

Molecular Shape and Polarity: Why 3D Structure Determines Behavior

STRUCTURE DRIVES PROPERTIES DRIVES THE REAL WORLD



Roadmap:

electron domains → molecular shape →
bond dipoles → net polarity → real-world behavior



Goals:

predict shape, predict polarity, explain everyday
and professional consequences



Anchor examples:

water dissolving salt, CO₂ nonpolar,
oil–water separation



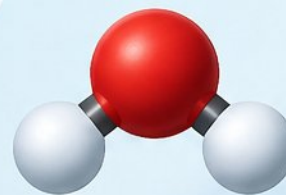
Prior knowledge check:

Lewis structures, electronegativity,
covalent and ionic bonding



Why it matters:

solubility, boiling point, drug delivery,
detergents, biological membranes



H₂O



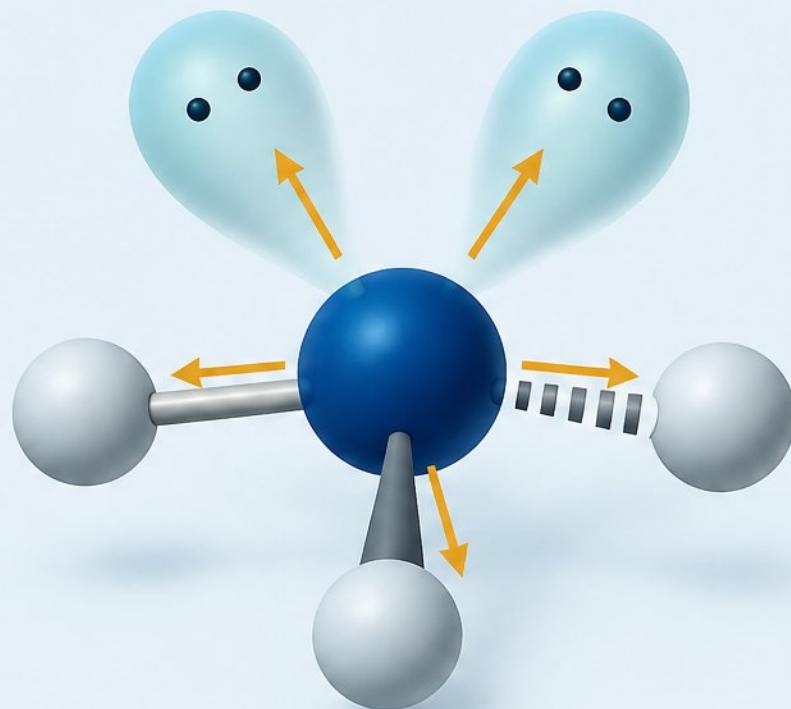
CO₂



Electron Domains and the VSEPR Model



- Electron domains: bonds (single, double, triple) and lone pairs; each counts as one
- Domains repel and spread out to minimize repulsion
- Steric number = bonded atoms + lone pairs on the central atom
- Repulsion hierarchy: lone pair–lone pair > lone pair–bond pair > bond pair–bond pair
- Method: draw Lewis structure, count domains, choose lowest-repulsion arrangement



Steric number

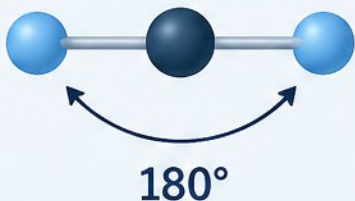
= bonded atoms + lone pairs
on the central atom

Electron Domain Geometries and Ideal Angles



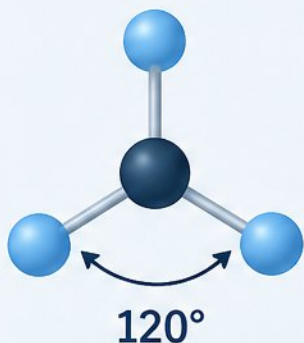
2 domains

linear



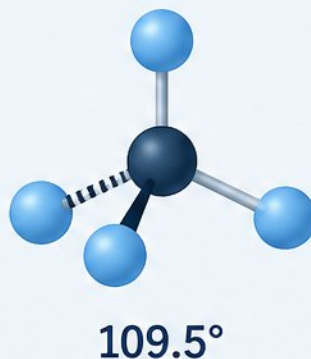
3 domains

trigonal planar



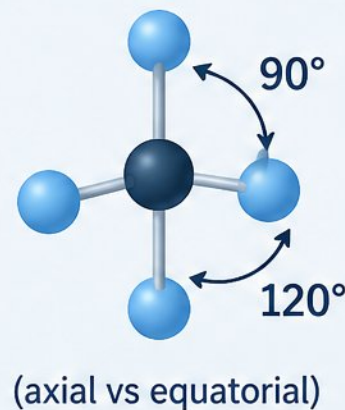
4 domains

tetrahedral



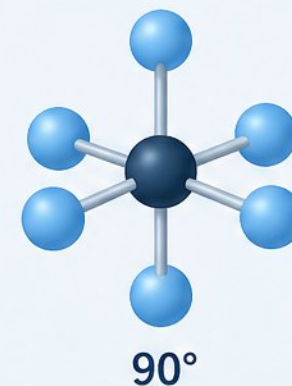
5 domains

trigonal bipyramidal



6 domains

octahedral



7-8 domains are advanced cases



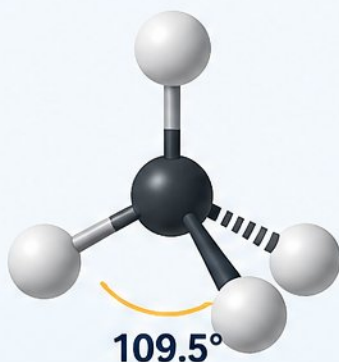
- Multiple bonds count as one domain;
- VSEPR is a simplified electrostatic model



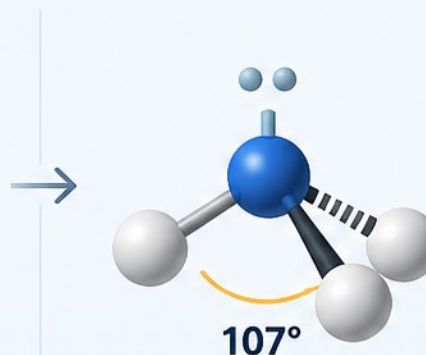
From Electron Domain Geometry to Molecular Geometry

- Molecular geometry names only atom positions; lone pairs stay but are invisible
- Four domains: 0, 1, 2 lone pairs → tetrahedral, trigonal pyramidal, bent
- Five domains: 1, 2, 3 lone pairs → seesaw, T-shaped, linear
- Six domains: 1 and 2 lone pairs → square pyramidal, square planar
- Lone pairs take more room, squeezing angles: CH_4 109.5° , NH_3 107° , H_2O 104.5°

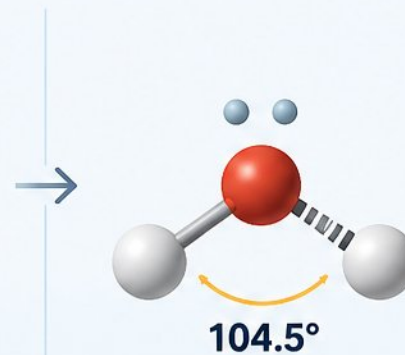
: Four Electron Domains (Tetrahedral Electron Geometry) :



Tetrahedral
(0 lone pairs)

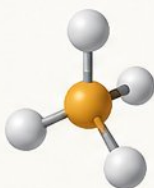


Trigonal pyramidal
(1 lone pair)

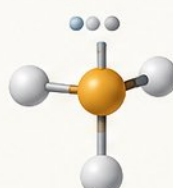


Bent
(2 lone pairs)

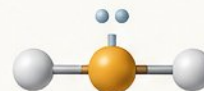
Five Electron Domains



Seesaw
(1 lone pair)

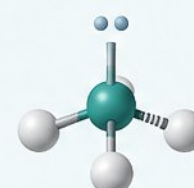


T-shaped
(2 lone pairs)



Linear
(3 lone pairs)

Six Electron Domains



Square pyramidal
(1 lone pair)

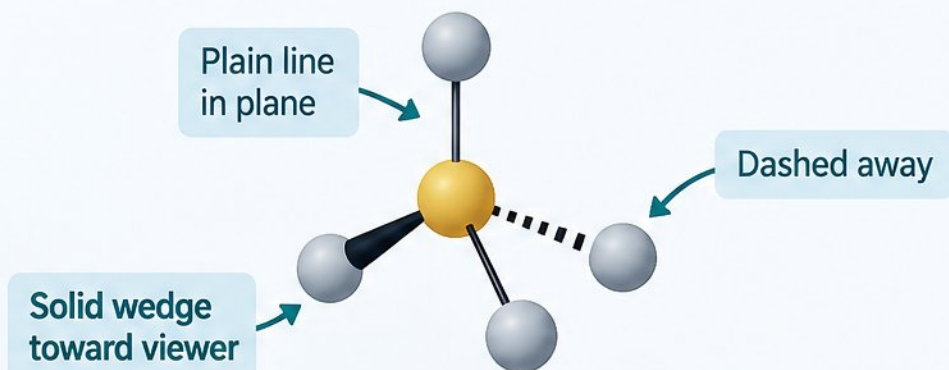


Square planar
(2 lone pairs)

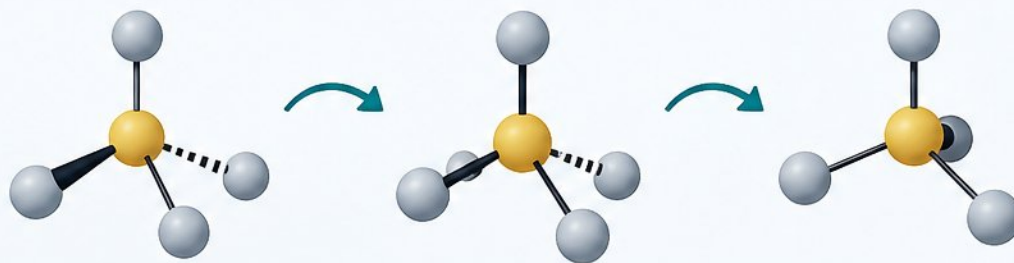
Reading and Drawing 3D Molecular Structures

- Wedge-dash: solid wedge toward viewer, dashed away, plain lines in plane
- Rotating a model changes the view, not the molecule — practice mental rotation
- Physical model kits and simulations build spatial reasoning better than flat drawings
- Electron geometry answers a domain count; molecular geometry answers atom positions
- Anchor shapes: linear, trigonal planar, bent, tetrahedral, trigonal pyramidal, seesaw, T-shaped, octahedral, square planar

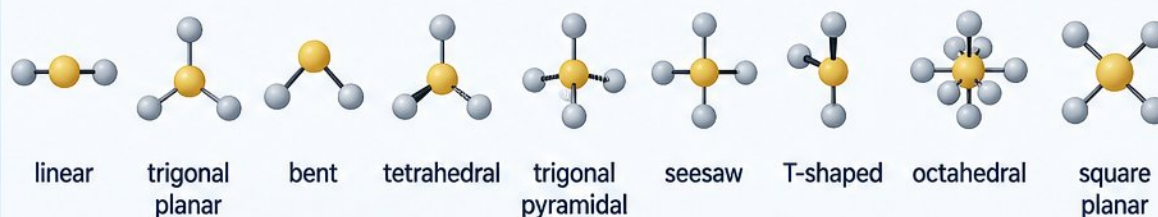
Wedge-Dash Convention (Tetrahedral Example)



Same Molecule, Different Views (Rotation)



Common Molecular Geometry Shapes



Electronegativity and Bond Polarity

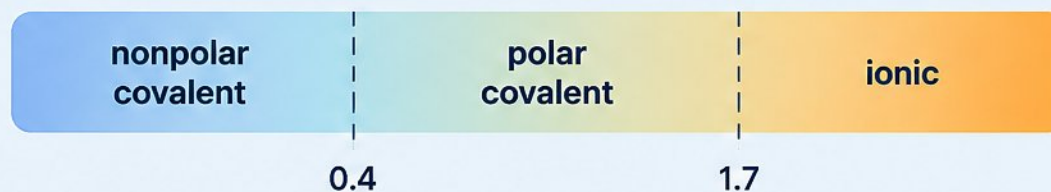


- Electronegativity: an atom's pull on shared electrons
- Increases across a period, decreases down a group
- $\Delta EN < 0.4$ nonpolar; 0.4–1.7 polar covalent; > 1.7 ionic
- Polar bonds carry $\delta+$ and $\delta-$, with a dipole arrow toward the more electronegative atom
- Examples: HCl polar; H₂O very polar O–H; C–Cl polar; C–H essentially nonpolar

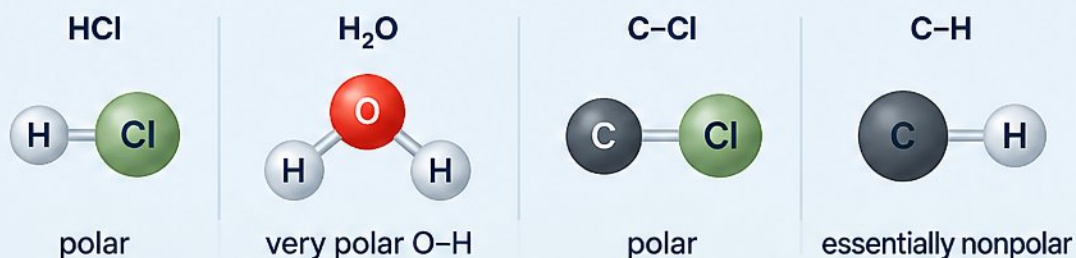
Electronegativity Trend



Bond Type by Electronegativity Difference (ΔEN)

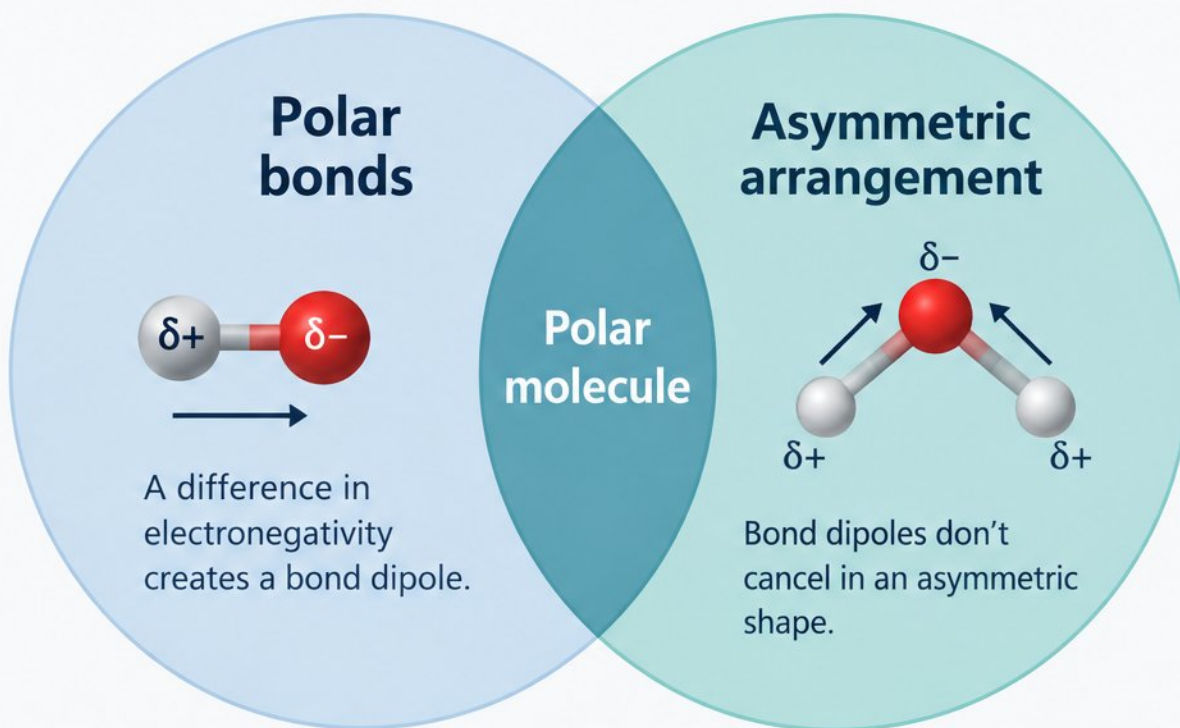


Examples



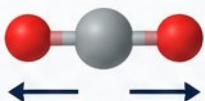
Molecular Polarity and Net Dipole Moments

- Molecular polarity needs polar bonds plus an asymmetric arrangement
- Bond dipoles add head to tail as vectors; the sum is the net dipole
- Symmetric polar bonds cancel: CO_2 linear, CCl_4 tetrahedral, BF_3 trigonal planar
- Asymmetric bonds usually don't cancel: H_2O bent, NH_3 pyramidal, CHCl_3 polar
- No polar bonds means a nonpolar molecule, whatever the geometry

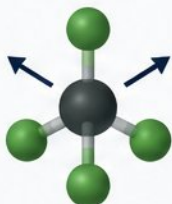


Symmetric polar bonds cancel

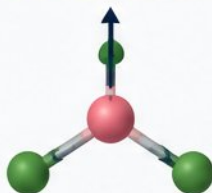
CO_2 linear



CCl_4 tetrahedral

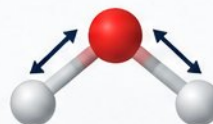


BF_3 trigonal planar

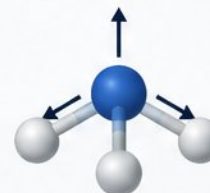


Asymmetric bonds usually don't cancel

H_2O bent



NH_3 pyramidal



CHCl_3 polar



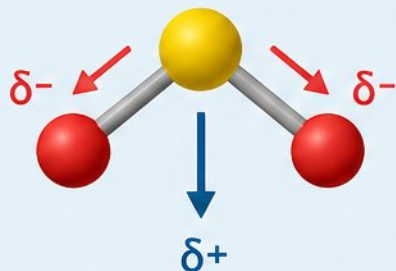
Symmetry, Lone Pairs, and Hard Cases

MOLECULAR SHAPE • DIPOLES • REAL-WORLD EXAMPLES

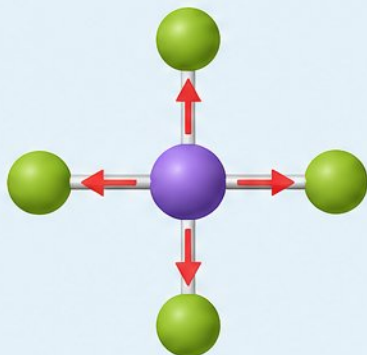
- **Symmetry** cancels identical bond dipoles: linear, trigonal planar, tetrahedral, square planar
- **Lone pairs** add to the net dipole even without being atoms: H_2O , NH_3 are polar
- **Expanded octets**: treat each central atom separately, then combine local dipoles
- **Hard cases**: SO_2 bent/polar, XeF_4 square planar/nonpolar, SF_4 seesaw/polar
- **Pitfalls**: polar bond $\neq$ polar molecule; ignoring lone pairs; reading 2D drawings as flat



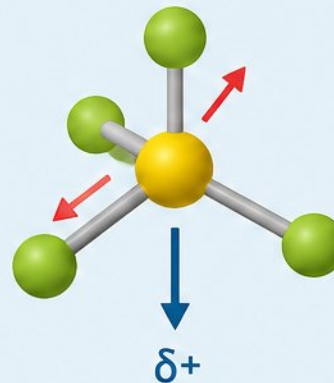
Bent / Polar



Square Planar / Nonpolar

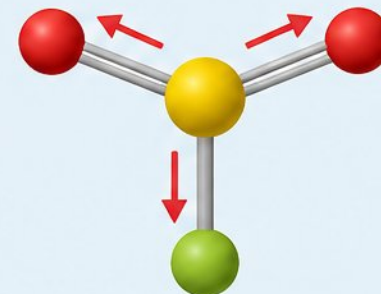


Seesaw / Polar



Expanded Octet Example

Central Atoms with Local Dipoles



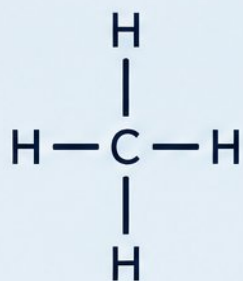
Decision Flowchart: Polar or Nonpolar?



1

Step 1:

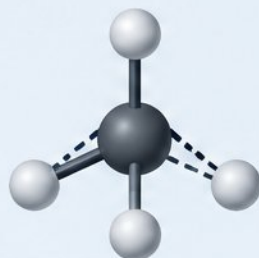
Draw the correct
Lewis structure



2

Step 2:

Count domains;
name the
molecular geometry



3

Step 3:

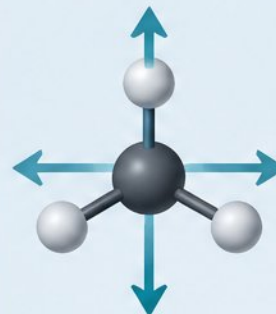
Check bond
polarity with
electronegativity
differences



4

Step 4:

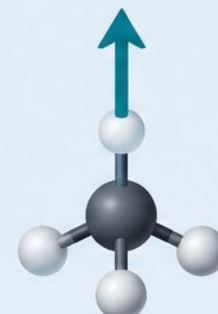
Look for symmetry
or lone pairs that
cancel or reinforce
dipoles



5

Step 5:

State your verdict;
sketch the net
dipole arrow



Intermolecular Forces and Physical Properties

- Force hierarchy: hydrogen bonding > dipole–dipole > London dispersion
- Stronger IMFs: higher melting and boiling points, lower vapor pressure
- H-bonding needs H on N, O, or F; explains water, NH_3 , HF anomalies
- Larger, more polarizable molecules: stronger dispersion forces
- Branching lowers boiling point; shape affects solid packing and melting point

Intermolecular Force Hierarchy

Hydrogen
bonding

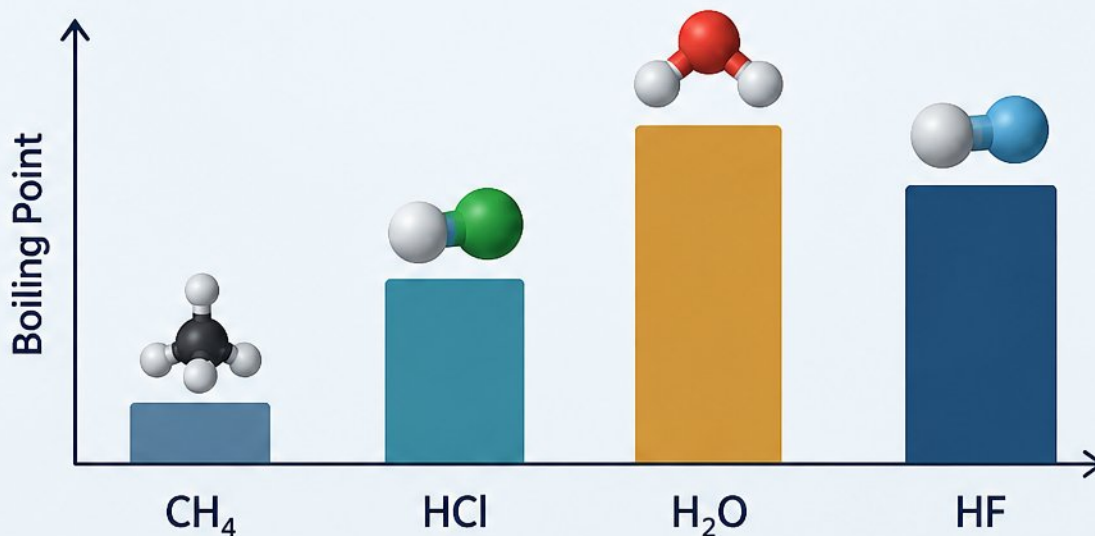
>

Dipole–dipole

>

London
dispersion

Boiling Points Reflect Intermolecular Forces



Stronger intermolecular forces lead to higher boiling points.

Like Dissolves Like: Solubility in Action

SAME POLARITY. STRONGER SOLUTIONS.



Polar solutes dissolve in polar solvents; nonpolar solutes dissolve in nonpolar solvents



Small alcohols mix with water; butanol onward separates as the tail grows



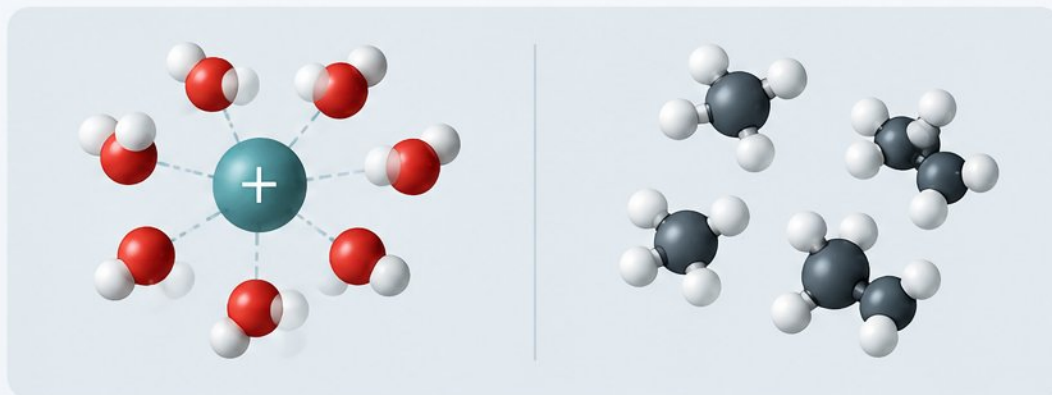
Water's ion-dipole interactions dissolve NaCl; hexane cannot stabilize ions



CO₂ is nonpolar yet water-soluble: it forms carbonic acid with water



Everyday pairings: water versus oil, ethanol versus hexane, soap removing grease



Applications in Biology, Medicine, and Materials



Hydrogen bonding holds DNA base pairs and drives protein folding; water is life's solvent



Lipophilicity ($\log P$) governs membrane permeability and delivery route



API polarity decides drug location in nanoemulsions and skin permeation



Molecular chameleons and polarity-switching prodrugs make polarity tunable



Surfactants pair polar heads with nonpolar tails; chromatography separates by polarity



Teaching Strategies, Demonstrations, and Misconceptions



PhET simulations plus physical models build 3D spatial reasoning



Let learners derive VSEPR arrangements by adding domains one at a time



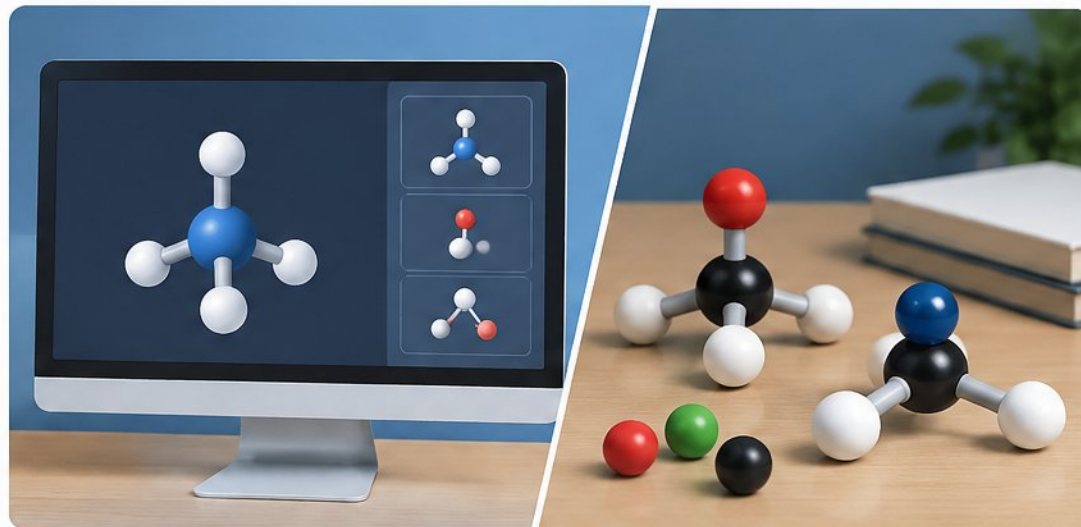
Low-cost demos: food coloring in water vs. hexane; charged balloon; oil-water



Misconceptions: polar bonds always mean polar molecule; lone pairs ignored; flat 2D drawings



Assess by predicting shape/polarity from formula and justifying with a model



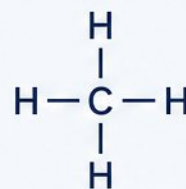
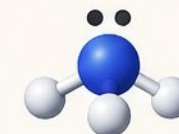
Common Misconceptions



Polar bonds always mean polar molecule



Lone pairs ignored

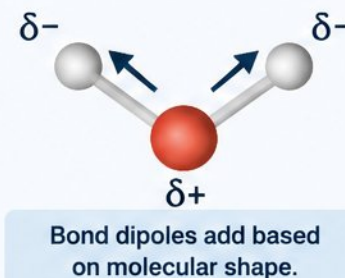


Flat 2D drawings



Guided Practice, Self-Check, and Summary

- **Worked examples:** CH₄, NH₃, H₂O, CO₂, CCl₄, CHCl₃, SO₂ — Lewis structure to polarity verdict
- **Error review:** misread symmetry, miscounted domains, misplaced lone pairs
- **Self-check quiz** with answers and reasoning, plus one-page summary rules
- **Transfer task:** defend shape and polarity of a molecule from your field
- **Takeaway:** shape plus bond dipoles determines polarity, which predicts behavior



Molecule	Lewis structure (dots = lone pairs)	Domain count	Geometry	Polarity verdict
CH ₄	<pre> H H — C — H H </pre>	4	Tetrahedral	Nonpolar
NH ₃	<pre> H H — N — H H </pre>	4	Trigonal pyramidal	Polar
H ₂ O	<pre> H H — O — H H </pre>	4	Bent	Polar
CO ₂	<pre> O = C = O : : : : : : </pre>	2	Linear	Nonpolar
CCl ₄	<pre> Cl Cl — C — Cl Cl </pre>	4	Tetrahedral	Nonpolar
CHCl ₃	<pre> Cl H — C — Cl Cl </pre>	4	Tetrahedral	Polar
SO ₂	<pre> O = S = O : : : : : : </pre>	3	Bent	Polar

Self-Check Quiz

Answer each question, then check the provided answers and reasoning.

1 What is the molecular geometry and polarity of CH₄?

2 What is the molecular geometry and polarity of NH₃?

3 Why is CO₂ nonpolar even though the C=O bonds are polar?

4 Which has a larger net dipole moment, H₂O or SO₂? Explain.

5 Choose a molecule from your field and defend its shape and polarity.



**One-page
summary
rules**

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