Bonding and structure

Ionic bonding and polarisation, covalent and dative bonding, giant structures of carbon, electronegativity and polarity, shapes of molecules, and metallic bonding.

Ionic bonding

Metals lose electrons to form **cations**, and non-metals gain electrons to form **anions**. A dot-and-cross diagram shows the outer electrons. In sodium chloride, the sodium atom gives its one outer electron to chlorine. The Na^+ ion is drawn with no outer electrons shown (its full second shell), and the Cl^- ion with eight outer electrons, in square brackets with the charge outside.

An ionic crystal is a **giant lattice** of ions. **Ionic bonding** is the strong net electrostatic attraction between oppositely charged ions in all directions.

Evidence for ions

- High melting temperatures, because a lot of energy is needed to overcome the attractions.
- Solids are brittle and do not conduct, but they **conduct when molten or dissolved**, because the ions are then free to move.
- Electron density maps show almost no electron density between the ions.
- **Migration of ions.** On a piece of damp filter paper, a coloured ion such as purple manganate(VII) moves towards the positive electrode, and blue copper(II) ions move towards the negative electrode.

Strength of ionic bonding

The attraction is stronger when ions have **higher charge** and **smaller radius**. MgO (Mg^{2+} and O^{2-}) has a much higher melting temperature than $NaCl$.

- Ionic radius **increases down a group**, because there is an extra shell.
- In a set of **isoelectronic ions** such as $N^{3-}, O^{2-}, F^-, Na^+, Mg^{2+}, Al^{3+}$ (all with 10 electrons) the radius **decreases** as the nuclear charge increases and pulls the same number of electrons in more tightly.

Polarisation

Polarisation is the distortion of the electron cloud of an anion by a cation. A cation has high **polarising power** when it is small and highly charged. An anion is **more polarisable** when it is large and highly

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charged, because its outer electrons are held less tightly. Polarisation gives some covalent character to an ionic bond.

> **NOTE**
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> Aluminium iodide has more covalent character than sodium fluoride, because Al^{3+} is small and highly charged and I^- is large and easily polarised.

Covalent bonding

A **covalent bond** is the strong electrostatic attraction between two nuclei and the shared pair of electrons between them. Evidence: giant covalent structures have very high melting temperatures, and electron density maps show a high density of electrons between the nuclei.

Dot-and-cross diagrams show single, double (O_2, C_2H_4) and triple (N_2) bonds.

A **dative covalent (coordinate) bond** is a covalent bond in which both shared electrons come from one atom. It is shown by an arrow from the donor. Examples are the ammonium ion, NH_4^+ (nitrogen's lone pair is donated to H^+), and Al_2Cl_6, where each aluminium accepts a lone pair from a chlorine.

Giant covalent structures of carbon

Structure	Bonding	Properties and uses
Diamond	Each carbon bonded to 4 others, tetrahedral	Very hard, high melting temperature, does not conduct. Used in cutting tools
Graphite	Layers of hexagons, each carbon bonded to 3 others; the fourth electron is delocalised; weak London forces between layers	Soft, layers slide (lubricant), conducts electricity along layers. Used in electrodes
Graphene	A single layer of graphite	Very strong, light, excellent conductor of electricity and heat; used in electronics and composites

Electronegativity and polarity

Electronegativity is the ability of an atom to attract the bonding pair of electrons in a covalent bond. It increases across a period and decreases down a group. Fluorine is the most electronegative element.

- If the two atoms have equal electronegativity, the bond is **non-polar**.
- If they differ, the bond is **polar**, with a partial charge $\delta+$ on the less electronegative atom and $\delta-$ on the other.
- If the difference is large enough, the electron pair is effectively transferred and the bond is **ionic**.

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Ionic and covalent bonding are the two ends of a continuum, with polar covalent bonds in between.

A **polar bond** is not the same as a **polar molecule**. A molecule is polar only if the bond dipoles do not cancel. CO_2 and CCl_4 have polar bonds but are non-polar molecules because of their symmetry; H_2O and NH_3 are polar molecules.

NOTE

A simple test is to bring a charged rod near a thin jet of liquid. Water and ethanol, which are polar, are deflected. Non-polar cyclohexane is not.

Shapes of molecules

Electron-pair repulsion theory: electron pairs around a central atom repel and take positions as far apart as possible. Lone pairs repel more than bonding pairs, so each lone pair reduces the bond angle (by about 2.5°).

Pairs (bonding + lone)	Shape	Bond angle	Examples
2 + 0	Linear	180°	$BeCl_2$, CO_2
3 + 0	Trigonal planar	120°	BCl_3, C_2H_4 (at each carbon)
4 + 0	Tetrahedral	109.5°	CH_4, NH_4^+
3 + 1	Pyramidal	107°	NH_3
2 + 2	Bent (V-shaped)	104.5°	H_2O
5 + 0	Trigonal bipyramidal	90° and 120°	PCl_5 (gas)
6 + 0	Octahedral	90°	SF_6

A double bond counts as one region of electron density.

TRY IT

Predict the shape and bond angle in the NH_2^- ion.

Nitrogen has 5 outer electrons. Add 2 for the two N–H bonds and 1 for the negative charge: $5 + 2 + 1 = 8$ electrons, which is 4 pairs. Two are bonding pairs and two are lone pairs, so the ion is bent, with a bond angle of about 104°. Always count the central atom's outer electrons, add one per bond, adjust for the charge, and divide by two to get the pairs.

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Bond length is the distance between the nuclei of two bonded atoms. **Bond angle** is the angle between two bonds at an atom.

Metallic bonding

A metal is a giant lattice of positive metal ions in a sea of **delocalised electrons**. **Metallic bonding** is the strong electrostatic attraction between the metal ions and the delocalised electrons.

- **Conducts electricity** because the delocalised electrons are free to move.
- **High melting temperature** because there is strong attraction to overcome throughout the lattice.
- **Malleable** because layers of ions can slide without breaking the attraction.

> **In explaining a property, link the structure (particles and forces) to the property. Say "mobile ions" for ionic liquids and "delocalised electrons" for metals and graphite.**

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