Chapter 4: Chemical bonding and structure fast facts

4.1 Ionic bonding and structure

Ionic compounds consist of ions held together in lattice structures by ionic bonds.

- An ion is a charged particle.
- The number of charges on an ion is equal to the number of electrons lost (positive ion) or gained (negative ion) by an atom.
- Metals lose electrons to form positive ions (cations); non-metals gain electrons to form negative ions (anions).
- The charge on an ion can usually be predicted from the group of the element in the Periodic Table; transition metal elements can form more than one ion.
- Common polyatomic ions include: OH^-, HCO_3^-, NO_3^-, CO_3^{2-}, SO_4^{2-}, PO_4^{3-}, NH_4^+.
- Ionic compounds consist of ions held together by forces of electrostatic attraction.
- Ionic compounds are electrically neutral, as they consist of a lattice in which the total number of positive charges is balanced by the total number of negative charges. The formula of the compound is expressed as its simplest ratio, e.g. the ions X^{m+} and Y^{n-} will form the compound X_nY_m.
- In the ionic lattice, each ion is surrounded by a fixed number of ions of the opposite charge, known as the coordination number.
- Ionic compounds usually have high melting and boiling points, and are more soluble in water than in non-polar solvents. They conduct electricity when molten or in aqueous solution but not when solid.

4.2 Covalent bonding

Covalent compounds form by the sharing of electrons.

- A covalent bond is the electrostatic attraction between a pair of electrons and positively charged nuclei.
- A molecule is a group of atoms held together by covalent bonds.
- Two pairs of shared electrons = double bond.
- Three pairs of shared electrons = triple bond.
- Increasing number of bonds $\Rightarrow$ shorter and stronger bonds.
- Polar bonds form when the two atoms bonded together have different electronegativity values.

4.3 Covalent structures

Lewis (electron dot) structures show the electron domains in the valence shell and are used to predict molecular shape.

- Lewis (electron dot) structures show all the valence electrons of the atoms in the molecule or polyatomic ion.
- The octet rule refers to the fact that most atoms form a stable arrangement with eight electrons in their outer shell.
- Exceptions to the octet rule include:

  less than an octet – $BeCl_2$, BF_3 (central atom very small)

  expanded octet – PCl_5, SF_6 (central atom from third period or beyond).
- VSEPR theory: the total number of electron domains determines their geometrical arrangement by maximum repulsion; the shape of the molecule then depends on the number of bonding pairs within this arrangement.

Number of charge centres	Number of bonding pairs	Shape of molecule
2	2	linear
3	3	planar triangular
3	2	V-shaped
4	4	tetrahedral
4	3	triangular pyramidal
4	2	V-shaped
5	5	triangular bipyramidal
5	4	see-saw
5	3	T-shaped
5	2	linear
6	6	octahedral
6	5	square pyramidal
6	4	square planar

- Resonance structures occur when there is more than one possible position for a double bond.
- Carbon, silicon, and silicon dioxide form giant covalent molecules.
- Carbon occurs as allotropes with different bonding within giant molecules – diamond, graphite, fullerene, and graphene.

- The polarity of a molecule depends on:
  i the polarities of its bonds
  ii its molecular shape – whether cancellation occurs between the polar bonds.
- Coordinate bonds form when both the shared electrons originate from the same atom.

4.4 Intermolecular forces

The physical properties of molecular substances result from different types of forces between their molecules.

- The forces between molecules are largely determined by the charge separation within the molecule:
  - non-polar molecules ⇒ London (dispersion) forces
  - polar molecules ⇒ dipole–dipole attraction
  - polar molecules in which H is bonded to O, N, or F ⇒ hydrogen bonding.
- van der Waals forces refer to London (dispersion) and dipole–dipole attractions.
- In order of strength:
  London (dispersion) < dipole–dipole < hydrogen bonding
- The stronger the intermolecular force, the lower the volatility (higher boiling point).
- Polar substances are more soluble in water and less soluble in non-polar solvents.
- Covalent compounds are generally not good electrical conductors, unless they are able to ionize in solution, e.g. HCl(aq).

	Covalent substances	Ionic compounds
Volatility	low	high
Electrical conductivity	low	high
Solubility in polar solvents	low	high
Solubility in non-polar solvents	high	low

4.5 Metallic bonding

Metallic bonds involve a lattice of cations with delocalized electrons.

- Metal atoms are held together by the electrostatic attraction between a lattice of positive ions and delocalized electrons.
- The strength of the metallic bond increases with the charge on the cation and decreases with the radius of the ion.
- The properties of metals – electrical and thermal conductivity, malleability, ductility – are a result of the delocalized electrons.
- Alloys form as a result of the non-directional bonding in metals and often have enhanced properties.

14.1 Further aspects of covalent bonding and structure

Larger structures and more in-depth explanations of binding systems often require more sophisticated concepts and theories of bonding.

- Sigma (σ) bonds form when atomic orbitals (s, p, or hybridized) overlap along the bond axis; all single bonds are σ bonds.
- Pi (π) bonds form when p atomic orbitals overlap laterally; the electron density is concentrated above and below the bond axis.
- Double bond = one σ bond and one π bond.
- Triple bond = one σ bond and two π bonds.
- Atoms in Period 3 and below can expand their octet using unoccupied d orbitals. This gives rise to molecules with 5 or 6 electron domains around the central atom.
- The number of resonance structures that can be drawn for a molecule is the same as the number of possible positions for a double bond.
- Delocalization of π electrons leads to greater stability and bonds of intermediate length and strength.
- Formal charge (FC) can be used to determine which of some possible structures is the preferred structure. The most stable structure is the one with the lowest values for formal charge for the atoms.
- FC = (number of valence electrons) –
  [½(number of bonding electrons) – (number of non-bonding electrons)]
- Ozone is a resonance hybrid with a bond order of 1.5. Oxygen is a diatomic molecule with a bond order of 2. Ozone is therefore dissociated by light of longer wavelength.
- The catalytic breakdown of ozone by CFCs and NO_x has contributed to significant depletion of the ozone layer.

14.2 Hybridization

Hybridization results from the mixing of atomic orbitals to form the same number of new equivalent hybrid orbitals that can have the same mean energy as the contributing atomic orbitals.

- Hybridization occurs when different atomic orbitals mix to form new atomic orbitals for bonding.
- The shape of hybridized orbitals:

  $sp^3 \Rightarrow$ tetrahedral

  $sp^2 \Rightarrow$ planar triangular

  $sp \Rightarrow$ linear