

Molecular Geometry & Bonding Theories

VSEPR shapes, bond angles, polarity, hybridization, sigma/pi bonds, and molecular-orbital basics.

01 Bond polarity

CORE RULE

Identical atoms → nonpolar bond; different electronegativity → polar bond. A small nonzero ΔEN (e.g. Cl–Br) still gives a real bond dipole even though the ΔEN classification bin calls it 'nonpolar covalent'.

02 Count electron domains

CORE RULE

On the central atom, count domains = bonding pairs (a single, double, or triple bond is ONE domain each) + lone pairs + any single-electron radical.

03 Electron geometry

REFERENCE

Domains	Electron geometry	Ideal angles
2	linear	180°
3	trigonal planar	120°
4	tetrahedral	109.5°
5	trigonal bipyramidal	90° / 120° / 180°
6	octahedral	90° / 180°

04 Molecular geometry

CORE RULE

Names the arrangement of BONDS only (lone pairs are invisible to the shape). Drop lone-pair domains from the parent electron geometry: e.g. bent, trigonal pyramidal, see-saw, T-shaped, square planar, square pyramidal.

05 Lone-pair repulsion

CORE RULE

Lone pairs repel more than bonding pairs, compressing angles below ideal: H₂O 104.5° and NH₃ 107° (vs 109.5°). More lone pairs → more compression.

06 Lone-pair placement

CORE RULE

Trigonal bipyramidal: lone pairs take equatorial sites (fewer 90° neighbours) → see-saw, T-shaped, linear. Octahedral: two lone pairs go trans (opposite) → square planar.

07 Molecular polarity

CORE RULE

Symmetric arrangement of identical polar bonds → dipoles cancel → nonpolar (CO₂, BF₃, CH₄, PF₅, SF₆). Asymmetric (usually a lone pair on the central atom) → polar (H₂O, NH₃, SO₂, SCl₄).

08 Hybridization

REFERENCE

Domains	Hybridization
2	sp
3	sp ²
4	sp ³
5	sp ³ d
6	sp ³ d ²

09 Sigma & pi bonds

CORE RULE

Single = 1 σ ; double = 1 σ + 1 π ; triple = 1 σ + 2 π . Every bonded connection (including each C–H) is one σ ; π count comes only from double and triple bonds.

10 MO bond order

CORE RULE

Bond order = (bonding e[−] – antibonding e[−]) / 2. Zero means no stable bond (Ne₂). Half-integers occur for odd species: O₂[−] = 1.5, O₂⁺ = 2.5.

11 MO 2p ordering

CORE RULE

For B₂, C₂, N₂ (and CO), s-p mixing puts π_{2p} BELOW σ_{2p} . For O₂, F₂, Ne₂ the order is conventional: σ_{2p} below π_{2p} .

12 Magnetism

CORE RULE

All electrons paired → diamagnetic (weakly repelled). Any unpaired electron → paramagnetic (attracted). O₂ has 2 unpaired electrons in π^*_{2p} → paramagnetic.