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CH 02

Chemical Bonding — VSEPR, Hybridisation & MO Theory

02

Count electron pairs to predict any shape, assign hybridisation, explain dipole moments and covalent character, and use MO theory for bond order and magnetism — with an exam trap gallery, graded MCQs and a one-page revision sheet.

WHAT YOU WILL BE ABLE TO DO

- Find the steric number and predict shape and bond angle for any molecule or ion
- Assign hybridisation from sp to sp^3d^3 and place lone pairs correctly
- Explain dipole moments (NH_3 vs NF_3, cis vs trans) and covalent character using Fajans' rules
- Use formal charge and resonance to find bond orders in ions like CO_3^{2-} and O_3
- Fill MO diagrams for second-period diatomics and get bond order, bond length and magnetism

INSIDE

A The big picture
B Counting electron pairs
C VSEPR shapes
D Hybridisation
E Formal charge and resonance
F Dipole moment and Fajans' rules

HOW TO USE THESE NOTES

IN ONE LINE The core idea of a section	**KEY IDEA** The concept to remember	**EXAM TRAP** Where marks are usually lost
SOLVED EXAMPLE Worked step by step	**CHECK YOURSELF** Quick self-test	**MEMORY HOOK** A line that sticks

SECTION A

The big picture

A

Four questions, asked in order, solve almost every bonding problem.

IN ONE LINE

Electron pairs around a central atom repel and spread as far apart as possible; lone pairs repel most. The arrangement fixes the hybridisation; MO theory then explains bond order and magnetism.

1. **How many electron pairs** surround the central atom? (steric number)
2. **How are they arranged** in space? (electron geometry → hybridisation)
3. **Where are the lone pairs?** (shape = where the atoms are)
4. **Do the bond dipoles cancel?** (dipole moment)

THINK OF IT LIKE THIS

Tie balloons together at their necks: two balloons point opposite ways, three make a flat triangle, four a tetrahedron. Electron pairs behave the same way. A lone pair is a fatter balloon — it squeezes the others closer together.

SECTION B

Counting electron pairs

B

Get this number right and the rest is a table look-up.

Steric number = bonded atoms + lone pairs on the central atom

Lone pairs = (valence electrons of central atom − one electron per bond to a monovalent atom ± charge) ÷ 2. Add one electron for each negative charge; remove one for each positive charge. Double-bonded oxygen uses two electrons of the central atom.

KEY IDEA

Repulsion order: lone pair–lone pair > lone pair–bond pair > bond pair–bond pair. That is why CH_4 (109.5°) > NH_3 (107°) > H_2O (104.5°).

SOLVED EXAMPLE 01 — COUNTING FOR AN ION

Find the steric number and shape of ICl_4^-.

SOLUTION

1. I has 7 valence electrons; add 1 for the negative charge = 8.
2. Four I–Cl bonds use 4 → 4 left = 2 lone pairs.
3. Steric number = 4 + 2 = 6 → octahedral electron geometry; the lone pairs sit opposite each other.

ANSWER Square planar, sp^3d^2.

SECTION C

C

VSEPR shapes

The whole chapter on one table.

SN	Lone pairs	Shape	Example	Angle
2	0	Linear	$BeCl_2$, CO_2	180°
3	0	Trigonal planar	BF_3, SO_3	120°
3	1	Bent	SO_2, O_3	about 117–119°
4	0	Tetrahedral	CH_4, NH_4^+, SO_4^{2-}	109.5°
4	1	Trigonal pyramidal	NH_3, XeO_3	107° (NH_3)
4	2	Bent	H_2O	104.5°
5	0	Trigonal bipyramidal	PCl_5	90°, 120°
5	1	See-saw	SF_4	
5	2	T-shaped	ClF_3	about 87.5°
5	3	Linear	XeF_2, I_3^-	180°
6	0	Octahedral	SF_6	90°
6	1	Square pyramidal	BrF_5, $XeOF_4$	
6	2	Square planar	XeF_4, ICl_4^-	90°
7	0	Pentagonal bipyramidal	IF_7	72°, 90°

KEY IDEA

In a trigonal bipyramid, lone pairs always go equatorial (they have 120° of room there, against 90° in the axial positions). That single rule gives SF_4 (see-saw), ClF_3 (T-shape) and XeF_2 (linear).

SOLVED EXAMPLE 02 — SHAPE OF CLF_3

Predict the shape of ClF_3.

SOLUTION

1. Cl: 7 valence electrons; 3 used in Cl–F bonds; 4 left = 2 lone pairs.
2. Steric number 5 → trigonal bipyramidal arrangement, sp^3d.
3. Both lone pairs equatorial; the three F atoms form a T.

ANSWER T-shaped; F–Cl–F angle slightly under 90°.

SOLVED EXAMPLE 03 — SHAPE OF XEO_3

Predict the shape of XeO_3.

SOLUTION

1. Xe: 8 valence electrons. Each Xe=O double bond uses 2 → 6 used, 2 left = 1 lone pair.
2. Steric number = 3 + 1 = 4 → sp^3.

ANSWER Trigonal pyramidal (like NH_3).

CHECK YOURSELF

C1 Give the shapes of SF_4 and I_3^-.

C2 Why is the bond angle in H_2O smaller than in NH_3?

Answers at the end of the chapter.

SECTION D

Hybridisation

D

Mixing orbitals to point where the electron pairs are.

Steric number	Hybridisation	Orbitals mixed	Electron geometry
2	sp	s + p	Linear
3	sp^2	s + 2p	Trigonal planar
4	sp^3	s + 3p	Tetrahedral
5	sp^3d	s + 3p + $d(z^2)$	Trigonal bipyramidal

Steric number	Hybridisation	Orbitals mixed	Electron geometry
6	sp^3d^2	s + 3p + $d(z^2)$ + $d(x^2-y^2)$	Octahedral
7	sp^3d^3	s + 3p + 3d	Pentagonal bipyramidal

- Solid PCl_5 is ionic: $[PCl_4]^+$ (sp^3, tetrahedral) and $[PCl_6]^-$ (sp^3d^2, octahedral).
- NO_2^+ is linear (sp); NO_2^- is bent (sp^2); NO_3^- is trigonal planar (sp^2).
- In ethyne each carbon is sp (linear, 180°), in ethene sp^2 (120°), in ethane sp^3 (109.5°).
- **s character:** sp (50%) > sp^2 (33%) > sp^3 (25%). More s character → shorter bond and more electronegative carbon: ethyne's C–H is the most acidic of the three.

SECTION E

E

Formal charge and resonance

Choosing the best Lewis structure, and averaging the ones that tie.

> Formal charge = valence electrons − non-bonding electrons − ½ (bonding electrons)
>
> The best structure has formal charges closest to zero, with negative charge on the more electronegative atom

Resonance: when two or more valid Lewis structures differ only in where electrons sit, the real molecule is an average (resonance hybrid). Bond order = total bonds between the atoms ÷ number of positions.

Species	Resonance structures	Bond order of each bond
O_3	2	1.5
CO_3^{2-}	3	1.33
NO_3^-	3	1.33
Benzene (C–C)	2 (Kekulé)	1.5

SOLVED EXAMPLE 04 — FORMAL CHARGES IN O_3

Find the formal charge on each oxygen in one Lewis structure of O_3 (O=O–O).

SOLUTION

1. Central O: 6 − 2 − ½(6) = +1.
2. Double-bonded terminal O: 6 − 4 − ½(4) = 0.
3. Single-bonded terminal O: 6 − 6 − ½(2) = −1.

ANSWER +1 on the centre, 0 and −1 on the ends; the two resonance forms average to a bond order of 1.5 for both O–O bonds.

SECTION F

F

Dipole moment and Fajans' rules

When charges separate, and when ionic bonds turn partly covalent.

Dipole moment (μ = charge × distance, in debye, D) is a **vector**: bond dipoles add or cancel according to the shape.

Zero dipole moment (symmetric)	Non-zero dipole moment
CO_2, BF_3, CH_4, CCl_4, PCl_5, SF_6, XeF_4, trans-1,2-dichloroethene	H_2O, NH_3, SO_2, $CHCl_3$, NF_3, cis-1,2-dichloroethene

KEY IDEA

NH_3 (1.47 D) vs NF_3 (0.23 D): in NH_3, N is more electronegative than H, so the bond moments point toward N — the same way as the lone pair's moment. They add. In NF_3 the bond moments point toward F, away from the lone pair, and partly cancel it.

Fajans' rules: covalent character in ionic compounds

- **Small, highly charged cation** polarises more: $Al^{3+} > Mg^{2+} > Na^+$. So $AlCl_3$ is far more covalent than NaCl.
- **Large anion** is more easily polarised: $I^- > Br^- > Cl^- > F^-$. So LiI is more covalent than LiF.
- **18-electron cations** (Cu^+, Ag^+) polarise more than noble-gas cations of similar size: CuCl is more covalent than NaCl.
- Covalent character lowers melting point and solubility in water.

CHECK YOURSELF

C3 Which has a larger dipole moment: cis- or trans-1,2-dichloroethene?

C4 Arrange in increasing covalent character: NaCl, $MgCl_2$, $AlCl_3$.

Answers at the end of the chapter.

SECTION G

Molecular orbital theory

G

The only model that explains why O_2 is magnetic.

$$\text{Bond order} = (Nb - Na) / 2$$

Nb = electrons in bonding MOs; Na = electrons in antibonding MOs

- Bond order 0 → no stable molecule (He_2, Ne_2).
- Higher bond order → shorter, stronger bond.
- Any unpaired electron → **paramagnetic**.

Filling order

Up to N_2 (B_2, C_2, N_2), s–p mixing: σ1s, σ∗1s, σ2s, σ∗2s, π2p (×2), σ2p, π∗2p (×2), σ∗2p

O_2 and F_2: σ1s, σ∗1s, σ2s, σ∗2s, σ2p, π2p (×2), π∗2p (×2), σ∗2p

Species	Electrons	Bond order	Unpaired e^-	Magnetism
H_2	2	1	0	Diamagnetic
He_2	4	0	0	Does not exist
B_2	10	1	2	Paramagnetic
C_2	12	2	0	Diamagnetic
N_2	14	3	0	Diamagnetic
N_2^+	13	2.5	1	Paramagnetic
O_2	16	2	2	Paramagnetic
O_2^+	15	2.5	1	Paramagnetic
O_2^-	17	1.5	1	Paramagnetic
O_2^{2-}	18	1	0	Diamagnetic
NO	15	2.5	1	Paramagnetic
CO	14	3	0	Diamagnetic

KEY IDEA

Bond length follows bond order in reverse: O_2^{2-} (1) > O_2^- (1.5) > O_2 (2) > O_2^+ (2.5). Liquid O_2 sticks between the poles of a magnet — the two unpaired π∗ electrons that Lewis structures can't show.

SOLVED EXAMPLE 05 — SUPEROXIDE ION

Find the bond order and magnetism of O_2^-.

SOLUTION

1. 17 electrons. Bonding: $\sigma1s^2$, $\sigma2s^2$, $\sigma2p^2$, $\pi2p^4$ = 10.
2. Antibonding: $\sigma*1s^2$, $\sigma*2s^2$, $\pi*2p^3$ = 7.
3. Bond order = (10 − 7)/2 = 1.5; one unpaired electron.

ANSWER Bond order 1.5; paramagnetic.

SOLVED EXAMPLE 06 — WHY B_2 IS PARAMAGNETIC

Use the filling order to explain why B_2 is paramagnetic but C_2 is not.

SOLUTION

1. B_2 has 10 electrons; after $\sigma1s^2$, $\sigma*1s^2$, $\sigma2s^2$, $\sigma*2s^2$ (8), two remain.
2. With s–p mixing, π2p (two orbitals) comes before σ2p: one electron in each π orbital (Hund's rule).
3. C_2 has two more electrons, which pair up in the π orbitals.

ANSWER B_2: 2 unpaired (paramagnetic). C_2: all paired (diamagnetic).

SECTION H

Hydrogen bonding

H

The weak bond with big consequences.

- Forms when H is bonded to **F, O or N** and is attracted to a lone pair on another F, O or N.
- **Intermolecular** H bonding raises boiling points: H_2O (373 K) vs H_2S (213 K); HF boils far above HCl.
- **Intramolecular** H bonding (within one molecule) lowers boiling point and water solubility: o-nitrophenol is steam-volatile, p-nitrophenol is not.
- Ice is less dense than water because H bonds lock molecules into an open cage.
- Explains DNA base pairing and protein folding.

SECTION I

Exam trap gallery

I

Where marks are lost in bonding questions.

✗ TRAP 01 · WHAT STUDENTS WRITE	✓ WHAT IS ACTUALLY CORRECT
H_2O is tetrahedral.	Its electron geometry is tetrahedral; its **shape** is bent.
WHY Shape describes atoms only, not lone pairs.	

✗ TRAP 02 · WHAT STUDENTS WRITE	✓ WHAT IS ACTUALLY CORRECT
In SF_4 the lone pair is axial.	The lone pair is equatorial → see-saw.
WHY Equatorial positions have more room (120° neighbours).	

✗ TRAP 03 · WHAT STUDENTS WRITE	✓ WHAT IS ACTUALLY CORRECT
XeF_4 is tetrahedral.	XeF_4 is square planar (SN 6, 2 lone pairs opposite).
WHY Count Xe's 8 valence electrons: 4 bonds + 2 lone pairs.	

✗ TRAP 04 · WHAT STUDENTS WRITE	✓ WHAT IS ACTUALLY CORRECT
O_2 is diamagnetic because all electrons pair in the Lewis structure.	O_2 is paramagnetic: two unpaired π^* electrons.
WHY Lewis structures can't show this; MO theory can.	

✗ TRAP 05 · WHAT STUDENTS WRITE	✓ WHAT IS ACTUALLY CORRECT
B_2 is diamagnetic.	B_2 is paramagnetic.
WHY s–p mixing puts $\pi 2p$ below $\sigma 2p$ up to N_2.	

✗ TRAP 06 · WHAT STUDENTS WRITE	✓ WHAT IS ACTUALLY CORRECT
A molecule with polar bonds has a dipole moment.	Not if the shape cancels them: CO_2, BF_3, CCl_4 have $\mu = 0$.
WHY Dipole moment is a vector sum.	

✗ TRAP 07 · WHAT STUDENTS WRITE	✓ WHAT IS ACTUALLY CORRECT
NF_3 has a larger dipole than NH_3 because F is more electronegative.	NH_3 (1.47 D) > NF_3 (0.23 D).
WHY In NF_3 the bond moments oppose the lone pair's moment.	

✗ TRAP 08 · WHAT STUDENTS WRITE	✓ WHAT IS ACTUALLY CORRECT
Bond order of C–O in CO_3^{2-} is 2.	1.33 (three resonance structures, four bonds).
WHY The double bond is shared over three positions.	

MEMORY HOOK

"**Lone pairs like the equator**" — in trigonal bipyramids, LPs go equatorial.

"**Up to N, pi first**" — B_2, C_2, N_2 fill π2p before σ2p.

"**FON makes H bonds**" — only F, O, N.

"**Small and charged, big and soft**" — Fajans: small, high-charge cation + large anion = covalent.

SECTION J

Practice MCQs

J

Levels: Easy, Moderate, Tough.

Q01 The shape of NH_3 is: [EASY]

(a) tetrahedral
(b) trigonal planar
(c) trigonal pyramidal
(d) T-shaped

Q02 Hybridisation of carbon in ethyne is: [EASY]

(a) sp
(b) sp^2
(c) sp^3
(d) sp^3d

Q03 Which molecule has zero dipole moment? [EASY]

(a) NH_3
(b) H_2O
(c) BF_3
(d) SO_2

Q04 Bond order of N_2 is: [EASY]

(a) 1
(b) 2
(c) 2.5
(d) 3

Q05 Which can form hydrogen bonds? [EASY]

(a) CH_4
(b) HCl
(c) NH_3
(d) PH_3

Q06 The shape of XeF_2 is: [MODERATE]

(a) bent
(b) linear
(c) T-shaped
(d) see-saw

Q07 Which is paramagnetic? [MODERATE]

(a) N_2
(b) C_2
(c) O_2^{2-}
(d) B_2

Q08 The correct order of bond angles is: [MODERATE]

(a) $H_2O > NH_3 > CH_4$
(b) $CH_4 > NH_3 > H_2O$
(c) $NH_3 > CH_4 > H_2O$
(d) $CH_4 > H_2O > NH_3$

Q09 Hybridisation of P in the $[PCl_6]^-$ ion is: [MODERATE]

(a) sp^3 (b) sp^3d
(c) sp^3d^2 (d) sp^3d^3

Q10 Most covalent among these is: [MODERATE]

(a) NaCl (b) $MgCl_2$
(c) $AlCl_3$ (d) KCl

Q11 Bond order of each C–O bond in CO_3^{2-} is: [MODERATE]

(a) 1 (b) 1.33
(c) 1.5 (d) 2

Q12 Which species has the shortest bond? [MODERATE]

(a) O_2^{2-} (b) O_2^-
(c) O_2 (d) O_2^+

Q13 ClF_3 has the shape: [TOUGH]

(a) trigonal planar (b) trigonal pyramidal
(c) T-shaped (d) see-saw

Q14 Which pair has the same shape? [TOUGH]

(a) XeF_4 and SF_4 (b) XeF_2 and I_3^-
(c) NH_3 and BF_3 (d) SO_2 and CO_2

Q15 o-Nitrophenol is more volatile than p-nitrophenol because of: [TOUGH]

(a) intermolecular H bonding in the ortho isomer (b) intramolecular H bonding in the ortho isomer
(c) larger dipole moment of the ortho isomer (d) higher molar mass of the para isomer

Answer key with explanations

Q01 **(c) trigonal pyramidal** — SN 4 with one lone pair.

Q02 **(a) sp** — Triple bond: two π bonds, linear.

Q03 **(c) BF_3** — Trigonal planar BF_3: bond dipoles cancel.

Q04 **(d) 3** — (10 - 4)/2 = 3.

Q05 **(c) NH_3** — H bonded to N.

Q06 **(b) linear** — SN 5 with 3 equatorial lone pairs.

Q07 **(d) B_2** — s–p mixing leaves two unpaired π2p electrons.

Q08 **(b) $CH_4 > NH_3 > H_2O$** — More lone pairs → stronger compression: 109.5° > 107° > 104.5°.

Q09 **(c) sp^3d^2** — SN 6, no lone pairs.

Q10 **(c) $AlCl_3$** — Al^{3+} is the smallest, most highly charged cation.

Q11 **(b) 1.33** — Four bonds shared over three positions.

Q12 **(d) O_2^+** — Highest bond order (2.5) → shortest.

Q13 **(c) T-shaped** — SN 5, two equatorial lone pairs.

Q14 **(b) XeF_2 and I_3^-** — Both linear (SN 5, three lone pairs).

Q15 **(b) intramolecular H bonding in the ortho isomer** — Intramolecular H bonding means the ortho molecules don't hold each other.

SECTION K

Advanced problems

K

Each combines two ideas from the chapter.

SOLVED EXAMPLE 07 — SHAPE AND POLARITY TOGETHER

Which of SF_4, XeF_4, CF_4 and SF_6 have a non-zero dipole moment?

SOLUTION

1. CF_4 (tetrahedral), SF_6 (octahedral), XeF_4 (square planar): symmetric → bond dipoles cancel.
2. SF_4: SN 5, one equatorial lone pair → see-saw → bond dipoles don't cancel.

ANSWER Only SF_4.

SOLVED EXAMPLE 08 — RANKING BY MO THEORY

Arrange N_2, N_2^+ and N_2^{2-} by bond length and identify which are paramagnetic.

SOLUTION

1. N_2: 14 e^-, bond order 3, diamagnetic.
2. N_2^+: 13 e^- (one fewer bonding), bond order 2.5, one unpaired.
3. N_2^{2-}: 16 e^- (two in π^*), bond order 2, two unpaired.

ANSWER Bond length $N_2^{2-} > N_2^+ > N_2$; N_2^+ and N_2^{2-} are paramagnetic.

Check-yourself answers

C1 SF_4: see-saw. I_3^-: linear.

C2 H_2O has two lone pairs; the extra lone pair–lone pair repulsion squeezes the H–O–H angle more.

C3 cis (the C–Cl dipoles add); trans cancels to zero.

C4 NaCl < $MgCl_2$ < $AlCl_3$.

QUICK REVISION

One-page revision

Read this page the night before the exam.

Counting

- SN = bonded atoms + lone pairs
- Add e^- for − charge, remove for + charge
- LP–LP > LP–BP > BP–BP
- CH_4 109.5° > NH_3 107° > H_2O 104.5°

Shapes to know

- SN 5: TBP, see-saw (SF_4), T (ClF_3), linear (XeF_2)
- SN 6: octahedral, sq. pyramidal (BrF_5), sq. planar (XeF_4)
- Lone pairs go equatorial in TBP
- XeO_3 pyramidal; ICl_4^- square planar

Hybridisation

- sp linear, sp^2 120°, sp^3 109.5°
- sp^3d TBP; sp^3d^2 octahedral; sp^3d^3 IF_7
- More s character → shorter bond
- Solid PCl_5 = $[PCl_4]^+[PCl_6]^-$

Polarity

- μ is a vector; symmetric shapes → 0
- NH_3 1.47 D > NF_3 0.23 D
- Fajans: small charged cation + big anion = covalent
- $AlCl_3$ > $MgCl_2$ > NaCl covalent

MO theory

- BO = (Nb − Na)/2
- Up to N_2: π2p below σ2p
- O_2 paramagnetic (2 unpaired); B_2 paramagnetic
- O_2^+ 2.5 > O_2 2 > O_2^- 1.5 > O_2^{2-} 1

Resonance and H bonds

- CO_3^{2-}, NO_3^-: BO 1.33; O_3, benzene: 1.5
- H bonds only via F, O, N
- Intramolecular H bond → more volatile (o-nitrophenol)
- Ice floats: open H-bonded cage

END OF NOTES · RAMGOVINDYADAV.COM