CHEMWHIZ QUICK REFERENCE

TOPIC 15

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: H_2O 104.5° and NH_3 107° (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 (CO_2, BF_3, CH_4, PF_5, SF_6). Asymmetric (usually a lone pair on the central atom) → polar (H_2O, NH_3, SO_2, SCl_4).

08 Hybridization — REFERENCE

Domains	Hybridization
2	sp
3	sp^2
4	sp^3
5	sp^3d
6	sp^3d^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 (Ne_2). Half-integers occur for odd species: O_2^- = 1.5, O_2^+ = 2.5.

11 MO 2p ordering — CORE RULE

For B_2, C_2, N_2 (and CO), s-p mixing puts π_2p BELOW σ_2p. For O_2, F_2, Ne_2 the order is conventional: σ_2p below π_2p.

12 Magnetism — CORE RULE

All electrons paired → diamagnetic (weakly repelled). Any unpaired electron → paramagnetic (attracted). O_2 has 2 unpaired electrons in π^*_2p → paramagnetic.