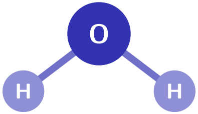
Chemical Bonding

A-Level Chemistry ▪ Topic 3

A-Level Chemistry



What we will cover

1 Electronegativity

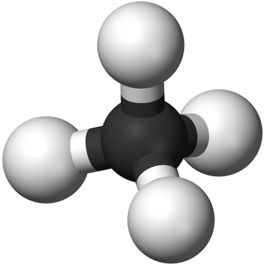
2 Ionic & metallic bonding

3 Covalent & coordinate bonds

4 Sigma & pi bonds

5 Shapes of molecules

6 Intermolecular forces



molecules in 3-D

1 Bonding types

Electronegativity

Electronegativity 电负性 is the power of an atom to attract bonding electrons towards itself. The difference in **Pauling electronegativity** 鲍林电负性 values predicts the bond type.

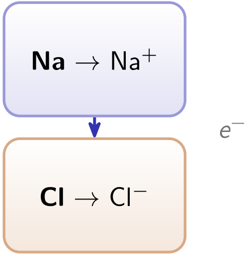
nuclear charge	**atomic radius**	**shielding**
more protons pull the pair more strongly	closer to the nucleus $\Rightarrow$ stronger pull	inner shells weaken the pull

> It rises across a period and falls down a group. Fluorine is the most electronegative element. A large difference $\Rightarrow$ ionic; a small difference $\Rightarrow$ covalent.

Ionic bonding

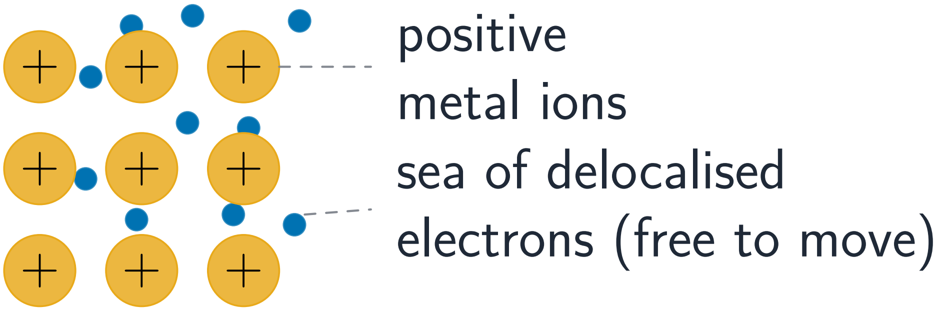
Ionic bonding 离子键 – positive **cations** 阳离子 and negative **anions** 阴离子 – is the electrostatic attraction between oppositely charged **ions** 离子. A metal gives electrons to a non-metal. The ions pack into a giant **lattice** 晶格 held in every direction.

> NaCl: sodium transfers its outer electron to chlorine → Na^+ and a full-octet Cl^-.



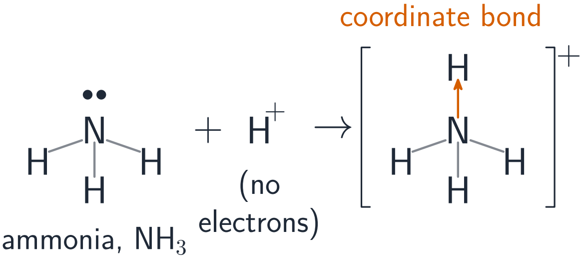
Metallic bonding

Metallic bonding 金属键 is the attraction between positive metal ions and a sea of **delocalised electrons** 离域电子. The free electrons explain why metals conduct and are strong.



2 Covalent bonding

Covalent and coordinate bonds



A **covalent bond** 共价键 is a shared pair of electrons.

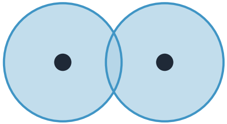
> In a **coordinate bond** 配位键 (dative) both electrons come from one atom – e.g. N's lone pair makes NH_4^+.

Sigma and pi bonds

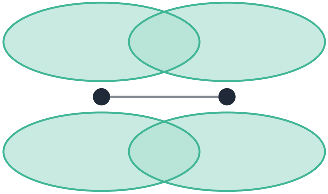
Covalent bonds form when **orbitals** 轨道 overlap:

- a **sigma bond** σ 键 – head-on **overlap** 重叠
- a **pi bond** π 键 – sideways p-orbital overlap

Double $= 1\sigma + 1\pi$; triple $= 1\sigma + 2\pi$. **Hybridisation** 杂化: sp, sp^2, sp^3.



σ bond:
head-on overlap



π bond: sideways overlap
of p orbitals

Bond energy and bond length

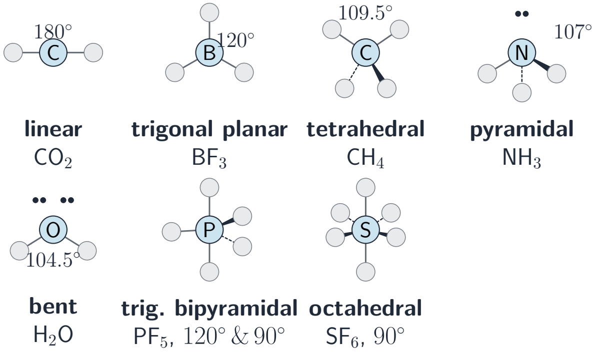
- **bond energy 键能** is the energy needed to break one mole of a particular covalent bond in the gas state.
- **bond length 键长** is the distance between the centres of the two bonded atoms.

Shapes of molecules

VSEPR theory 价层电子对互斥理论: electron pairs push apart as far as possible.

> A **lone pair** 孤对电子 repels harder than a bonding pair, squeezing the **bond angle** 键角 ($\sim 2.5°$ each) – so NH_3 is $107°$, H_2O $104.5°$.

Shapes of molecules, in detail



The seven shapes from VSEPR theory; the lone pairs on NH_3 and H_2O push harder, squeezing the bond angle below 109.5°

The shapes, and the angles that come with them

Linear	CO_2 – two bonding regions, $180°$.
Trigonal planar	BF_3 – three regions, $120°$, all in one plane.
Tetrahedral	CH_4 – four regions, $109.5°$. Lone pairs push harder: NH_3 is pyramidal at $107°$, H_2O bent at $104.5°$.
Trigonal bipyramidal	PF_5 – five regions, $120°$ in the plane and $90°$ to the axis.
Octahedral	SF_6 – six regions, all $90°$.

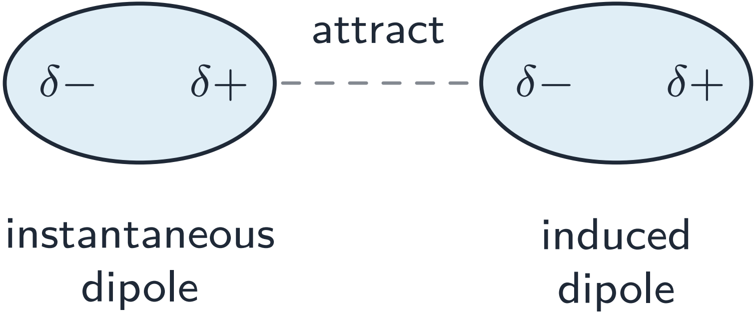
> Count the regions of electron density around the central atom, then subtract for lone pairs. The last two shapes need an atom that can expand the octet.

3 Intermolecular forces

Intermolecular forces

A bond is **polar** 极性 if the atoms differ in electronegativity (a **dipole** 偶极).

- **London forces** 伦敦色散力 – between all molecules; stronger with more electrons
- permanent dipole forces – between polar molecules



Van der Waals' forces, and when a molecule is polar

Van der Waals' forces

Van der Waals' forces 范德华力 is the general name for all intermolecular forces. There are two main types.

London dispersion

The instantaneous dipole–induced dipole force, or **London dispersion force** 伦敦色散力. Moving electrons make a brief **instantaneous dipole** 瞬时偶极, which induces a matching **induced dipole** 诱导偶极 next door. It acts between all molecules.

Permanent dipole

Between molecules that are always polar, because each carries a **permanent dipole** 永久偶极.

Dipole moment

If the bond dipoles in a molecule do not cancel, the whole molecule has a **dipole moment** 偶极矩 and is polar – which is why CO_2 is not, and H_2O is.

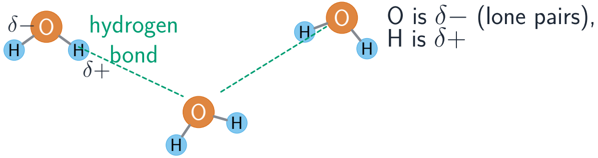
Shape decides polarity: identical bonds arranged symmetrically cancel, however polar each bond is on its own.

Bond polarity and dipoles

When two atoms with different electronegativity share a bond, the electrons sit closer to the more electronegative atom.

> The bond then has a **polarity 极性**: one end is slightly negative ($\delta-$) and the other slightly positive ($\delta+$).

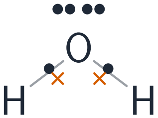
Hydrogen bonding



Hydrogen bonding 氢键 forms when H is bonded to N, O or F and meets a lone pair on N, O or F.

> It gives water a high **boiling point** 沸点, high **surface tension** 表面张力, and makes ice less dense (so it floats).

Dot-and-cross diagrams



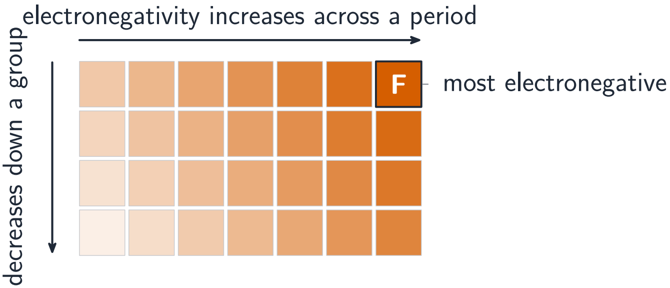
H_2O: 2 bonding pairs + 2 lone pairs

N_2: triple bond (3 shared pairs)

- • electron from one atom
- × electron from the other

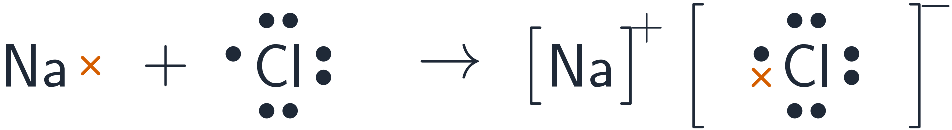
> Covalent dot-and-cross: each shared pair is one electron from each atom. Water has two bonding pairs and two lone pairs; nitrogen shares three pairs (a triple bond)

Electronegativity, continued



Electronegativity rises across a period and falls down a group, so fluorine is the most electronegative element

Ionic bonding, continued



sodium gives its outer electron (×) to chlorine

> Ionic bonding in NaCl: sodium transfers its single outer electron to chlorine, giving Na^{+} and a full-octet Cl^{-}

Ionic bonding, continued (2)

A real crystal of rock salt (halite, NaCl); the cubic shapes mirror the giant ionic lattice inside

Exam tips

- For **shapes**, count bonding pairs and lone pairs, name the shape, then give the exact bond angle (e.g. NH_3: pyramidal, $107°$) – each lone pair lowers the angle by about $2.5°$.
- A **dative (coordinate) bond** has both electrons from one atom (e.g. NH_4^+, H_3O^+); draw the arrow from the lone pair.
- Name the intermolecular force precisely: **hydrogen bonding** needs H bonded to N, O or F; otherwise it is permanent-dipole or induced-dipole (van der Waals). Never call van der Waals forces "bonds".
- Explain a physical property by stating **which forces are broken**, not just "strong bonds".

4 Recap

Worked example – shape of a molecule

Predict the shape and bond angle of NH_3.

- N has 5 outer electrons: 3 bond pairs + 1 **lone pair** 孤对电子 = 4 electron pairs.
- 4 pairs repel to a **tetrahedral** arrangement $(109.5°)$.
- A lone pair repels more than a bond pair, so the angle closes.
- Name the shape from the atoms only: pyramidal, $\approx 107°$.

Count electron pairs for the arrangement, then name the shape from the atoms. Each lone pair closes the angle by about $2.5°$.

Topic 3 – key takeaways

1 Bond types

ionic, metallic, covalent (& coordinate)

2 Sigma & pi

single 1σ; double $1\sigma 1\pi$; triple $1\sigma 2\pi$

3 Shapes

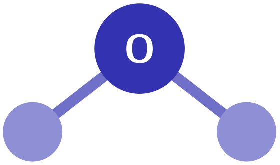
VSEPR; lone pairs squeeze the angle

4 Forces

London, dipole, hydrogen bonding

Check yourself

1. Which is the most electronegative element?
2. In a coordinate bond, where do both electrons come from?
3. How many sigma and pi bonds in a triple bond?
4. Why does ice float on water?



Answers **1.** fluorine **2.** one atom (a lone pair) **3.** one σ and two π **4.** hydrogen bonds hold an open structure (less dense)