paramagnetism of oxygen is explained by __________________ orbital theory.

Case Studies: Linking Symmetry, Geometry, and MO Theory

Molecule	Point Group (Symmetry)	Molecular Geometry	MO Theory Insight	Chemical/Physical Outcome
Water (H_2O)	C_{2v}	**Bent** (104.5°)	The $2s$ and $2p$ orbitals of Oxygen hybridize and mix with Hydrogen $1s$ orbitals.	**Highly Polar:** The C_{2v} symmetry does not cancel bond dipoles, leading to a net dipole and hydrogen bonding.
Carbon Dioxide (CO_2)	$D_{\infty h}$	**Linear** (180°)	Overlap of C and O orbitals creates two sets of degenerate π bonds.	**Non-Polar:** The $D_{\infty h}$ symmetry includes a center of inversion (i); the polar $C=O$ vectors perfectly cancel out.
Oxygen (O_2)	$D_{\infty h}$	**Linear** (Diatomic)	The highest occupied orbitals are two π^* **antibonding** orbitals, each holding one electron.	**Paramagnetism:** MO theory correctly predicts two unpaired electrons, explaining why liquid O_2 is magnetic.

Box 3.4: Case studies linking symmetry, geometry, and orbital theory

Water (H_2O): bent geometry → polarity explained by symmetry and geometry
Carbon dioxide (CO_2): linear geometry → non-polar behaviour explained by symmetry
Oxygen (O_2): molecular orbital diagram → paramagnetism explained by unpaired electrons

Pilot questions 3.4

Only orbitals with compatible __________ can overlap effectively to form strong bonds.
A. Energy
B. Symmetry
C. Polarity
D. Geometry
(Linked to SLO 3.5)

A higher __________ indicates greater stability in molecular orbital theory.
A. Bond angle
B. Bond order
C. Bond length
D. Bond polarity
(Linked to SLO 3.5)

The paramagnetism of oxygen is explained by __________ orbital theory.
A. Valence
B. Hybridisation
C. Molecular
D. Symmetry
(Linked to SLO 3.5)

Give one example of a molecule where symmetry and geometry explain polarity.
(Linked to SLO 3.2, SLO 3.5)

Explain how molecular orbital theory accounts for the stability of nitrogen compared to oxygen.
(Linked to SLO 3.3, SLO 3.5)

Series Summary

This Series on **Symmetry, Molecular Geometry and Molecular Orbital Theory** was designed to help you connect fundamental concepts of molecular structure with the theories that explain chemical behaviour. You began by exploring the principles of symmetry, learning about symmetry elements and operations, and how they are applied in molecular classification. Building on this, you studied molecular geometry, examining common shapes, their symmetry properties, and how geometry influences chemical behaviour. You then moved into molecular orbital theory, where you learned how atomic orbitals combine to form molecular orbitals, distinguished between bonding and antibonding orbitals, and constructed diagrams for simple diatomic molecules. Finally, you integrated these ideas by linking symmetry, geometry, and orbital theory to explain stability, reactivity, and observable properties through case studies.

By completing this Series, you should now be able to **define symmetry and identify its elements (SLO 3.1)**, **explain the relationship between symmetry and molecular geometry (SLO 3.2)**, **describe molecular orbital formation and distinguish bonding from antibonding orbitals (SLO 3.3)**, **construct molecular orbital diagrams for simple diatomic molecules (SLO 3.4)**, and **evaluate how symmetry, geometry, and molecular orbital theory collectively explain molecular stability and reactivity (SLO 3.5)**. These outcomes ensure you can connect theoretical models with experimental evidence, giving you a comprehensive understanding of how molecular structure governs chemical properties.

Glossary of Terms

Antibonding orbitals: Molecular orbitals formed when atomic orbitals overlap destructively, reducing electron density between nuclei and destabilising the molecule.

Bonding orbitals: Molecular orbitals formed when atomic orbitals overlap constructively, increasing electron density between nuclei and stabilising the molecule.

Bond order: A measure of bond strength calculated as half the difference between the number of electrons in bonding and antibonding orbitals.

Molecular geometry: The three-dimensional arrangement of atoms in a molecule, determined by bonding and lone pairs of electrons.

Molecular orbital diagrams: Visual representations showing the relative energy levels of molecular orbitals formed from atomic orbitals, used to explain bond order and magnetic properties.

Molecular orbital theory (MOT): A theory that explains bonding by considering how atomic orbitals combine to form molecular orbitals that extend over the entire molecule.

Orbital overlap: The interaction of atomic orbitals that leads to the formation of molecular orbitals, influenced by symmetry and geometry.

Point group: A classification system that groups molecules based on their symmetry elements, used in spectroscopy and bonding studies.

Symmetry: The balanced arrangement of parts of a molecule in space, where certain operations such as rotation or reflection leave the molecule unchanged.

Symmetry elements: Features of a molecule, such as an axis, plane, or point, about which symmetry operations can be performed.

Symmetry operations: Actions such as rotation, reflection, or inversion that leave a molecule unchanged.

Concept Check Questions [Series 3]

Objective Questions

Which of the following is a symmetry operation that leaves a molecule unchanged?
A. Rotation
B. Translation
C. Expansion
D. Compression
(Linked to SLO 3.1)

Methane (CH_4) belongs to which point group due to its tetrahedral symmetry?
A. C_2v
B. Td
C. D∞h
D. C_3v
(Linked to SLO 3.2)

Constructive overlap of atomic orbitals produces:
A. Antibonding orbitals
B. Bonding orbitals
C. Hybrid orbitals
D. Core orbitals
(Linked to SLO 3.3)

The bond order of a molecule is calculated as half the difference between electrons in:
A. Core and valence orbitals
B. Bonding and antibonding orbitals
C. s and p orbitals
D. Inner and outer orbitals
(Linked to SLO 3.4)

The paramagnetism of oxygen (O_2) is explained by the presence of unpaired electrons in:
A. Bonding orbitals
B. Antibonding orbitals
C. Hybrid orbitals
D. Core orbitals
(Linked to SLO 3.5)

Short-Answer Questions

Define symmetry in chemistry and explain why it is important.
(Linked to SLO 3.1)

Describe how molecular geometry influences the polarity of water compared with carbon dioxide.
(Linked to SLO 3.2)

Explain the difference between bonding and antibonding orbitals.
(Linked to SLO 3.3)

Construct the molecular orbital diagram for nitrogen (N_2) and state its bond order.
(Linked to SLO 3.4)

Give one example of how symmetry influences orbital overlap in diatomic molecules.
(Linked to SLO 3.5)

Long-Answer Questions

Analyse how symmetry and molecular geometry together explain the chemical behaviour of water and methane.
(Linked to SLO 3.2 & 3.5)

Evaluate the role of molecular orbital theory in predicting stability and reactivity, using oxygen (O_2) as a case study.
(Linked to SLO 3.4 & 3.5)

Assess how symmetry, geometry, and molecular orbital theory collectively provide a complete picture of molecular properties, using case studies of water, methane, and oxygen.
(Linked to SLO 3.5)

Answers to Concept Check Questions [Series 3]

Objective Questions

A. Rotation
B. Td
B. Bonding orbitals
B. Bonding and antibonding orbitals
B. Antibonding orbitals

Short-Answer Questions

Symmetry in chemistry is the balanced arrangement of parts of a molecule where certain operations leave it unchanged. It is important because it helps classify molecules and predict their properties.

Water's bent geometry makes it polar, allowing hydrogen bonding, while carbon dioxide's linear geometry makes it non-polar.

Bonding orbitals stabilise molecules through constructive overlap, while antibonding orbitals destabilise them through destructive overlap.
The molecular orbital diagram for N_2 shows a bond order of 3, explaining its strong triple bond.
In diatomic molecules, only orbitals with compatible symmetry, such as s and p orbitals aligned along the bond axis, can overlap effectively.

Long-Answer Questions

Question 1

Basic response: Symmetry and geometry explain water's polarity and methane's stability. Water's bent geometry and C_2v symmetry lead to hydrogen bonding, while methane's tetrahedral geometry and Td symmetry allow strong sp^3 orbital overlap.
Value-added response: Outstanding learners may expand by discussing how these properties influence solubility, boiling points, and reactivity in organic and inorganic chemistry.

Question 2

Basic response: Molecular orbital theory explains oxygen's paramagnetism due to unpaired electrons in antibonding orbitals, and predicts its bond order of 2.
Value-added response: Learners may extend by linking this to oxygen's role in combustion and biological processes, showing how MOT connects theory with real-world behaviour.

Question 3

Basic response: Symmetry, geometry, and MOT together explain molecular properties. Water's bent geometry explains polarity, methane's tetrahedral geometry explains stability, and oxygen's MOT diagram explains paramagnetism.
Value-added response: Learners may expand by discussing how these theories are applied in spectroscopy, quantum chemistry, and materials science, demonstrating their broader relevance.

Answers to Pilot Questions [Series 3]

Part 3.1: Fundamentals of Symmetry in Chemistry

Symmetry
Operation
Point
Water (H_2O) → C_2v
Symmetry helps classify molecules, predict properties, and explain chemical behaviour

Part 3.2: Molecular Geometry and Bonding

Molecular geometry
Linear
Polar

Methane (CH_4) → Td
Water's bent geometry makes it polar and enables hydrogen bonding, while carbon dioxide's linear geometry makes it non-polar

Part 3.3: Introduction to Molecular Orbital Theory

Bonding
Bond order
Paramagnetism
Nitrogen (N_2) → bond order = 3
Bonding orbitals concentrate electron density between nuclei, while antibonding orbitals reduce electron density between nuclei

Part 3.4: Linking Symmetry, Geometry, and Molecular Orbital Theory

Symmetry
Bond order
Molecular
Water (H_2O) → bent geometry explains polarity
Nitrogen is stable due to a bond order of 3, while oxygen is less stable and paramagnetic due to unpaired electrons in antibonding orbitals

---

References and Attributions [Series 3]

Textual Sources

Atkins, P., & Friedman, R. (2011). *Molecular Quantum Mechanics* (5th ed.). Oxford University Press.
Levine, I. N. (2014). *Quantum Chemistry* (7th ed.). Pearson.
McQuarrie, D. A. (2008). *Quantum Chemistry*. University Science Books.
IUPAC. (1997). *Compendium of Chemical Terminology (the "Gold Book")*.

Illustrations (Figures, Plates, Tables, Boxes)

Figure 3.1 Symmetry in methane molecule
AI prompt: "Generate a labelled diagram showing the symmetrical tetrahedral structure of methane with equal bond angles."
Search string: "methane molecule symmetry diagram OER"

Plate 3.1 Common symmetry elements in molecules
AI prompt: "Create an image showing examples of symmetry elements in molecules, including mirror plane and rotation axis."
Search string: "symmetry elements in molecules diagram OER"

Box 3.1 Examples of point groups
AI prompt: "Generate a table listing examples of molecules and their point groups, including H_2O, NH_3, CH_4, and CO_2."
Search string: "examples of molecular point groups chemistry OER"

Figure 3.2 Relationship between symmetry and molecular geometry
AI prompt: "Generate a labelled diagram comparing methane with tetrahedral symmetry and water with bent geometry."
Search string: "molecular geometry symmetry methane water OER"

Plate 3.2 Common molecular geometries and their symmetry properties
AI prompt: "Create an image showing common molecular geometries such as linear, trigonal planar, tetrahedral, trigonal bipyramidal, and octahedral with symmetry labels."
Search string: "common molecular geometries symmetry chemistry OER"

Box 3.2 Influence of geometry on chemical behaviour
AI prompt: "Generate a table summarising how molecular geometry influences polarity and chemical behaviour, including H_2O, CO_2, and NH_3."
Search string: "molecular geometry polarity chemical behaviour OER"

Figure 3.3 Formation of bonding and antibonding molecular orbitals
AI prompt: "Generate a labelled diagram showing constructive overlap forming bonding orbitals and destructive overlap forming antibonding orbitals."
Search string: "bonding and antibonding molecular orbitals diagram OER"

Plate 3.3 Bonding and antibonding orbital electron density
AI prompt: "Create an image showing electron density distribution in bonding orbitals (between nuclei) and antibonding orbitals (outside nuclei)."
Search string: "bonding vs antibonding orbital electron density OER"

Box 3.3 Examples of molecular orbital diagrams
AI prompt: "Generate a table summarising molecular orbital diagrams for H_2, N_2, and O_2, including bond order and magnetic properties."
Search string: "molecular orbital diagrams H2 N2 O2 OER"

Figure 3.4 Symmetry and orbital overlap
AI prompt: "Generate a labelled diagram showing orbital overlap with symmetry compatibility, including s-s and p-p overlap."
Search string: "symmetry orbital overlap chemistry diagram OER"

Plate 3.4 Predicting stability and reactivity using molecular orbital theory
AI prompt: "Create an image showing molecular orbital diagrams for N_2 and O_2 with bond orders and magnetic properties indicated."
Search string: "molecular orbital diagrams N2 O2 bond order OER"

Box 3.4 Case studies linking symmetry, geometry, and orbital theory
AI prompt: "Generate a table summarising case studies linking symmetry, geometry, and molecular orbital theory, including H_2O, CO_2, and O_2."
Search string: "case studies symmetry geometry molecular orbital theory OER"

Notes on Attribution

AI-generated illustrations are documented with prompts and should be noted with the generation date and platform used.
Where OERs are used, attribution must comply with the licence terms of the source.

References are presented in APA style for consistency.

Course code: CHM 214

- **Course title:** Structure and Bonding
- **Course credit load:** 2 Units (C: LH 30)
- **Series titles:**

  Quantum States, Orbitals, Shape and Energy
  Valence Theory, Electron Repulsion and Atomic Spectra
  Symmetry, Molecular Geometry and Molecular Orbital Theory
  Methods of Determining Molecular Shape, Bond Lengths and Angles
  Structure and Chemistry of Representative Main Group Compound

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Suggested Outline

Part 4.1: Theoretical Approaches to Determining Molecular Shape

Sub-Part 4.1.1: Valence Shell Electron Pair Repulsion (VSEPR) model
Sub-Part 4.1.2: Limitations of theoretical models
Sub-Part 4.1.3: Role of hybridisation in predicting shapes

Part 4.2: Experimental Methods for Determining Molecular Geometry

Sub-Part 4.2.1: X-ray crystallography
Sub-Part 4.2.2: Electron diffraction
Sub-Part 4.2.3: Spectroscopic techniques (infrared and Raman)

Part 4.3: Determination of Bond Lengths

Sub-Part 4.3.1: Definition and significance of bond length
Sub-Part 4.3.2: Experimental measurement methods
Sub-Part 4.3.3: Factors affecting bond length (bond order, electronegativity, resonance)

Part 4.4: Determination of Bond Angles

Sub-Part 4.4.1: Definition and importance of bond angles
Sub-Part 4.4.2: Experimental measurement methods
Sub-Part 4.4.3: Influence of lone pairs and multiple bonds on bond angles

Introduction

In the last Series, we explored symmetry, molecular geometry, and molecular orbital theory, which together provided a framework for understanding how molecules are structured and why they behave in particular ways. Building on that foundation, this Series focuses on the practical methods used to determine molecular shape, bond lengths, and bond angles. These measurements are essential in chemistry because they provide direct evidence of molecular structure and help validate theoretical models.

The aim of this Series is to equip you with knowledge of both theoretical and experimental approaches to determining molecular geometry, bond lengths, and bond angles. By the end, you will be able to explain how these methods are applied, interpret their results, and appreciate their significance in predicting chemical behaviour.

We shall commence this Series by examining theoretical approaches to determining molecular shape, including the VSEPR model and hybridisation. Next, we will move on to experimental methods such as X-ray crystallography, electron diffraction, and spectroscopic techniques. Following that, we will consider how bond lengths are defined, measured, and influenced by factors such as bond order and resonance. Finally, we will wrap up by exploring bond angles, their measurement, and how lone pairs and multiple bonds affect them. This progression will provide you with a comprehensive understanding of how chemists determine and interpret molecular structures.

Series Learning Outcomes

Upon completing this Series, you should be able to:

SLO 4.1 explain the principles of theoretical approaches such as the VSEPR model and hybridisation for predicting molecular shape,
SLO 4.2 analyse the limitations of theoretical models in determining molecular geometry,
SLO 4.3 describe experimental methods used to determine molecular geometry, including X-ray crystallography, electron diffraction, and spectroscopy,
SLO 4.4 define bond length and demonstrate how it is measured using experimental techniques,
SLO 4.5 evaluate the factors that influence bond length, such as bond order, electronegativity, and resonance,
SLO 4.6 define bond angle and explain its importance in molecular structure, and
SLO 4.7 assess how lone pairs and multiple bonds affect bond angles in molecules.

4.1 Theoretical Approaches to Determining Molecular Shape

4.1.1 Valence Shell Electron Pair Repulsion (VSEPR) model

The **Valence Shell Electron Pair Repulsion (VSEPR) model** is a theoretical approach used to predict the shape of molecules. It is based on the idea that electron pairs around a central atom repel each other and will arrange themselves as far apart as possible to minimise repulsion. This arrangement determines the geometry of the molecule. For example, methane (CH_4) adopts a tetrahedral shape because its four bonding pairs of electrons spread out evenly around the central carbon atom.

Fill in the blank: The VSEPR model predicts molecular shape by assuming that electron pairs __________________ each other.

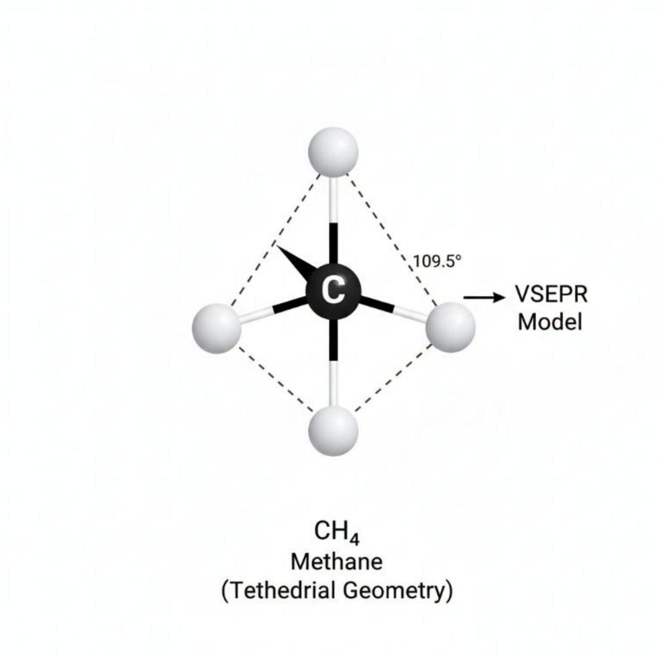

Figure 4.1: Tetrahedral geometry of methane predicted by VSEPR

AI prompt: “Generate a labelled diagram showing methane molecule with tetrahedral geometry explained by VSEPR model.”
Search string: “VSEPR model methane tetrahedral geometry OER”

4.1.2 Limitations of theoretical models

While the VSEPR model is useful, it has limitations. It does not always accurately predict bond angles, especially when lone pairs or multiple bonds are present. It also struggles with molecules involving transition metals, where d-orbitals play a role in bonding. Furthermore, VSEPR does not explain the electronic basis of bonding, which is better addressed by molecular orbital theory.

Fill in the blank: The VSEPR model cannot explain __________________ properties of molecules such as oxygen.

Limitation Category	Description of the Failure	Examples
Delocalized Electrons	VSEPR assumes electrons are "fixed" between two atoms (localized). It cannot account for resonance or delocalization where electrons are spread over several nuclei.	**Benzene (C_6H_6)** or the **Carbonate ion (CO_3^{2-})**.
Magnetic Properties	VSEPR focuses strictly on geometry and cannot predict whether a molecule is paramagnetic (attracted to magnets) or diamagnetic.	**Oxygen (O_2)**: VSEPR suggests it is diamagnetic, but it is actually paramagnetic.
Complex Molecules	The model becomes less accurate as the size and number of multiple bonds increase, as it doesn't account for the subtle orbital interactions in transition metals or heavy elements.	**Transition metal complexes** (e.g., $[Fe(H_2O)_6]^{2+}$) and molecules with significant steric bulk.
Relative Bond Strengths	It does not provide information on bond lengths or the actual energy required to break bonds; it only predicts the angles between them.	Comparing the stability of N_2 vs. F_2.
Isoelectronic Species	VSEPR sometimes predicts identical shapes for isoelectronic species that actually differ due to nuclear charge effects.	Comparing CH_4, NH_4^+, and BH_4^-.

Box 4.1: Limitations of the VSEPR model

Struggles with molecules containing delocalised electrons
Cannot explain magnetic properties
Less accurate for complex molecules with multiple bonds

4.1.3 Role of hybridisation in predicting shapes

Hybridisation is another theoretical approach that helps explain molecular shapes. It involves the mixing of atomic orbitals (such as s and p orbitals) to form new hybrid orbitals that are better suited for bonding. For example, in methane (CH_4), the carbon atom undergoes sp^3 hybridisation, producing four equivalent orbitals that form a tetrahedral shape. Hybridisation complements the VSEPR model by providing an electronic explanation for observed geometries.

Fill in the blank: In methane, carbon undergoes __________ hybridisation to form four equivalent orbitals.

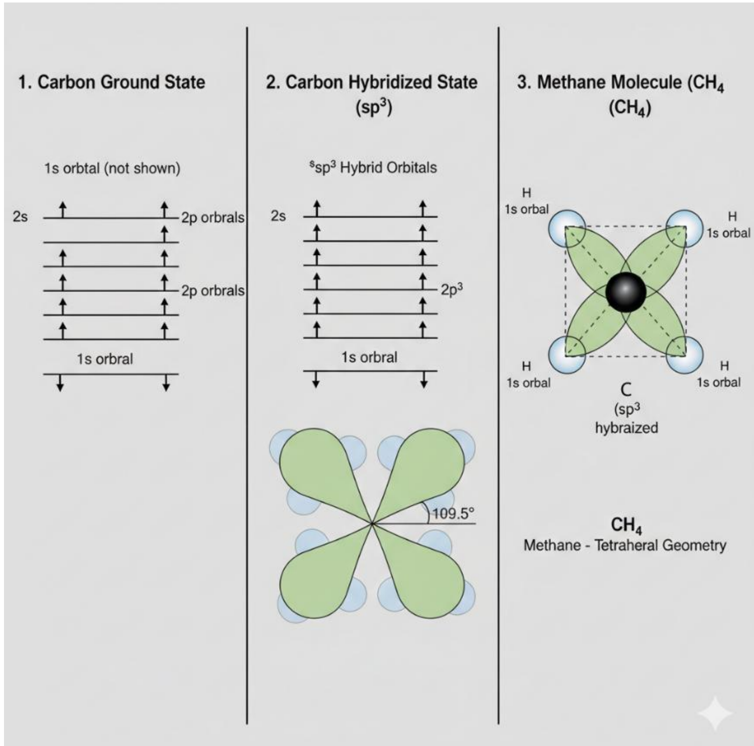

Plate 4.1: Hybridisation of carbon in methane

Pilot questions 4.1

The VSEPR model predicts molecular shape by assuming that electron pairs __________ each other.

A. Attract
B. Repel
C. Neutralise
D. Share
(Linked to SLO 4.1)

The VSEPR model cannot explain __________ properties of molecules such as oxygen.

A. Polarity
B. Magnetic
C. Bonding
D. Symmetry
(Linked to SLO 4.2)

In methane, carbon undergoes __________ hybridisation to form four equivalent orbitals.

A. sp^2
B. sp^3
C. sp
D. sp^3d
(Linked to SLO 4.1)

Give one limitation of the VSEPR model when predicting molecular geometry.
(Linked to SLO 4.2)

Explain how hybridisation complements the VSEPR model in predicting molecular shapes.
(Linked to SLO 4.1, SLO 4.2)

4.2 Experimental Methods for Determining Molecular Geometry

4.2.1 X-ray crystallography

X-ray crystallography is one of the most powerful experimental techniques used to determine molecular geometry. In this method, X-rays are directed at a crystal of the substance. The X-rays are diffracted by the electrons in the atoms, producing a diffraction pattern. By analysing this pattern, scientists can determine the three-dimensional arrangement of atoms in the molecule. This technique provides highly accurate bond lengths and angles, making it invaluable in structural chemistry.

Fill in the blank: X-ray crystallography determines molecular geometry by analysing the __________________ pattern produced when X-rays interact with a crystal.

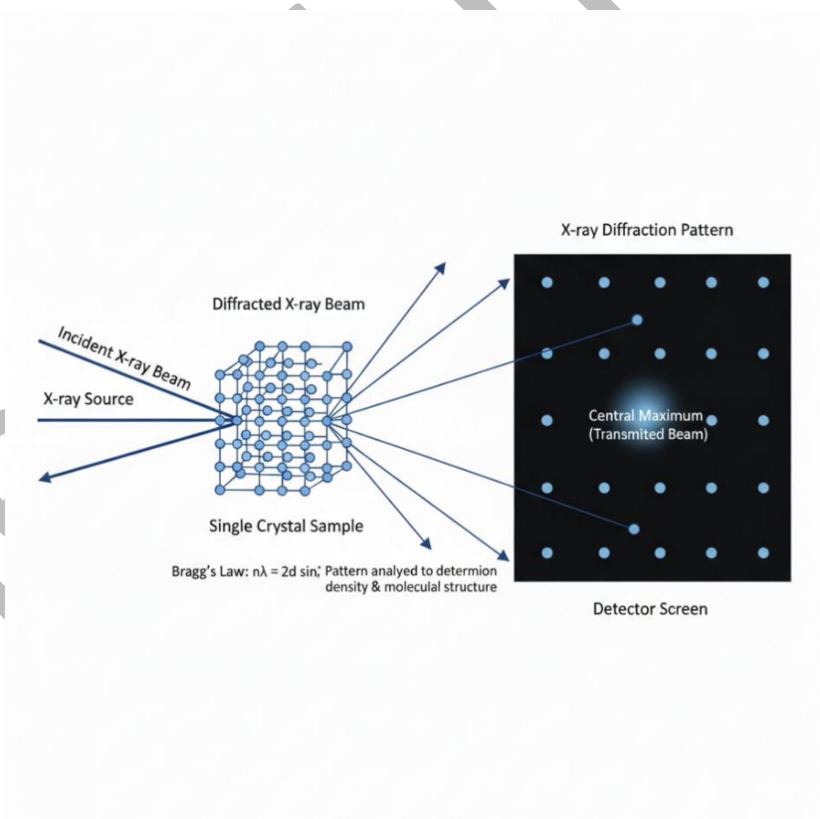

Figure 4.2: Principle of X-ray crystallography

4.2.2 Electron diffraction

Electron diffraction is a technique used to study the geometry of molecules in the gas phase. A beam of electrons is directed at a gaseous sample, and the electrons are scattered by the atoms. The scattering pattern provides information about bond lengths and angles. Unlike X-ray crystallography, electron diffraction does not require crystalline samples, making it useful for studying small molecules in the gas phase.

Fill in the blank: Electron diffraction is particularly useful for studying molecules in the __________________ phase.

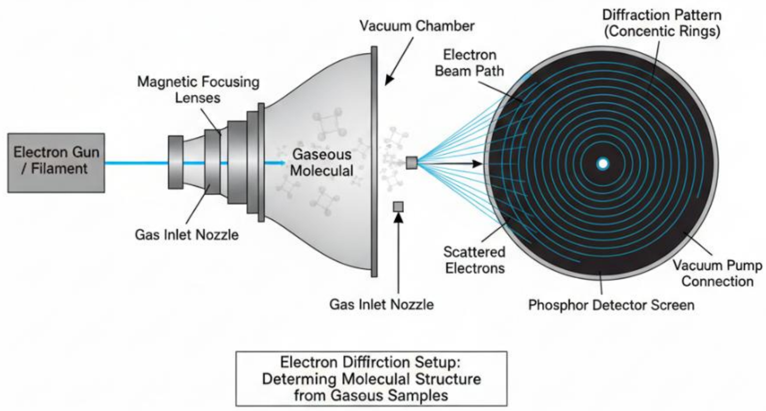

Plate 4.2: Electron diffraction experiment setup

4.2.3 Spectroscopic techniques (infrared and Raman)

Spectroscopy involves studying how molecules interact with light. Infrared (IR) and Raman spectroscopy are particularly useful for determining molecular geometry. In IR spectroscopy, molecules absorb infrared radiation, causing vibrations that depend on bond lengths and angles. Raman spectroscopy, on the other hand, measures the scattering of light as molecules vibrate. Together, these techniques provide complementary information about molecular structure and geometry.

Fill in the blank: Infrared spectroscopy measures the absorption of __________________ radiation by molecules.

Summary of Spectroscopic Applications for Molecular Geometry

Feature	Infrared (IR) Spectroscopy	Raman Spectroscopy	Structural Significance
Selection Rule	Requires a **change in dipole moment.**	Requires a **change in polarizability.**	Determines which vibrations "show up" based on molecular symmetry.
Primary Sensitivity	Polar bonds (e.g., $C-O$, $N-H$, $O-H$).	Non-polar bonds (e.g., $C=C$, $N=N$, $S-S$).	Identifies both the "connectors" and the "backbone" of the molecule.
Symmetry Analysis	Best for detecting **asymmetric** vibrations.	Best for detecting **symmetric** vibrations.	Helps identify the "point group" (the mathematical shape) of the molecule.
Bond Geometry	Vibrational modes (bending/stretching) indicate bond angles.	Complements IR by revealing "IR-inactive" modes.	Combined data allows for the calculation of force constants and indirect bond lengths.

Box 4.2: Applications of spectroscopic techniques

Infrared spectroscopy: identifies vibrational modes and functional groups
Raman spectroscopy: complements infrared by detecting vibrations that are IR-inactive
Both methods: provide indirect evidence of bond lengths and angles

Pilot questions 4.2

X-ray crystallography determines molecular geometry by analysing the __________ pattern produced when X-rays interact with a crystal.

A. Absorption
B. Diffraction
C. Reflection
D. Emission
(Linked to SLO 4.3)

Electron diffraction is particularly useful for studying molecules in the __________ phase.

A. Solid
B. Liquid
C. Gas
D. Plasma
(Linked to SLO 4.3)

Infrared spectroscopy measures the absorption of __________ radiation by molecules.

A. Ultraviolet
B. Infrared
C. Visible
D. Microwave
(Linked to SLO 4.3)

Give one advantage of electron diffraction compared to X-ray crystallography.
(Linked to SLO 4.3)

Explain how Raman spectroscopy complements infrared spectroscopy in studying molecular geometry.
(Linked to SLO 4.3)

4.3 Determination of Bond Lengths

4.3.1 Definition and significance of bond length

Bond length is the average distance between the nuclei of two bonded atoms. It is a fundamental property of molecules because it reflects the strength and nature of the bond. Shorter bond lengths usually indicate stronger bonds, while longer bond lengths suggest weaker interactions. Bond length also influences physical properties such as melting point, boiling point, and reactivity. For example, the bond length in a triple bond is shorter than that in a double bond, which in turn is shorter than a single bond.

Fill in the blank: The average distance between the nuclei of two bonded atoms is called ___________________.

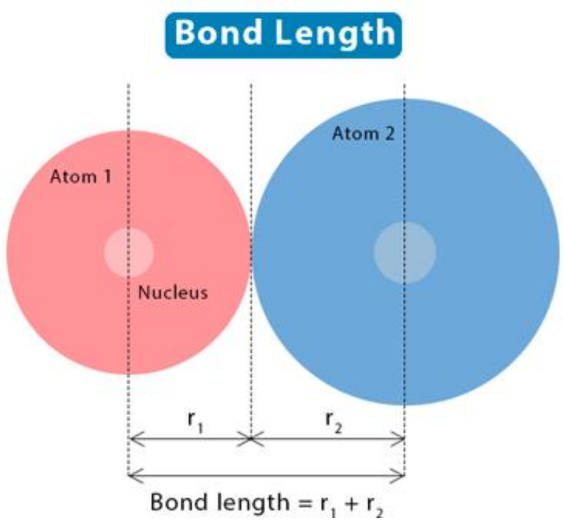

Figure 4.3: Representation of bond length between two nuclei

4.3.2 Experimental measurement methods

Bond lengths are determined using experimental techniques such as **X-ray crystallography**, **electron diffraction**, and **spectroscopy**. X-ray crystallography provides precise bond length measurements in crystalline solids, while electron diffraction is useful for gaseous molecules. Spectroscopic methods, such as infrared spectroscopy, can indirectly provide bond length information by analysing vibrational frequencies. These techniques complement each other, ensuring accurate determination across different states of matter.

Fill in the blank: Bond lengths in crystalline solids are most accurately measured using __________________ crystallography.

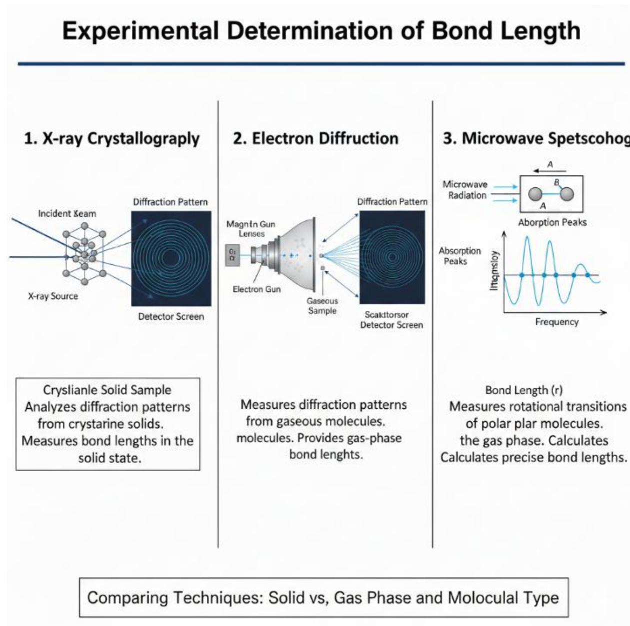

Plate 4.3: Experimental methods for measuring bond length

4.3.3 Factors affecting bond length

Several factors influence bond length:

Bond order: Higher bond order (triple > double > single) results in shorter bond lengths.

Electronegativity: When atoms have high electronegativity differences, bonds may be shorter due to stronger attraction.

Resonance: In molecules with resonance structures, bond lengths are intermediate between single and double bonds. For example, in benzene, all carbon–carbon bonds have equal length due to resonance.

Fill in the blank: A higher bond __________________ results in a shorter bond length.

Factor	Mechanism of Influence	Impact on Bond Length
Bond Order	Represents the number of shared electron pairs between two atoms.	**Inverse Relationship:** Higher bond order (e.g., triple vs. single) increases nuclear attraction, pulling atoms closer.
Electronegativity	The ability of an atom to attract shared electrons toward itself.	**Shortening Effect:** A large difference ($\Delta\chi$) creates partial charges (δ^+, δ^-), adding electrostatic attraction that shortens the bond.
Resonance	The delocalization of electrons across multiple adjacent bonds.	**Averaging Effect:** Results in "fractional" bond orders, creating lengths intermediate between single and double bonds.
Atomic Radius	The inherent size of the atoms involved in the bond.	**Direct Relationship:** Larger atoms have valence electrons further from the nucleus, resulting in longer bonds.
Hybridization	The type of orbital overlap (e.g., sp, sp^2, sp^3).	**S-Character Effect:** Higher "s-character" (like sp) keeps electrons closer to the nucleus, shortening the bond.

Box 4.3: Factors affecting bond length

Bond order: higher bond order → shorter bond length
Electronegativity: differences affect electron distribution and bond distance
Resonance: delocalisation leads to intermediate bond lengths

Pilot questions 4.3

The average distance between the nuclei of two bonded atoms is called:

A. Bond angle
B. Bond length
C. Bond order
D. Bond energy
(Linked to SLO 4.4)

Bond lengths in crystalline solids are most accurately measured using __________ crystallography.

A. Electron
B. X-ray
C. Neutron
D. Infrared
(Linked to SLO 4.4)

A higher bond __________ results in a shorter bond length.

A. Angle
B. Order
C. Energy
D. Polarity
(Linked to SLO 4.5)

Give one factor that influences bond length apart from bond order.
(Linked to SLO 4.5)

Explain how resonance affects bond length in molecules.
(Linked to SLO 4.5)

4.4 Determination of Bond Angles

4.4.1 Definition and importance of bond angles

Bond angle is the angle formed between two bonds that originate from the same atom. It is a key feature of molecular geometry because it determines the overall shape of the molecule. Bond angles influence physical and chemical properties such as polarity, reactivity, and intermolecular interactions. For example, the bond angle in water (H_2O) is approximately 104.5°, which contributes to its bent geometry and polarity.

Fill in the blank: The angle formed between two adjacent bonds originating from the same atom is called __________________.

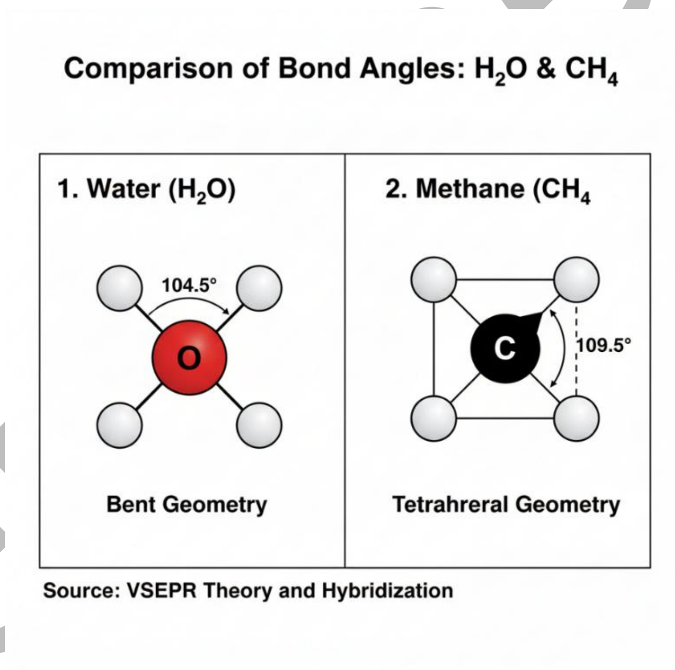

Figure 4.4: Bond angles in water and methane

4.4.2 Experimental measurement methods

Bond angles can be determined using several experimental techniques. **X-ray crystallography** provides precise bond angles in crystalline solids by analysing atomic positions. **Electron diffraction** is used for gaseous molecules, while **spectroscopic methods** such as infrared and

Raman spectroscopy provide indirect evidence of bond angles through vibrational frequencies. These methods complement each other depending on the physical state of the sample.

Fill in the blank: Bond angles in crystalline solids are most accurately measured using __________________ crystallography.

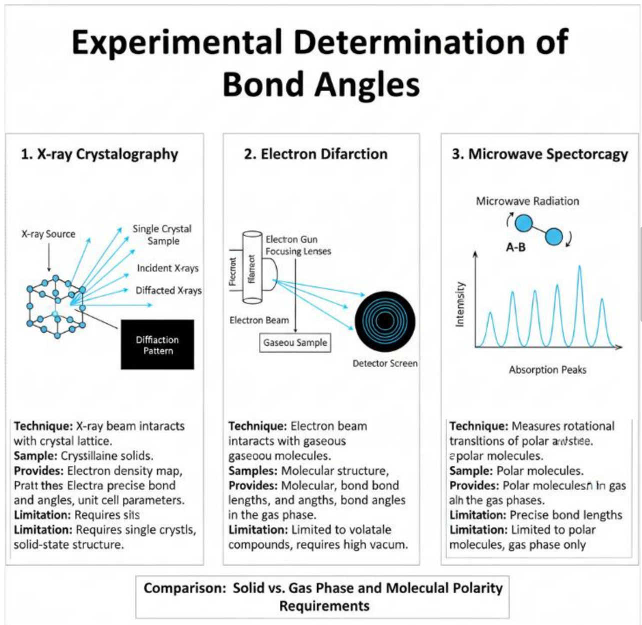

Plate 4.4: Experimental methods for determining bond angles

4.4.3 Influence of lone pairs and multiple bonds on bond angles

Bond angles are not fixed; they can be influenced by factors such as lone pairs and multiple bonds. **Lone pairs** of electrons occupy more space than bonding pairs, pushing bonds closer together and reducing bond angles. For example, in ammonia (NH_3), the bond angle is about 107°, smaller than the ideal tetrahedral angle of 109.5°, due to the lone pair on nitrogen. **Multiple bonds** increase electron density between atoms, which can expand bond angles adjacent to them. These variations explain why real molecules often deviate from idealised geometries.

Fill in the blank: Lone pairs of electrons occupy more space than bonding pairs, causing bond angles to __________________.

Molecule	Basic Geometry	Key Feature	Observed Bond Angle	Effect on Structure
Methane (CH_4)	Tetrahedral	4 Single Bonds (Reference)	109.5°	The ideal angle for maximum separation of four equal domains.
Ammonia (NH_3)	Trigonal Pyramidal	1 Lone Pair	107°	The lone pair "spreads out," pushing the three $N-H$ bonds closer together.
Water (H_2O)	Bent	2 Lone Pairs	104.5°	Two lone pairs exert even greater repulsion, compressing the $H-O-H$ angle further.
Ethene (C_2H_4)	Trigonal Planar	1 Double Bond	121.3° (H-C=C)	The high electron density of the double bond pushes the $C-H$ bonds away.

Box 4.4: Influence of lone pairs and multiple bonds on bond angles

Ammonia (NH_3): lone pair reduces bond angle to 107°
Water (H_2O): two lone pairs reduce bond angle to 104.5°
Ethene (C_2H_4): double bond increases repulsion, affecting bond angles around carbon

Pilot questions 4.4

The angle formed between two adjacent bonds originating from the same atom is called:
A. Bond length
B. Bond angle
C. Bond order
D. Bond energy
(Linked to SLO 4.6)

Bond angles in crystalline solids are most accurately measured using __________ crystallography.
A. Electron
B. X-ray
C. Neutron
D. Infrared
(Linked to SLO 4.6)

Lone pairs of electrons occupy more space than bonding pairs, causing bond angles to __________.
A. Increase
B. Decrease
C. Remain constant
D. Double
(Linked to SLO 4.7)

Give one example of a molecule where lone pairs reduce bond angles.
(Linked to SLO 4.7)

Explain how multiple bonds influence bond angles in molecules such as ethene. (Linked to SLO 4.7)

Series Summary

This Series on **Methods of Determining Molecular Shape, Bond Lengths and Angles** was designed to show you how chemists use both theoretical models and experimental techniques to understand molecular structure. You began with theoretical approaches, learning how the VSEPR model and hybridisation predict molecular shapes, while also recognising the limitations of these models. You then explored experimental methods such as X-ray crystallography, electron diffraction, and spectroscopy, which provide precise measurements of molecular geometry. Building on this, you studied how bond lengths are defined, measured, and influenced by factors such as bond order, electronegativity, and resonance. Finally, you examined bond angles, their importance in molecular structure, how they are measured, and how lone pairs and multiple bonds affect them.

By completing this Series, you should now be able to **explain theoretical approaches such as VSEPR and hybridisation (SLO 4.1)**, **analyse the limitations of these models (SLO 4.2)**, **describe experimental methods for determining molecular geometry (SLO 4.3)**, **define and measure bond lengths (SLO 4.4)**, **evaluate factors influencing bond length (SLO 4.5)**, **define bond angles and explain their importance (SLO 4.6)**, and **assess how lone pairs and multiple bonds affect bond angles (SLO 4.7)**. These outcomes ensure you can connect theory with experiment, giving you a well-rounded understanding of how molecular structure is determined and how it influences chemical behaviour.

Glossary of Terms

Bond angle: The angle formed between two bonds that originate from the same atom, which determines the overall shape of a molecule.

Bond length: The average distance between the nuclei of two bonded atoms, reflecting the strength and nature of the bond.

Bond order: A measure of the number of chemical bonds between a pair of atoms; higher bond order usually means shorter and stronger bonds.

Electron diffraction: An experimental technique where electrons are scattered by atoms in a gaseous sample, producing patterns that reveal molecular geometry.

Electronegativity: The tendency of an atom to attract electrons in a chemical bond, which can influence bond length and polarity.

Hybridisation: The mixing of atomic orbitals (such as s and p orbitals) to form new hybrid orbitals that explain molecular shapes and bonding.

Infrared spectroscopy (IR): A technique that measures how molecules absorb infrared radiation, providing information about bond vibrations and geometry.

Lone pair: A pair of valence electrons not involved in bonding, which can influence bond angles by repelling bonding pairs more strongly.

Resonance: A phenomenon where electrons are delocalised across multiple structures, resulting in bond lengths that are intermediate between single and double bonds.

Raman spectroscopy: A technique that measures the scattering of light as molecules vibrate, complementing infrared spectroscopy in determining molecular geometry.

Valence Shell Electron Pair Repulsion (VSEPR) model: A theoretical model that predicts molecular shape by assuming electron pairs around a central atom repel each other and arrange themselves to minimise repulsion.

X-ray crystallography: An experimental method that uses X-ray diffraction patterns from crystals to determine precise molecular geometry, including bond lengths and angles.

Concept Check Questions [Series 4]

Objective Questions

The VSEPR model predicts molecular shape by assuming that electron pairs __________________ each other.
(Linked to SLO 4.1)

Which experimental technique is most accurate for determining bond lengths in crystalline solids?
A. Infrared spectroscopy
B. Electron diffraction
C. X-ray crystallography
D. Raman spectroscopy
(Linked to SLO 4.3 & 4.4)

In benzene, resonance causes all carbon–carbon bonds to have __________________ lengths.
(Linked to SLO 4.5)

Lone pairs of electrons reduce bond angles because they occupy more __________________ than bonding pairs.
(Linked to SLO 4.7)

Infrared spectroscopy determines molecular geometry by measuring how molecules absorb __________________ radiation.
(Linked to SLO 4.3)

Short-Answer Questions

Define bond length and explain why it is significant in molecular chemistry.
(Linked to SLO 4.4)

State one limitation of the VSEPR model in predicting molecular geometry.
(Linked to SLO 4.2)

Describe how hybridisation complements the VSEPR model in predicting molecular shapes.
(Linked to SLO 4.1)

Give one example of a molecule where lone pairs reduce bond angles and explain the effect.
(Linked to SLO 4.7)

Explain how multiple bonds influence bond angles in molecules.
(Linked to SLO 4.7)

Long-Answer Questions

Analyse how theoretical approaches such as VSEPR and hybridisation help predict molecular shape, and discuss their limitations.
(Linked to SLO 4.1 & 4.2)

Evaluate the role of experimental methods (X-ray crystallography, electron diffraction, and spectroscopy) in determining molecular geometry, highlighting their strengths and weaknesses.
(Linked to SLO 4.3)

Assess how bond lengths and bond angles together influence molecular stability and chemical behaviour, using examples such as water, methane, and benzene.
(Linked to SLO 4.4, 4.5, 4.6 & 4.7)

Answers to Concept Check Questions [Series 4]

Objective Questions

Repel
C. X-ray crystallography
Equal
Space
Infrared

Short-Answer Questions

Bond length is the average distance between the nuclei of two bonded atoms. It is significant because it reflects bond strength and influences physical properties such as melting point, boiling point, and reactivity.

VSEPR does not accurately predict bond angles when lone pairs or transition metal d-orbitals are involved.

Hybridisation explains the electronic basis of bonding, showing how orbitals mix to form shapes consistent with VSEPR predictions.

In ammonia (NH_3), the lone pair on nitrogen reduces the bond angle from the ideal 109.5° to about 107°.

Multiple bonds increase electron density, which can expand adjacent bond angles compared with single bonds.

Long-Answer Questions

Question 1

Basic response: VSEPR predicts shapes by minimising electron pair repulsion, while hybridisation explains orbital mixing. Limitations include difficulty with transition metals and lone pairs.

Value-added response: Learners may extend by discussing how molecular orbital theory provides a more complete explanation of bonding and geometry.

Question 2

Basic response: X-ray crystallography provides precise data for solids, electron diffraction is useful for gases, and spectroscopy gives indirect information. Each method complements the others.

Value-added response: Outstanding learners may expand by comparing resolution, accessibility, and cost, and by linking these methods to applications in drug design and materials science.

Question 3

Basic response: Bond lengths and angles define molecular geometry, influencing stability and reactivity. Water's bent geometry makes it polar, methane's tetrahedral geometry makes it stable, and benzene's resonance stabilises its structure.

Value-added response: Learners may extend by discussing how these structural features affect intermolecular forces, solubility, and spectroscopic behaviour, connecting theory to practical applications in chemistry and biology.

Answers to Pilot Questions [Series 4]

Part 4.1: Theoretical Approaches to Determining Molecular Shape

Repel
Magnetic
sp^3 hybridisation
It cannot explain magnetic properties or molecules with delocalised electrons
Hybridisation provides a quantum mechanical explanation that complements the VSEPR model

Part 4.2: Experimental Methods for Determining Molecular Geometry

Diffraction
Gas
Infrared
It can be used for gaseous molecules, unlike X-ray crystallography which requires crystals
Raman spectroscopy detects vibrations that are IR-inactive, complementing infrared spectroscopy

Part 4.3: Determination of Bond Lengths

Bond length
X-ray
Order
Electronegativity differences or resonance
Resonance delocalises electrons, leading to intermediate bond lengths

Part 4.4: Determination of Bond Angles

Bond angle
X-ray
Decrease
Ammonia (NH_3) or water (H_2O)
Multiple bonds increase electron density, which repels adjacent bonds more strongly and alters bond angles

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References and Attributions [Series 4]

Textual Sources

Atkins, P., & Friedman, R. (2011). *Molecular Quantum Mechanics* (5th ed.). Oxford University Press.
McQuarrie, D. A. (2008). *Quantum Chemistry*. University Science Books.
Levine, I. N. (2014). *Quantum Chemistry* (7th ed.). Pearson.
IUPAC. (1997). *Compendium of Chemical Terminology (the "Gold Book")*.

Illustrations (Figures, Plates, Tables, Boxes)

Figure 4.1 Tetrahedral geometry of methane predicted by VSEPR
AI prompt: "Generate a labelled diagram showing methane molecule with tetrahedral geometry explained by VSEPR model."
Search string: "VSEPR model methane tetrahedral geometry OER"

Box 4.1 Limitations of the VSEPR model
AI prompt: "Generate a table summarising the limitations of the VSEPR model, including delocalised electrons, magnetic properties, and complex molecules."
Search string: "limitations of VSEPR model chemistry OER"

Plate 4.1 Hybridisation of carbon in methane
AI prompt: "Create an image showing sp^3 hybridisation in carbon forming four equivalent orbitals arranged tetrahedrally."
Search string: "sp3 hybridisation carbon methane diagram OER"

Figure 4.2 Principle of X-ray crystallography
AI prompt: "Generate a labelled diagram showing X-ray beams diffracting through a crystal lattice to produce a diffraction pattern."
Search string: "X-ray crystallography principle diagram OER"

Plate 4.2 Electron diffraction experiment setup
AI prompt: "Create an image showing electron diffraction setup with electron beam scattering through a gaseous sample."
Search string: "electron diffraction molecular geometry diagram OER"

Box 4.2 Applications of spectroscopic techniques
AI prompt: "Generate a table summarising applications of infrared and Raman spectroscopy in determining molecular geometry."
Search string: "infrared Raman spectroscopy molecular geometry OER"

Figure 4.3 Representation of bond length between two nuclei
AI prompt: "Generate a labelled diagram showing bond length measurement between two bonded atoms."
Search string: "bond length measurement diagram chemistry OER"

Plate 4.3 Experimental methods for measuring bond length
AI prompt: "Create an image comparing X-ray crystallography, electron diffraction, and spectroscopy for measuring bond length."
Search string: "methods of measuring bond length chemistry OER"

Box 4.3 Factors affecting bond length
AI prompt: "Generate a table summarising factors affecting bond length, including bond order, electronegativity, and resonance."
Search string: "factors affecting bond length chemistry OER"

Figure 4.4 Bond angles in water and methane
AI prompt: "Generate a labelled diagram showing bond angles in water (104.5°) and methane (109.5°)."
Search string: "bond angle water methane diagram OER"

Plate 4.4 Experimental methods for determining bond angles
AI prompt: "Create an image comparing X-ray crystallography, electron diffraction, and spectroscopy for measuring bond angles."
Search string: "methods of measuring bond angles chemistry OER"

Box 4.4 Influence of lone pairs and multiple bonds on bond angles
AI prompt: "Generate a table summarising how lone pairs and multiple bonds influence bond angles, including NH_3, H_2O, and C_2H_4."
Search string: "lone pairs multiple bonds bond angle chemistry OER"

Notes on Attribution

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References are presented in APA style for consistency.

Course code: CHM 214

- **Course title:** Structure and Bonding
- **Course credit load:** 2 Units (C: LH 30)
- **Series titles:**

  Quantum States, Orbitals, Shape and Energy
  Valence Theory, Electron Repulsion and Atomic Spectra
  Symmetry, Molecular Geometry and Molecular Orbital Theory
  Methods of Determining Molecular Shape, Bond Lengths and Angles
  Structure and Chemistry of Representative Main Group Compound

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Suggested Outline

Part 5.1: Introduction to Main Group Elements

Sub-Part 5.1.1: Position of main group elements in the periodic table
Sub-Part 5.1.2: General properties and trends across periods and groups
Sub-Part 5.1.3: Importance of main group compounds in chemistry and industry

Part 5.2: Structure and Chemistry of Group 1 and Group 2 Compounds

Sub-Part 5.2.1: Alkali metals (Group 1) – structures, bonding, and reactivity
Sub-Part 5.2.2: Alkaline earth metals (Group 2) – structures, bonding, and reactivity
Sub-Part 5.2.3: Comparative trends between Groups 1 and 2

Part 5.3: Structure and Chemistry of Group 13 and Group 14 Compounds

Sub-Part 5.3.1: Boron and aluminium compounds – bonding and applications
Sub-Part 5.3.2: Carbon and silicon compounds – bonding, allotropes, and reactivity
Sub-Part 5.3.3: Comparative trends within Groups 13 and 14

Part 5.4: Structure and Chemistry of Group 15 and Group 16 Compounds

Sub-Part 5.4.1: Nitrogen and phosphorus compounds – bonding and reactivity
Sub-Part 5.4.2: Oxygen and sulphur compounds – bonding, allotropes, and reactivity
Sub-Part 5.4.3: Comparative trends within Groups 15 and 16

Part 5.5: Structure and Chemistry of Group 17 and Group 18 Compounds

Sub-Part 5.5.1: Halogens (Group 17) – bonding, reactivity, and applications

Sub-Part 5.5.2: Noble gases (Group 18) – bonding, compounds, and uses
Sub-Part 5.5.3: Comparative trends between Groups 17 and 18

Introduction

In the last Series, we examined methods of determining molecular shape, bond lengths, and bond angles, which provided a foundation for understanding how chemists investigate molecular structures. Building on that knowledge, this Series turns to the **structure and chemistry of representative main group compounds**, which are among the most widely studied and practically important substances in chemistry. These compounds are central to everyday applications ranging from materials and energy to biological systems, making their study highly relevant to the overall course.

The aim of this Series is to introduce you to the structural features and chemical behaviour of main group compounds across different groups of the periodic table. By the end, you will be able to explain their bonding, identify periodic trends, and evaluate their reactivity and applications.

We shall commence this Series by exploring the position of main group elements in the periodic table and their general properties. Next, we will study the structure and chemistry of Group 1 and Group 2 compounds, followed by Groups 13 and 14, where elements such as boron, aluminium, carbon, and silicon play key roles. Subsequently, we will continue with Groups 15 and 16, focusing on nitrogen, phosphorus, oxygen, and sulphur compounds. Finally, we will wrap up by examining Groups 17 and 18, considering the chemistry of halogens and noble gases. This progression will provide you with a comprehensive understanding of the representative compounds of the main group elements.

Series Learning Outcomes

Upon completing this Series, you should be able to:

SLO 5.1 describe the position of main group elements in the periodic table and explain their general properties and trends,
SLO 5.2 explain the structure, bonding, and reactivity of Group 1 (alkali metals) and Group 2 (alkaline earth metals) compounds,
SLO 5.3 analyse the bonding and applications of Group 13 (boron and aluminium) compounds,
SLO 5.4 evaluate the structural features, allotropes, and reactivity of Group 14 (carbon and silicon) compounds,
SLO 5.5 explain the bonding and reactivity of Group 15 (nitrogen and phosphorus) compounds,
SLO 5.6 describe the structural features, allotropes, and reactivity of Group 16 (oxygen and sulphur) compounds,
SLO 5.7 analyse the bonding, reactivity, and applications of Group 17 (halogen) compounds, and
SLO 5.8 evaluate the bonding, compounds, and uses of Group 18 (noble gases).

5.1 Introduction to Main Group Elements

5.1.1 Position of main group elements in the periodic table

The **main group elements** are those found in Groups 1, 2, and 13 to 18 of the periodic table. They include alkali metals, alkaline earth metals, and non-metals such as halogens and noble gases. These elements are characterised by having their valence electrons in the s and p orbitals, which largely determine their chemical behaviour. Their position in the periodic table reflects recurring trends in properties such as ionisation energy, electronegativity, and atomic radius.

Fill in the blank: The main group elements are found in Groups __________ of the periodic table.

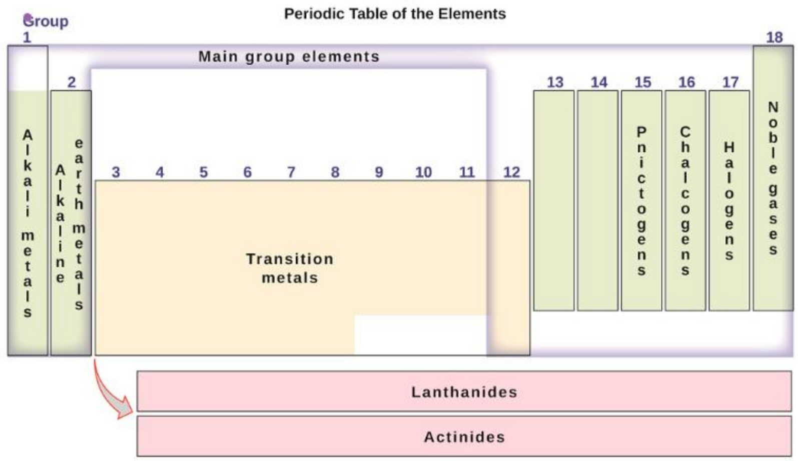

Figure 5.1: Position of main group elements in the periodic table

5.1.2 General properties and trends across periods and groups

Main group elements display clear **periodic trends**, which are predictable changes in properties across periods (rows) and groups (columns). For example, atomic radius decreases across a period due to increasing nuclear charge, while it increases down a group as new electron shells are added. Ionisation energy generally increases across a period and decreases down a group. Electronegativity follows a similar trend, with fluorine being the most electronegative element. These trends help chemists predict reactivity and bonding behaviour.

Fill in the blank: Atomic radius generally __________ across a period and __________ down a group.

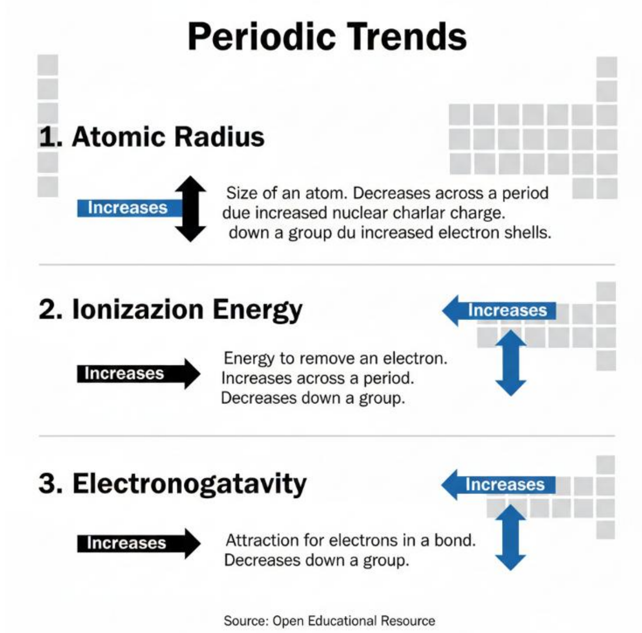

Plate 5.1: Periodic trends in main group elements

5.1.3 Importance of main group compounds in chemistry and industry

Compounds of main group elements are essential in both chemistry and industry. For instance, sodium chloride ($NaCl$) is vital in food preservation and chemical manufacturing, while calcium carbonate ($CaCO_3$) is used in construction and as a raw material in cement. Carbon compounds form the basis of organic chemistry, while silicon compounds are crucial in electronics and semiconductors. Halogen compounds are widely used in disinfectants, and noble gases find applications in lighting and medical imaging.

Fill in the blank: Silicon compounds are especially important in the __________ industry.

Industrial Applications of Key Main Group Compounds

Compound	Common Name / Category	Primary Industry	Specific Uses & Applications
Sodium Chloride (NaCl)	Table Salt / Halite	Food & Chemical	Food preservation and seasoning; primary feedstock for the "chlor-alkali" process to produce chlorine gas and sodium hydroxide (NaOH).
Calcium Carbonate (CaCo3)	Limestone / Calcite	Construction & Materials	Principal component of cement and mortar; used as a "flux" in steelmaking and as a pH neutralizer in environmental treatment.
Silicon Dioxide (SiO2)	Silica / Quartz	Glass & Electronics	Main ingredient in glass manufacturing; essential for producing silicon wafers for semi-conductors and optical fibers.
Phosphates (e.g., $Ca_3(PO4)_2$	Phosphate Rock	Agriculture	Crucial component of NPK fertilizers; used in the production of phosphoric acid and animal feed supplements.
Magnesium Oxide (MgO)	Magnesia	Refractories	Used to line high-temperature furnaces and kilns due to its extremely high melting point and stability.
Aluminum Oxide (Al_2O_3)	Alumina	Manufacturing	Primary source of aluminum metal; used as an abrasive (corundum) and as a catalyst support in chemical reactions.

Box 5.1: Examples of main group compounds in daily life

Sodium chloride (NaCl): food and chemical industry
Calcium carbonate ($CaCO_3$): construction and materials
Silicon dioxide (SiO_2): glass and electronics
Phosphates: fertilisers and agriculture

Pilot questions 5.1

The main group elements are found in Groups __________ of the periodic table.
A. 1, 2, and 13–18
B. 3–12
C. Only 1 and 2
D. Only 17 and 18
(Linked to SLO 5.1)

Atomic radius generally __________ across a period and __________ down a group.
A. Increases; decreases
B. Decreases; increases
C. Remains constant; decreases
D. Increases; remains constant
(Linked to SLO 5.1)

Silicon compounds are especially important in the __________ industry.
A. Textile
B. Electronics
C. Food
D. Agriculture
(Linked to SLO 5.1)

Give one example of a main group compound used in construction.
(Linked to SLO 5.1)

Explain why main group elements are called “representative elements.”
(Linked to SLO 5.1)

5.2 Structure and Chemistry of Group 1 and Group 2 Compounds

5.2.1 Alkali metals (Group 1) – structures, bonding, and reactivity

Alkali metals are the elements in Group 1 of the periodic table, including lithium, sodium, potassium, rubidium, caesium, and francium. They have one valence electron in the outermost s-orbital, which makes them highly reactive. Their structures are typically metallic, with atoms arranged in a body-centred cubic lattice. Bonding in alkali metals is metallic, characterised by a sea of delocalised electrons that allow conductivity. Reactivity increases down the group, with lithium being the least reactive and caesium among the most reactive.

Fill in the blank: Alkali metals are highly reactive because they have __________ valence electron.

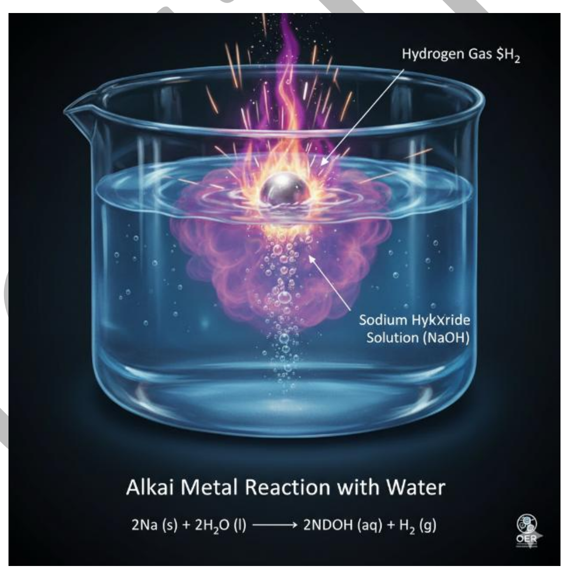

Figure 5.2: Reaction of sodium with water

AI prompt: “Generate a labelled diagram showing sodium reacting with water to produce sodium hydroxide and hydrogen gas.”
Search string: “alkali metals reaction with water diagram OER”

5.2.2 Alkaline earth metals (Group 2) – structures, bonding, and reactivity

Alkaline earth metals are the elements in Group 2 of the periodic table, including beryllium, magnesium, calcium, strontium, barium, and radium. They have two valence electrons in the outermost s-orbital, which makes them less reactive than alkali metals but still chemically active. Their structures are metallic, often arranged in a hexagonal close-packed or cubic lattice. Bonding is metallic, similar to Group 1, but stronger due to the presence of two valence electrons. Reactivity increases down the group, with beryllium being relatively inert compared to barium.

Fill in the blank: Alkaline earth metals form __________ cations when they lose their two valence electrons.

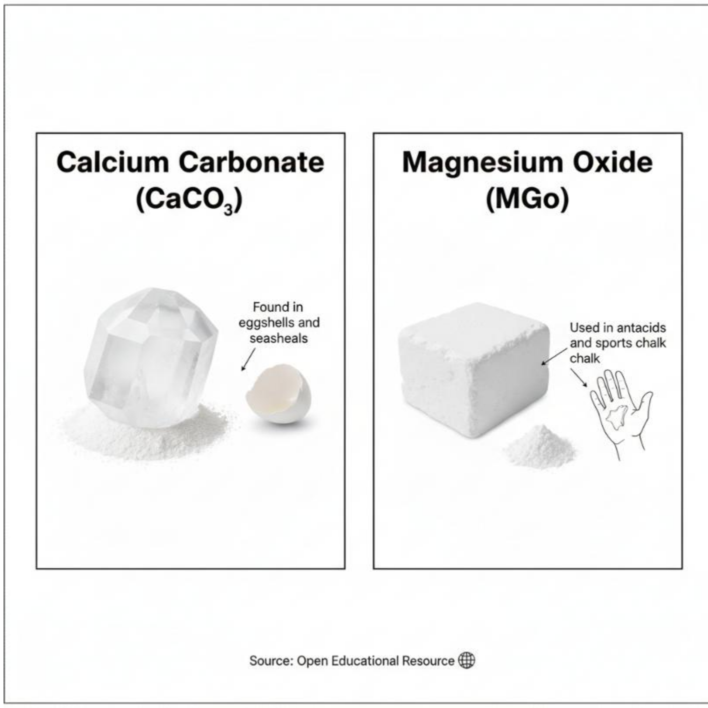

Plate 5.2: Common compounds of alkaline earth metals

5.2.3 Comparative trends between Groups 1 and 2

When comparing Groups 1 and 2, several trends emerge. Alkali metals are more reactive than alkaline earth metals because they need to lose only one electron to achieve stability, whereas Group 2 elements must lose two. Group 1 compounds, such as sodium chloride, are often soluble and form strong electrolytes. Group 2 compounds, such as calcium carbonate, are less soluble but play vital roles in biological and geological systems. Both groups form ionic compounds, but Group 2 compounds tend to have higher lattice energies due to the +2 charge of their cations.

Fill in the blank: Group 1 metals are generally __________ reactive than Group 2 metals.

Comparison of Group 1 and Group 2 Elements

Property	Group 1 (Alkali Metals)	Group 2 (Alkaline Earth Metals)
Valence Electrons	1 (ns^1)	2 (ns^2)
Reactivity	**Extremely High**; increases down the group. Must be stored in oil.	**High**, but less than Group 1. Requires higher energy to remove two electrons.
Common Ion Formed	+1 Cations (M^+)	+2 Cations (M^{2+})
Compound Types	Simple **ionic compounds** (e.g., $LiCl$, Na_2O).	More **complex ionic lattices**; some covalent character in lighter elements (e.g., $BeCl_2$).
Melting/Boiling Points	Relatively **low** (soft metals).	**Higher** than Group 1 due to stronger metallic bonding.
Solubility	Most compounds (salts) are **highly soluble** in water.	Many compounds (like carbonates and sulfates) are **insoluble or sparingly soluble**.

Box 5.2: Comparative trends between Groups 1 and 2

Group 1: one valence electron, highly reactive, form simple ionic compounds
Group 2: two valence electrons, less reactive, form more complex compounds
Both: metallic, form cations, and produce ionic lattices

Pilot questions 5.2

Alkali metals are highly reactive because they have __________ valence electron.

A. One
B. Two
C. Three
D. Four
(Linked to SLO 5.2)

Alkaline earth metals form __________ cations when they lose their two valence electrons.

A. Monovalent
B. Divalent
C. Trivalent
D. Neutral
(Linked to SLO 5.2)

Group 1 metals are generally __________ reactive than Group 2 metals.

A. More
B. Less
C. Equally
D. Not
(Linked to SLO 5.2)

Give one example of a common compound of an alkaline earth metal.

(Linked to SLO 5.2)

Explain why Group 1 metals react more vigorously with water compared to Group 2 metals. (Linked to SLO 5.2)

5.3 Structure and Chemistry of Group 13 and Group 14 Compounds

5.3.1 Boron and aluminium compounds – bonding and applications

Boron is unique among Group 13 elements because it forms covalent compounds rather than simple ionic ones. Its compounds, such as borates and boron hydrides, often feature electron-deficient bonding, meaning they do not follow the octet rule strictly. **Aluminium**, on the other hand, forms predominantly ionic compounds such as aluminium oxide (Al_2O_3), which is widely used in materials science. Both boron and aluminium compounds are important in industry, with boron used in glass and detergents, and aluminium in packaging and construction.

Fill in the blank: Boron compounds are often described as __________ because they do not strictly follow the octet rule.

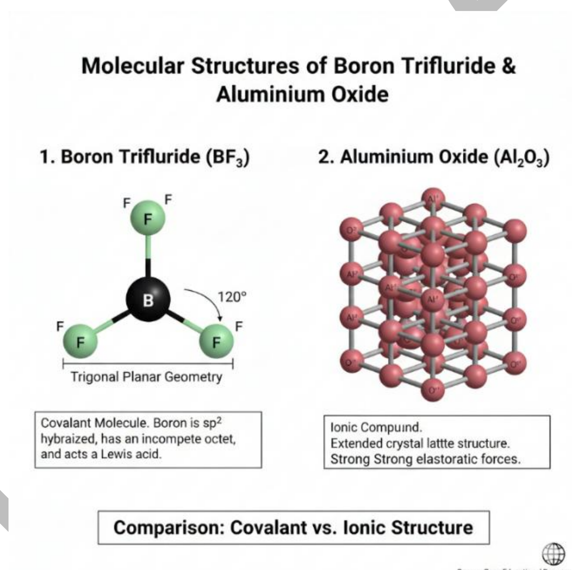

Figure 5.3: Structures of representative boron and aluminium compounds

5.3.2 Carbon and silicon compounds – bonding, allotropes, and reactivity

Carbon is unique in its ability to form multiple allotropes, such as diamond, graphite, graphene, and fullerenes. Diamond has a three-dimensional tetrahedral network with strong covalent bonds, making it extremely hard. Graphite consists of layers of hexagonal carbon atoms with delocalised electrons, giving it electrical conductivity. **Silicon**, in Group 14, also forms extended covalent networks, such as in quartz (SiO_2). Silicon compounds are less versatile than carbon but are crucial in semiconductors and glass production.

Fill in the blank: Diamond, graphite, and graphene are examples of carbon __________.

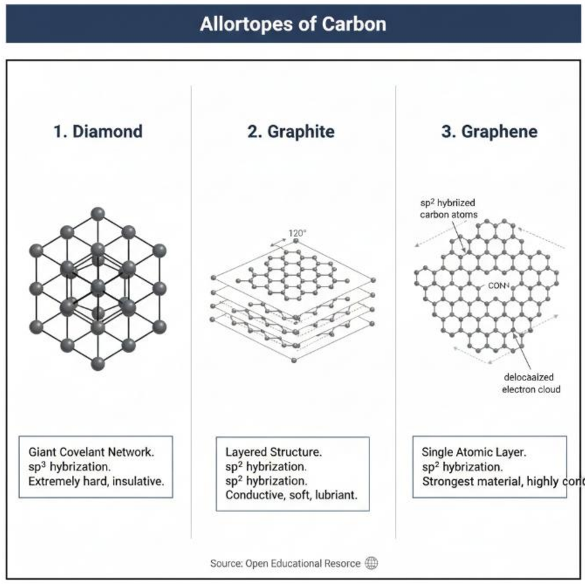

Plate 5.3: Allotropes of carbon

5.3.3 Comparative trends within Groups 13 and 14

Group 13 elements generally form compounds with +3 oxidation states, but heavier members like thallium show +1 due to the inert pair effect. Group 14 elements typically form compounds with +4 oxidation states, but heavier members like lead show +2 for the same reason. Bonding trends also differ: boron forms covalent compounds, while aluminium forms ionic compounds with covalent character. Carbon forms diverse allotropes and organic compounds, while silicon is more restricted but vital in materials science.

Fill in the blank: The tendency of heavier elements to show lower oxidation states, such as +1 or +2, is explained by the __________ effect.

Comparison of Groups 13 and 14: Oxidation States & Bonding

Feature	Group 13 (Boron Group)	Group 14 (Carbon Group)
Valence Configuration	ns^2np^1	ns^2np^2
Max Oxidation State	**+3** (Loss of all 3 valence e^-)	**+4** (Loss/Sharing of all 4 valence e^-)
Inert Pair State	**+1** (Loss of only p electron)	**+2** (Loss of only p electrons)
Primary Bonding	Covalent (lighter) to Ionic (heavier)	Covalent (lighter) to Ionic (heavier)
Inert Pair Impact	$Tl(I)$ is more stable than $Tl(III)$	$Pb(II)$ is more stable than $Pb(IV)$
Relativistic Effects	High in Thallium ($Z = 81$)	High in Lead ($Z = 82$)

Box 5.3: Comparative trends in Groups 13 and 14

Group 13: common oxidation state +3, inert pair effect leads to +1 in heavier elements

Group 14: common oxidation state +4, inert pair effect leads to +2 in heavier elements
Both groups: bonding and reactivity influenced by periodic trends and relativistic effects

Pilot questions 5.3

Boron compounds are often described as __________ because they do not strictly follow the octet rule.
A. Electron-deficient
B. Electron-rich
C. Ionic
D. Metallic
(Linked to SLO 5.3)

Diamond, graphite, and graphene are examples of carbon __________.
A. Isotopes
B. Allotropes
C. Ions
D. Compounds
(Linked to SLO 5.4)

The tendency of heavier elements to show lower oxidation states, such as +1 or +2, is explained by the __________ effect.
A. Shielding
B. Inert pair
C. Resonance
D. Hybridisation
(Linked to SLO 5.3 and SLO 5.4)

Give one industrial use of aluminium oxide (Al_2O_3).
(Linked to SLO 5.3)

Explain why silicon dioxide (SiO_2) is important in materials science.
(Linked to SLO 5.4)

5.4 Structure and Chemistry of Group 15 and Group 16 Compounds

5.4.1 Nitrogen and phosphorus compounds – bonding and reactivity

Nitrogen is a non-metal in Group 15 with five valence electrons. It commonly forms covalent bonds, as seen in ammonia (NH_3), where nitrogen shares electrons with hydrogen. Nitrogen also forms multiple bonds, such as the triple bond in nitrogen gas (N_2), which makes it very stable. **Phosphorus**, also in Group 15, has larger atomic size and lower electronegativity, allowing it to form extended structures like phosphorus pentachloride (PCl_5) and allotropes such as white and red phosphorus. Nitrogen compounds are vital in fertilisers and explosives, while phosphorus compounds are used in detergents and matches.

Fill in the blank: The stability of nitrogen gas (N_2) is due to the presence of a __________ bond between the two atoms.

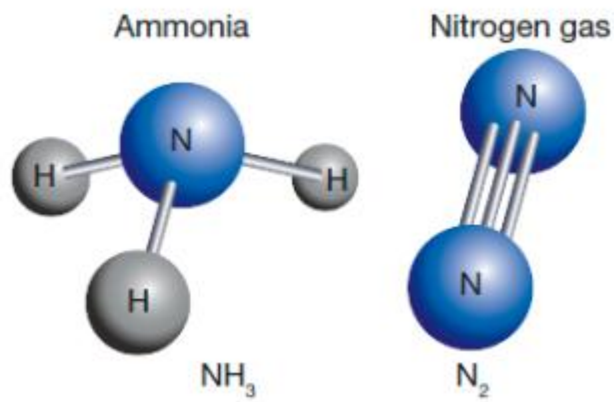

Figure 5.4: Bonding in nitrogen and ammonia

5.4.2 Oxygen and sulphur compounds – bonding, allotropes, and reactivity

Oxygen is a Group 16 element with six valence electrons. It forms diatomic molecules (O_2) with a double bond, making it essential for respiration and combustion. Oxygen also forms allotropes such as ozone (O_3), which protects life by absorbing harmful ultraviolet radiation. **Sulphur**, another Group 16 element, exists in several allotropes, including rhombic and monoclinic sulphur. It forms compounds such as hydrogen sulphide (H_2S) and sulphur dioxide (SO_2), which are important in industry but can also cause pollution.

Fill in the blank: The most common allotropes of sulphur are __________ and __________ sulphur.

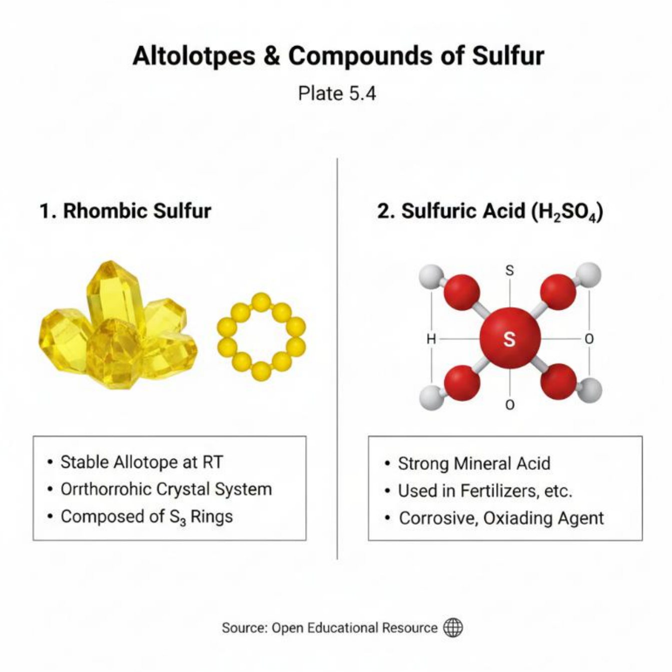

Plate 5.4: Allotropes and compounds of Sulphur

5.4.3 Comparative trends within Groups 15 and 16

Group 15 elements generally form compounds with oxidation states ranging from –3 to +5, while Group 16 elements range from –2 to +6. The tendency of heavier elements in both groups to show lower oxidation states is explained by the **inert pair effect**, where the outermost s-electrons are less likely to participate in bonding. This trend is particularly evident in bismuth (Group 15) and polonium (Group 16).

Fill in the blank: The reluctance of heavier elements to use their outermost s-electrons in bonding is known as the __________ effect.

Comparison of Groups 15 and 16: Oxidation States & Trends

Feature	Group 15 (Pnictogens)	Group 16 (Chalcogens)
Valence Configuration	ns^2np^3	ns^2np^4
Common Negative State	-3 (e.g., NH_3, PH_3)	-2 (e.g., H_2O, H_2S)
Max Positive State	+5 (e.g., HNO_3, PCl_5)	+6 (e.g., H_2SO_4, SF_6)
Inert Pair State	+3 (e.g., $BiCl_3$)	+4 (e.g., TeO_2, SeO_2)
Heaviest Element	Bismuth (Bi)	Polonium (Po)
Inert Pair Impact	$Bi(V)$ is highly oxidizing; $Bi(III)$ is very stable.	$Po(VI)$ is rare; $Po(IV)$ is the most stable state.

Box 5.4: Comparative trends in Groups 15 and 16

Group 15: oxidation states –3 to +5, inert pair effect in heavier elements
Group 16: oxidation states –2 to +6, inert pair effect in heavier elements
Both groups: essential compounds in biological and industrial systems

Pilot questions 5.4

The stability of nitrogen gas (N_2) is due to the presence of a __________ bond between the two atoms.
A. Single
B. Double
C. Triple
D. Ionic
(Linked to SLO 5.5)

The most common allotropes of sulphur are __________ and __________ sulphur.
A. Rhombic; monoclinic
B. Cubic; tetragonal
C. Amorphous; crystalline
D. Hexagonal; cubic
(Linked to SLO 5.6)

The reluctance of heavier elements to use their outermost s-electrons in bonding is known as the __________ effect.
A. Shielding
B. Inert pair
C. Resonance
D. Hybridisation
(Linked to SLO 5.5 and SLO 5.6)

Give one example of a phosphorus compound important in agriculture.
(Linked to SLO 5.5)

Explain why sulphuric acid (H_2SO_4) is considered an important industrial compound.
(Linked to SLO 5.6)

5.5 Structure and Chemistry of Group 17 and Group 18 Compounds

5.5.1 Halogens (Group 17) – bonding, reactivity, and applications

Halogens are the elements in Group 17 of the periodic table, including fluorine, chlorine, bromine, iodine, and astatine. They are highly reactive non-metals with seven valence electrons, which makes them eager to gain one electron to achieve a stable octet. Their compounds, such as sodium chloride (NaCl) and hydrogen chloride (HCl), are common and widely used. Halogens are strong oxidising agents, and their reactivity decreases down the group. Applications include disinfectants, bleaching agents, and pharmaceuticals.

Fill in the blank: Halogens are highly reactive because they have __________ valence electrons.

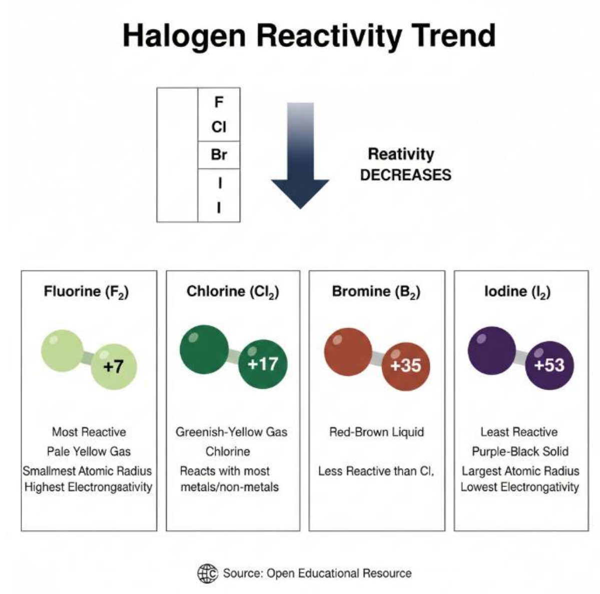

Figure 5.5: Reactivity trend of halogens in Group 17

AI prompt: "Generate a labelled diagram showing the reactivity trend of halogens from fluorine to iodine."
Search string: "halogen reactivity trend periodic table OER"

5.5.2 Noble gases (Group 18) – bonding, compounds, and uses

Noble gases are the elements in Group 18: helium, neon, argon, krypton, xenon, and radon. They have complete valence shells, making them chemically inert under most conditions. Bonding in noble gases is rare, but compounds such as xenon fluorides (XeF_2, XeF_4) demonstrate that heavier noble gases can form stable compounds under specific conditions. Noble gases are used in lighting (neon signs), shielding gases in welding (argon), and medical imaging (xenon). Their inertness makes them valuable in applications where reactivity must be avoided.

Fill in the blank: Noble gases are generally inert because they have __________ valence shells.

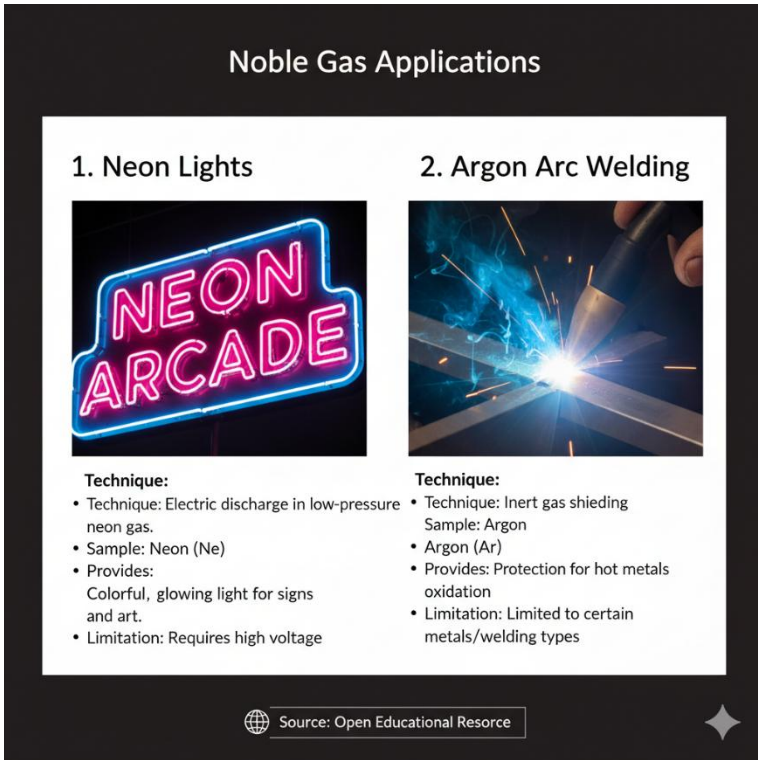

Plate 5.5: Applications of noble gases

5.5.3 Comparative trends between Groups 17 and 18

Group 17 elements are highly reactive non-metals, while Group 18 elements are chemically inert. Halogens readily form ionic and covalent compounds, whereas noble gases rarely form compounds. Reactivity decreases down Group 17, while stability increases down Group 18. Halogens are essential in everyday life, from water purification to pharmaceuticals, while noble gases are indispensable in lighting, electronics, and medical technologies.

Fill in the blank: The reactivity of halogens __________ down the group, while noble gases remain largely __________.

Comparison of Halogens and Noble Gases

Feature	Group 17: Halogens	Group 18: Noble Gases
Valence Electrons	7 (ns^2np^5)	8 (ns^2np^6)*
Chemical Nature	**Highly Reactive**; strong oxidizing agents.	**Inert / Unreactive**; extremely stable.
Diatomic vs. Monatomic	Exist as **diatomic molecules** (e.g., F_2, Cl_2).	Exist as **monatomic atoms** (e.g., He, Ne, Ar).
Reactivity Trend	**Decreases** down the group.	Remains **extremely low** (slight increase in heavier elements).
Common Ion State	-1 Anions (X^-)	Usually **0** (No ions formed).
Bonding Style	Ionic and Covalent.	Limited covalent compounds (mostly Xe and Kr).

Box 5.5: Comparative trends between Groups 17 and 18

Group 17: seven valence electrons, highly reactive, strong oxidising agents
Group 18: full valence shells, inert, limited compound formation in heavier elements
Contrast: halogens show decreasing reactivity down the group, noble gases remain stable

Pilot questions 5.5

Halogens are highly reactive because they have __________ valence electrons.
A. Five
B. Six
C. Seven
D. Eight
(Linked to SLO 5.7)

Noble gases are generally inert because they have __________ valence shells.
A. Empty
B. Half-filled
C. Full
D. Unstable
(Linked to SLO 5.8)

The reactivity of halogens __________ down the group, while noble gases remain largely __________.
A. Increases; reactive
B. Decreases; inert
C. Remains constant; unstable
D. Decreases; reactive
(Linked to SLO 5.7 and SLO 5.8)

Give one industrial application of chlorine.
(Linked to SLO 5.7)

Explain why xenon can form compounds while helium cannot.
(Linked to SLO 5.8)

Series Summary

This Series on **Structure and Chemistry of Representative Main Group Compounds** was designed to help you understand the periodic trends, bonding, reactivity, and applications of elements in Groups 1 to 18. Beginning with an introduction to the main group elements, you explored their position in the periodic table, general properties, and industrial importance. You then examined the structures and chemistry of Group 1 and Group 2 compounds, comparing their reactivity and bonding. Moving forward, you studied Group 13 and 14 compounds, focusing on boron, aluminium, carbon, and silicon, including their unique bonding features and allotropes. The Series continued with Group 15 and 16 compounds, highlighting nitrogen, phosphorus, oxygen, and sulphur, their allotropes, and comparative trends. Finally, you analysed Group 17 halogens and Group 18 noble gases, contrasting their reactivity and uses in everyday life and industry.

By completing this Series, you should now be able to **describe the position and properties of main group elements (SLO 5.1)**, **explain the bonding and reactivity of Groups 1 and 2 compounds (SLO 5.2)**, **analyse the bonding and applications of Group 13 compounds (SLO 5.3)**, **evaluate the structures and reactivity of Group 14 compounds (SLO 5.4)**, **explain the bonding and reactivity of Group 15 compounds (SLO 5.5)**, **describe the structural features and allotropes of Group 16 compounds (SLO 5.6)**, **analyse the bonding and applications of Group 17 compounds (SLO 5.7)**, and **evaluate the bonding and uses of Group 18 compounds (SLO 5.8)**. These outcomes ensure you can connect periodic trends with practical applications, giving you a comprehensive understanding of the chemistry of the main group elements.

Glossary of Terms

Alkaline earth metals: Elements in Group 2 of the periodic table, such as magnesium and calcium, which have two valence electrons and form metallic structures with moderate reactivity.

Allotropes: Different structural forms of the same element, such as diamond and graphite for carbon, or oxygen and ozone for oxygen.

Atomic radius: The distance from the nucleus of an atom to the outermost electrons, which generally decreases across a period and increases down a group.

Bonding: The way atoms are held together in compounds, which can be ionic (transfer of electrons), covalent (sharing of electrons), or metallic (delocalised electrons).

Halogens: Elements in Group 17 of the periodic table, including fluorine, chlorine, bromine, and iodine, which are highly reactive non-metals with seven valence electrons.

Inert pair effect: The tendency of heavier elements in Groups 13 to 16 to show lower oxidation states because their outermost s-electrons are less likely to participate in bonding.

Ionisation energy: The energy required to remove an electron from an atom, which increases across a period and decreases down a group.

Main group elements: Elements in Groups 1, 2, and 13 to 18 of the periodic table, characterised by valence electrons in the s and p orbitals.

Noble gases: Elements in Group 18 of the periodic table, such as helium, neon, and argon, which have complete valence shells and are chemically inert.

Oxidation state: The charge an atom appears to have in a compound, reflecting how many electrons it has gained or lost.

Periodic trends: Predictable changes in properties of elements across periods and groups, such as atomic radius, ionisation energy, and electronegativity.

Reactivity: The tendency of an element to undergo chemical reactions, influenced by factors such as valence electrons and atomic size.

Valence electrons: Electrons in the outermost shell of an atom that determine its chemical properties and bonding behaviour.

Concept Check Questions [Series 5]

Objective Questions

The main group elements are found in Groups __________________ of the periodic table.
(Linked to SLO 5.1)

Which of the following compounds is electron-deficient?
A. Boron trifluoride (BF_3)
B. Sodium chloride ($NaCl$)
C. Calcium carbonate ($CaCO_3$)
D. Neon (Ne)
(Linked to SLO 5.3)

Graphite conducts electricity because it contains __________________ electrons that move freely between layers.
(Linked to SLO 5.4)

Ozone (O_3) protects life on Earth by absorbing harmful __________________ radiation.
(Linked to SLO 5.6)

Noble gases are chemically inert because they have __________________ valence shells.
(Linked to SLO 5.8)

Short-Answer Questions

Define alkali metals and explain why they are highly reactive.
(Linked to SLO 5.2)

State one industrial application of aluminium compounds.
(Linked to SLO 5.3)

Describe why diamond is hard but graphite is soft.
(Linked to SLO 5.4)

Give one example of a phosphorus compound and its common use.
(Linked to SLO 5.5)

Explain why xenon can form compounds while helium cannot.
(Linked to SLO 5.8)

Long-Answer Questions

Analyse the periodic trends in Groups 1 and 2, focusing on reactivity, bonding, and solubility of their compounds.
(Linked to SLO 5.2)

Evaluate the structural features and applications of carbon allotropes, comparing them with silicon compounds.
(Linked to SLO 5.4)

Assess the similarities and differences between halogens and noble gases in terms of bonding, reactivity, and industrial applications.
(Linked to SLO 5.7 & 5.8)

Answers to Concept Check Questions [Series 5]

Objective Questions

Groups 1, 2, and 13–18
A. Boron trifluoride (BF_3)
Delocalised
Ultraviolet
Complete

Short-Answer Questions

Alkali metals are Group 1 elements with one valence electron. They are highly reactive because they easily lose this electron to form stable cations.
Aluminium compounds are used in packaging (aluminium foil), construction (aluminium oxide in ceramics), and catalysis.
Diamond is hard due to its three-dimensional tetrahedral covalent network, while graphite is soft because of weak forces between layers.
Phosphorus pentachloride (PCl_5) is used in the manufacture of detergents and matches.
Xenon can form compounds because its outer electrons are less tightly held, whereas helium's small size and complete shell make it inert.

Long-Answer Questions

Question 1

Basic response: Group 1 elements are more reactive than Group 2 because they need to lose only one electron. Group 1 compounds are generally soluble and form strong electrolytes, while Group 2 compounds are less soluble but have higher lattice energies.
Value-added response: Learners may extend by discussing biological roles of Group 2 compounds (e.g., calcium in bones) and industrial uses of Group 1 compounds (e.g., sodium hydroxide in soap making).

Question 2

Basic response: Carbon allotropes such as diamond, graphite, and graphene show diverse structures and properties. Diamond is hard, graphite conducts electricity, and graphene is strong and flexible. Silicon compounds, such as quartz, form extended covalent networks but are less versatile.
Value-added response: Outstanding learners may extend by linking carbon allotropes to modern applications (nanotechnology, electronics) and silicon compounds to semiconductors and solar cells.

Question 3

Basic response: Halogens are highly reactive non-metals that form ionic and covalent compounds, while noble gases are inert and rarely form compounds. Halogens are used in disinfectants and pharmaceuticals, while noble gases are used in lighting and medical imaging.
Value-added response: Learners may extend by explaining how xenon compounds challenge the idea of noble gas inertness and by comparing environmental impacts of halogen compounds with the safe applications of noble gases.

Answers to Pilot Questions [Series 5]

Part 5.1: Introduction to Main Group Elements

1, 2, and 13–18
Decreases; increases
Electronics
Calcium carbonate ($CaCO_3$)
They are called representative elements because they display typical periodic trends and chemical behaviours.

Part 5.2: Structure and Chemistry of Group 1 and Group 2 Compounds

One
Divalent
More
Calcium carbonate ($CaCO_3$) or magnesium oxide (MgO)

Group 1 metals have only one valence electron, which is easily lost, making them more reactive with water than Group 2 metals.

Part 5.3: Structure and Chemistry of Group 13 and Group 14 Compounds

Electron-deficient
Allotropes
Inert pair
Used in construction materials and abrasives
Silicon dioxide (SiO_2) is important because it is a major component of glass and semiconductors.

Part 5.4: Structure and Chemistry of Group 15 and Group 16 Compounds

Triple
Rhombic; monoclinic
Inert pair
Phosphates (used in fertilisers)
Sulphuric acid is important as a key industrial chemical used in fertilisers, detergents, and manufacturing.

Part 5.5: Structure and Chemistry of Group 17 and Group 18 Compounds

Seven
Full
Decreases; inert
Chlorine is used in water treatment and disinfectants.
Xenon can form compounds because its outer electrons are more easily polarised, while helium's small size and full shell make it completely inert.

References and Attributions [Series 5]

Textual Sources

Atkins, P., & Jones, L. (2010). *Chemical Principles: The Quest for Insight* (5th ed.). Oxford University Press.
Housecroft, C. E., & Sharpe, A. G. (2018). *Inorganic Chemistry* (5th ed.). Pearson.
IUPAC. (1997). *Compendium of Chemical Terminology (the "Gold Book").*

Illustrations (Figures, Plates, Tables, Boxes)

Figure 5.1 Position of main group elements in the periodic table
AI prompt: "Generate a labelled periodic table highlighting Groups 1, 2, and 13–18 as main group elements."
Search string: "periodic table main group elements diagram OER"

Plate 5.1 Periodic trends in main group elements
AI prompt: "Create an image showing periodic trends in atomic radius, ionisation energy,

and electronegativity across periods and down groups."
Search string: "periodic trends atomic radius ionisation energy electronegativity OER"

Box 5.1 Examples of main group compounds in daily life
AI prompt: "Generate a table listing examples of main group compounds and their uses, including NaCl, $CaCO_3$, SiO_2, and phosphates."
Search string: "examples of main group compounds and uses OER"

Figure 5.2 Reaction of sodium with water
AI prompt: "Generate a labelled diagram showing sodium reacting with water to produce sodium hydroxide and hydrogen gas."
Search string: "alkali metals reaction with water diagram OER"

Plate 5.2 Common compounds of alkaline earth metals
AI prompt: "Create an image showing examples of alkaline earth metal compounds such as calcium carbonate and magnesium oxide."
Search string: "alkaline earth metals compounds examples OER"

Box 5.2 Comparative trends between Groups 1 and 2
AI prompt: "Generate a table comparing properties of Group 1 and Group 2 elements, including valence electrons, reactivity, and compound types."
Search string: "comparison of Group 1 and Group 2 elements chemistry OER"

Figure 5.3 Structures of representative boron and aluminium compounds
AI prompt: "Generate a labelled diagram showing the structure of boron trifluoride and aluminium oxide."
Search string: "boron trifluoride aluminium oxide structure OER"

Plate 5.3 Allotropes of carbon
AI prompt: "Create an image showing the structures of diamond, graphite, and graphene as carbon allotropes."
Search string: "carbon allotropes diamond graphite graphene OER"

Box 5.3 Comparative trends in Groups 13 and 14
AI prompt: "Generate a table comparing oxidation states and bonding trends in Groups 13 and 14, including inert pair effect."
Search string: "Group 13 Group 14 oxidation states inert pair effect OER"

Figure 5.4 Bonding in nitrogen and ammonia
AI prompt: "Generate a labelled diagram showing the triple bond in nitrogen gas and the structure of ammonia."
Search string: "nitrogen triple bond ammonia structure OER"

Plate 5.4 Allotropes and compounds of sulphur
AI prompt: "Create an image showing rhombic sulphur crystals and the molecular structure of sulphuric acid."
Search string: "sulphur allotropes rhombic monoclinic sulphuric acid OER"

Box 5.4 Comparative trends in Groups 15 and 16
AI prompt: "Generate a table comparing oxidation states and inert pair effect in Groups

15 and 16."
Search string: "Group 15 Group 16 oxidation states inert pair effect OER"

Figure 5.5 Reactivity trend of halogens in Group 17
AI prompt: "Generate a labelled diagram showing the reactivity trend of halogens from fluorine to iodine."
Search string: "halogen reactivity trend periodic table OER"

Plate 5.5 Applications of noble gases
AI prompt: "Create an image showing neon lights and argon shielding gas in welding as applications of noble gases."
Search string: "noble gases applications neon argon OER"

Box 5.5 Comparative trends between Groups 17 and 18
AI prompt: "Generate a table comparing properties of halogens and noble gases, including valence electrons, reactivity, and applications."
Search string: "comparison halogens noble gases chemistry OER"

Notes on Attribution

AI-generated illustrations are documented with prompts and should be noted with the generation date and platform used.
Where OERs are used, attribution must comply with the licence terms of the source.
References are presented in APA style for consistency.