

Chemical Bonding and Molecular Structure: one-page cheat sheet

NEET Chemistry · Unit 3 · Inorganic Chemistry

1 • Octet rule & formal charge

$$\text{F.C.} = V - L - \frac{1}{2}S$$

O₃ central O +1; double-bonded O 0; single-bonded O -1

Incomplete BeH₂, BF₃, AlCl₃ (central atom has fewer than 8 electrons)

Odd electron NO, NO₂

Expanded PF₅ (10), SF₆ (12): Period 3 onwards, empty *d*-orbitals

Trap • The octet rule cannot explain shapes or noble-gas compounds such as XeF₂, XeF₄, KrF₂.

2 • Ionic bond & Fajans' rules

Favoured by low ionisation enthalpy, high electron gain enthalpy, high lattice enthalpy

Lattice enthalpy energy to separate 1 mol of crystal into gaseous ions (NaCl: +788 kJ mol⁻¹)

More covalent when	Order
small cation	LiCl > NaCl > KCl
large anion	LiI > LiBr > LiCl > LiF
high charges	AlCl ₃ > MgCl ₂ > NaCl
18-electron cation	Cu ⁺ , Ag ⁺ > Na ⁺ , K ⁺

3 • Bond parameters & dipole moment

Bond order BO ∝ bond enthalpy ∝ 1/bond length

Resonance hybrid is more stable; CO₃²⁻ C–O bond order 1.33; O₃ O–O 128 pm

Dipole $\mu = Q \times r$; 1 D = 3.336 × 10⁻³⁰ C m

$\mu = 0$ CO₂, BF₃, BeF₂, CH₄, CCl₄, SF₆, XeF₄, *p*-dichlorobenzene

Trap • NH₃ (1.47 D): lone-pair dipole adds to N–H dipoles. NF₃ (0.23 D): it opposes them.

4 • VSEPR shapes & hybridisation

Repulsion: lp–lp > lp–bp > bp–bp. Steric number = σ bonds + lone pairs on the central atom: 2 *sp*, 3 *sp*², 4 *sp*³, 5 *sp*³*d*, 6 *sp*³*d*².

Type	Hyb.	Shape	Examples
AB ₂	<i>sp</i>	linear	BeCl ₂ , CO ₂
AB ₃	<i>sp</i> ²	trigonal planar	BF ₃ , SO ₃
AB ₂ E	<i>sp</i> ²	bent	SO ₂ , O ₃
AB ₄	<i>sp</i> ³	tetrahedral	CH ₄ , NH ₄ ⁺
AB ₃ E	<i>sp</i> ³	pyramidal	NH ₃ (107°), PCl ₃
AB ₂ E ₂	<i>sp</i> ³	bent	H ₂ O (104.5°)
AB ₅	<i>sp</i> ³ <i>d</i>	trigonal bipyramidal	PCl ₅
AB ₄ E	<i>sp</i> ³ <i>d</i>	see-saw	SF ₄
AB ₃ E ₂	<i>sp</i> ³ <i>d</i>	T-shaped	ClF ₃ , BrF ₃
AB ₂ E ₃	<i>sp</i> ³ <i>d</i>	linear	XeF ₂ , I ₃ ⁻
AB ₆	<i>sp</i> ³ <i>d</i> ²	octahedral	SF ₆
AB ₅ E	<i>sp</i> ³ <i>d</i> ²	square pyramidal	BrF ₅ , IF ₅
AB ₄ E ₂	<i>sp</i> ³ <i>d</i> ²	square planar	XeF ₄

Trap • In *sp*³*d* shapes the lone pairs sit in **equatorial** positions.

Six traps to remember

- Octet rule cannot explain shapes or noble-gas compounds.
- Smaller cation, larger anion, higher charge: more covalent character.
- Lone pairs in *sp*³*d* shapes go equatorial; XeF₂ is linear.

5 • σ and π bonds

σ head-on overlap along the axis; stronger

π sideways overlap of parallel *p*-orbitals

C–C ethane 1 σ ; ethene 1 σ + 1 π ; ethyne 1 σ + 2 π ; C₂ molecule: **two π bonds** and no σ bond

*dsp*² square planar, e.g. [Ni(CN)₄]²⁻; *sp*³*d*² and *d*²*sp*³ give octahedral

6 • Molecular orbital theory

$$\text{BO} = \frac{N_b - N_a}{2}$$

≤ 14 *e*⁻ B₂, C₂, N₂: $\pi 2p < \sigma 2p_z$ (2s–2p mixing)

> 14 *e*⁻ O₂, F₂: $\sigma 2p_z < \pi 2p$

Species	<i>e</i> ⁻	BO	Magnetism
N ₂	14	3	diamagnetic
O ₂ ⁺	15	2.5	paramagnetic
O ₂	16	2	paramagnetic
O ₂ ⁻	17	1.5	paramagnetic
O ₂ ²⁻	18	1	diamagnetic

Trap • BO = 0 (He₂, Be₂) means the molecule does not exist. A higher BO gives a **shorter** bond.

7 • Hydrogen bonding

Strength F–H...F > O–H...O > N–H...N

Intermolecular HF, H₂O, alcohols, *p*-nitrophenol: raises boiling point and viscosity

Intramolecular *o*-nitrophenol, salicylaldehyde: lowers boiling point, steam volatile

8 • Quick orders

Bond angle CH₄ (109.5°) > NH₃ (107°) > H₂O (104.5°)

Group 15 hydrides NH₃ > PH₃ > AsH₃ > SbH₃

Bond length C–C > C=C > C≡C

Bond enthalpy C–C < C=C < C≡C

Seen in NEET 2022

Which has the maximum lone pair–lone pair repulsion?

SF₄ : 1 IF₅ : 1 ClF₃ : 2 XeF₂ : 3

Count lone pairs on the central atom: **XeF₂**.

- $\mu = 0$ for symmetrical molecules; NH₃ has more dipole than NF₃.
- O₂⁺ is **paramagnetic** (BO 2.5); BO 0 means no molecule.
- Intramolecular H-bonding lowers boiling point; intermolecular raises it.