



OCR (A) Chemistry A-level

Module 2: Foundations in Chemistry

Notes

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2.1 atomic structure and isotopes

- Isotopes: atoms of same element w/ different no of neutrons + different masses
- Mass number = $p + n$, atomic number = p
- Different isotopes react in similar ways: have same number of electrons, chemical reactions involve electrons & number neutrons has no effect on reactions
- Heavy water: used to control nuclear processes, for heavy water ${}^2_1\text{H}$ isotopes (deuterium /D) formula can be written D_2O . slightly higher mpt, bpt + density. If all water were heavy water, would see ice more often since higher mpt
- Cations: +ve, anions: -ve

2.2 relative masses

- Mass defect: small amount of mass lost due to strong nuclear force holding together protons/neutrons
- Relative isotopic mass: mass of an isotope relative to 1/12 mass of an atom carbon-12
- Relative atomic mass: weighted mean mass of an atom of an element relative to 1/12 mass of an atom of carbon-12
- % abundances isotopes can be found w/ mass spectrometer. Work by:
 - Sample placed in mass spec, vapourised then ionised to form +ve ions
 - Ions accelerated (heavier move more slowly + difficult to deflect so ions of different isotopes separated)
 - Ions detected as a mass to charge ratio (m/z). Greater the abundance, greater the signal
 - For ion w/ +1 charge, ratio equivalent to relative isotopic mass

2.3 formulae and equations

- Binary compound: contains 2 elements only. To name: change ending 2nd element to -ide. Metals come first in ionic compound names
- Polyatomic ions: an ion w/ more than one element bonded together:
 - Ammonium NH_4^+
 - Hydroxide OH^- , nitrate NO_3^- , nitrite NO_2^- , hydrogencarbonate HCO_3^- , manganate (VII) (permanganate) MnO_4^-
 - Carbonate CO_3^{2-} , sulfate SO_4^{2-} , sulfite SO_3^{2-} , dichromate (VI) $\text{Cr}_2\text{O}_7^{2-}$
 - Phosphate PO_4^{3-}
- Diatomic molecules: H_2 , N_2 , O_2 , F_2 , Cl_2 , Br_2 , I_2
- Other small molecules: P_4 or S_8 (normal practise to write as S)

3.1 amount of substance and the mole

- Avogadro constant: number of particles in each mol of carbon-12
- One mole: amount of substance that contains 6.02×10^{23} particles
- Molar mass: mass in g in each mole of a substance (units = g mol^{-1})
- $n = m / M_r$

3.2 determination of formulae

- Molecular formula: no of atoms of each element in a molecule
- Empirical formula: simplest whole number ratio of atoms of each element in a compound (important for giant crystalline structures where it would be impossible to use actual numbers- used for metals, some non metals (e.g. C) and ionic compounds)





- Relative molecular mass: compares mass molecule w/ mass carbon-12
- Relative formula mass: compares mass formula unit w/ mass carbon-12
- Analysis: investigating chemical composition of substance
- Water of crystallisation: water molecules which are part of crystalline structure
- When hydrated crystals are heated, bonds holding water w/in crystals are broken + water driven off
 - E.g. $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ (s) (blue) \rightarrow CuSO_4 (s) (white) + $5\text{H}_2\text{O}$ (l)
- Experimentally finding formula hydrated salt:
 - Weigh empty crucible, then add hydrated salt & reweigh
 - Use pipe clay triangle to support crucible on a tripod. Heat for 1 min strong, 3 mins gentle
 - Leave to cool then weigh
- Accuracy of experimental formula: assumes all water has been lost (solution= heat to constant mass) & assumes no further decomposition (difficult if no colour change)

3.3 moles and volume

- 1 mol dm^{-3} sol contains 1 mol of solute dissolved in each 1 dm^3 solution
- $\text{mol} = \text{conc} \times \text{vol}$
- Standard solution= solution of a known conc. Prepared by: dissolving exact mass solute in solvent + making it up to an exact volume
- Can have mass conc (g dm^{-3}), $\text{mol dm}^{-3} \rightarrow \text{mass dm}^{-3}: \times \text{Mr}$
- Molar gas volume V_m : the volume per mole of gas molecules a stated temperature and pressure ($24 \text{ dm}^3 \text{ mol}^{-1}$ at RTP)
- RTP: about 20°C and 101 kPa
- Assumptions for molecules making up ideal gas: random motion, elastic collisions, negligible size, no intermolecular forces
- $pV = nRT$:
 - p = pressure Pa (kPa to Pa $\times 10^3$)
 - V = vol m^3 (cm^3 to $\text{m}^3 \times 10^{-6}$ // dm^3 to $\text{m}^3 \times 10^{-3}$)
 - n = mol of gas
 - R = ideal gas constant $8.314 \text{ J mol}^{-1} \text{ K}^{-1}$
 - T = temp in K
- Experimentally finding a relative molecular mass of volatile liquid (liquid room temp, boils below 100°C):
 - Add sample liquid to small syringe via needle + weigh
 - Inject into gas syringe through self-sealing rubber cap + reweigh small syringe to find mass added
 - Place in boiling water bath (100°C). Liquid vapourises + record pressure
 - Use ideal gas eq to find moles, then use moles & mass to find Mr

3.4 reacting quantities

- Stoichiometry: ratio of amount/moles each substance in balanced eq
- Experimentally identifying unknown metal:
 - Weigh sample metal + add to conical flask
 - Add known conc + vol HCl to flask + quickly replace bung





- Measure max vol gas in syringe, work out moles gas then use eq to find moles unknown, use moles + mass to find Mr
- Theoretical yield: maximum possible product if all reactants converted to product
- May not achieve theoretical yield because:
 - Reaction may not go to completion
 - Side reactions may take place
 - Purification may lead to loss of product
- Percentage yield = $\frac{\text{actual yield}}{\text{theoretical yield}} \times 100$
- Limiting reagent: reactant not in excess which will be used up first + stop reaction. Calculations must use limiting reagent
- Atom economy: measure of how well atoms have been utilised
- Atom economy = $\frac{\text{sum molar masses desired product}}{\text{sum molar masses all products}} \times 100$
- High atom economy: large proportion desired products, few waste products, important for sustainability - make most of resources. Makes industrial processes more efficient, preserves raw material + reduces waste
- Atom economy only part of sustainability: should use readily available reactants w/ low obtaining costs & depends on percentage yield

4.1 acids, bases and neutralisation

- Strong acid fully dissociates in aq solution, weak acid partially dissociates in aq solution
- Alkali: base that dissolves in water releasing OH^- ions into solution
- Neutralisation of an acid: the H^+ ions react w/ a base to form a salt + water. H^+ replaced by metal or ammonium ions from base
- with alkalis, all reactants for neutralisation are aq. Ionic eq: $\text{H}^+ + \text{OH}^- \rightarrow \text{H}_2\text{O}$

4.2 acid-base titrations

- Titration: technique to accurately measure vol one solution reacting exactly with another
- Can be used to check purity - important for pharmaceuticals etc
- Volumetric flask typical tolerances: $100 \text{ cm}^3 \pm 0.2 \text{ cm}^3$, $250 \text{ cm}^3 \pm 0.3 \text{ cm}^3$
- Experimentally preparing standard solutions:
 - Solid weighed + dissolved in beaker using less distilled water than needed to fill volumetric flask
 - Transfer to volumetric flask + last traces rinsed into flask with distilled water
 - Add distilled water dropwise until bottom of meniscus matches up with mark
 - Flask inverted slowly several times to mix, if not titration results will be inconsistent
- Typical tolerances pipette: $10 \text{ cm}^3 \pm 0.04 \text{ cm}^3$, $25 \text{ cm}^3 \pm 0.06$. Burette: $50 \text{ cm}^3 \pm 0.1$
- Burette recorded to nearest half division, to 2dp (last 5 or 0)
- Acid-base titration procedure:
 - Add measured volume one solution to conical flask w/ pipette
 - Add other solution to burette, record initial reading
 - Add few drops indicator to conical flask
 - Run solution from burette into conical flask, swirling it, until it reaches the end point





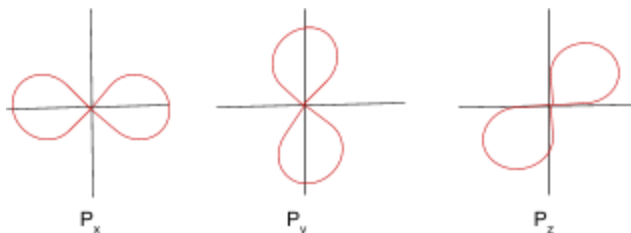
- Record final reading.
- 1st titre carried out quickly to get approx, then repeat accurately adding solution dropwise as end point approached. Carry out until two accurate titres are concordant (within 0.1 cm^3)

4.3 redox

- Sign for oxidation number placed before the number
- Oxidation numbers:
 - O -2
 - H +1
 - F -1
 - Ions: charge on ions
 - Special cases: H in metal hydrides: -1, O in peroxides -1, O bonded to F +2
- Roman numerals used for compounds w/ elements that form different ions w/ different charges
- Reduction: gain of electrons (decrease oxd no), oxidation: loss of electrons (increase oxd no)

5.1 electron structure

- shells=energy levels, energy increases as shell number increases
- Principal quantum number: the shell number or energy levels number
- Atomic orbital: region around the nucleus that can hold up to 2 electrons w/ opposite spins (make up shells)
- S- sphere, P-dumbbell, can have 3 separate orbitals P_x , P_y , P_z



- Orbitals of same type are grouped as sub-shells
- Two electrons in an orbital must have opposite spins (up/down)
- Periodic table can be divided into blocks corresponding to highest energy subshell
- 4s sub shell at lower energy than 3s, so is filled first. Once filled, energy 3d falls below 4s, so it empties before

5.2 ionic bonding and structure

- Ionic bonding: the electrostatic attraction between positive and negative ions
- High melting point and boiling point: high temp needed to provide large quantity energy needed to overcome strong electrostatic attraction between ions
- Melting points higher for lattices with greater charges on ions, because of stronger attraction between ions
- Many dissolve in polar solvents (e.g. water), they break down the lattice + surround each ion in solution. If made of ions with strong charges, attraction too strong to be broken down

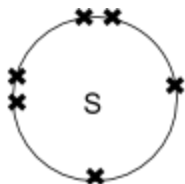




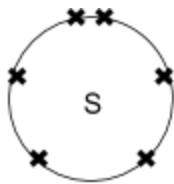
- Solubility depends on relative strengths attractions w/in lattice & attraction between ions + water molecules so predictions of solubility should be treated with caution
- Solid state: ions in fixed position, no mobile charge carriers so doesn't conduct electricity
- liquid/molten: solid lattice breaks down so ions free to move as mobile charge carriers so can conduct electricity
- Ions in tooth enamel removed in acid conditions, gaps can allow tooth decay to develop. Saliva helps neutralise acidic food + replace ions but not always enough so toothpaste contains fluoride ions

5.3 covalent bonding

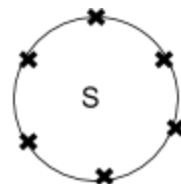
- Covalent bonding: strong electrostatic attraction between a shared pair of electrons and the nuclei of bonded atoms
- Attraction is localised between electrons
- In BF_3 , there are 6 electrons in boron's outer shell → bonding predictions can't be made solely on noble gas structure
- For phosphorus, sulfur and fluorine their outer electrons are in $n=3$ outer shell, which can hold up to 18 electrons, so more electrons are available for bonding. This means you can get: PF_3 PF_5 SF_2 SF_4 SF_6 ClF ClF_3 ClF_5 ClF_7 .
- Different numbers unpaired electrons → different possibilities of compounds (e.g. sulfur)



2 unpaired
electrons, 2
bonds possible

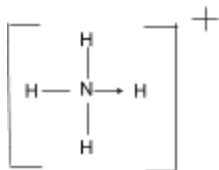


4 unpaired
electrons, 4
bonds possible



6 unpaired
electrons, 6
bonds possible

- Double covalent bond: electrostatic attraction is between 2 shared pairs of electrons and the nuclei of bonding atoms e.g. O_2 or CO_2
- Triple covalent bond: electrostatic attraction is between 3 shared pairs of electrons and the nuclei of bonded atoms e.g. N_2 or HCN
- Dative covalent/coordinate bond: covalent bond in which shared pair of electrons has been supplied by one of the bonding atoms only. Shown by → arrow, e.g. NH_4^+



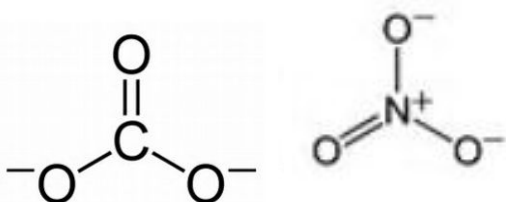
6.1 shapes of molecules and ions

- Electron pair repulsion theory:
 - Electron pairs surrounding central atom determine molecule/ion shape
 - Pairs repel each other so they are arranged as far apart as possible
 - Arrangement minimises repulsion, so holds atoms in definite shape
 - Different number of electron pairs → different shape

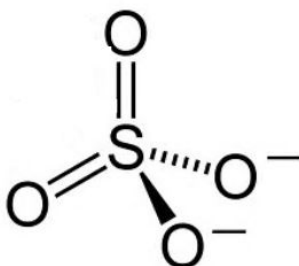




- Solid line=in plane of paper, wedge=comes out of plane of paper, dotted=goes into plane
- Lone pair slightly closer to central atom + occupies more space than bonded atom → repels more strongly than bonding pair.
- Bond angle is reduced by about 2.5° per lone pair
- CH_4 = tetrahedral 109.5° , NH_3 pyramidal 107° , H_2O nonlinear 104.5°
- Multiple bonds treated as a bonding region
- Different shapes/bond angles: *
 - 2: 180° , linear e.g. CO_2
 - 3: 120° , trigonal planar e.g. BF_3
 - 4: 109.5° , tetrahedral e.g. CH_4
 - 6: 90° , octahedral e.g. SF_6
- Ammonium ion has 4 bonding pairs so tetrahedral
- CO_3^{2-} and NO_3^- ions are trigonal planar*



- SO_4^{2-} ions are tetrahedral



6.2 electronegativity and polarity

- Electronegativity: attraction of a bonded atom for the pair of electrons in a covalent bond
- Pauling scale (& pauling electronegativity values) used to compare electronegativity
- Increases upwards + across towards fluorine (F, O, N, Cl most, group 1 least)
- If electronegativity difference is large, bond becomes ionic rather than covalent
- Non-polar bond: bonded electron pair shared equally between bonded atoms (when atoms same element/ similar electronegativity)
- Pure covalent bond: bonded atoms are same element
- Polar covalent bond: bonded electron pair shared unequally (different atoms with different electronegativity). More electronegative has greater attraction for bonded pair electrons.
- Polar bonds are polarised with $\delta+/-$ signs (dipoles)
- Permanent dipole: dipole in a polar covalent bond which doesn't change





- Polar bonds may reinforce one another to produce larger dipole over whole molecule or cancel out:
 - H_2O : polar- OH bonds have permanent dipole, act in opposite directions but don't exactly oppose each other, overall O end is δ^- and H end is δ^+
 - CO_2 : nonpolar- C=O bonds have permanent dipole, act in opposite directions + exactly oppose each other, overall dipoles cancel
- Ionic lattices dissolving in polar solvents: water molecules attract +/- ions, ionic lattice breaks down as dissolves, water molecules surround ions, + ions attracted towards δ^- oxygen of water & - ions attracted to δ^+ hydrogen

6.3 intermolecular forces

- Intermolecular forces: weak interactions between dipoles of different molecules
- Induced dipole-dipole interactions (London forces):
 - Exist between all molecules, only temporary
 - Movement electrons produces changing dipole in any molecule, at any instant an instantaneous dipole will exist but position shifts constantly
 - Instantaneous dipole induces a dipole on neighbouring molecule, which induces dipoles on further molecules, they then attract one another
 - More electrons in each molecule \rightarrow larger instantaneous + induced dipoles \rightarrow greater induced dipole-dipole interactions \rightarrow stronger attractive forces (explains increased bpt noble gases)
- Permanent dipole-dipole interactions:
 - Act between permanent dipoles in polar molecules
 - Mean boiling point of polar molecules is much greater: have both London and permanent dipole-dipole interactions, extra energy needed to break additional permanent interactions, so boiling point is higher
- Simple molecular substance: made of of simple molecules (small units w/ definite number of atoms). In solid state form simple molecular lattices, held together by weak intermolecular forces, but atoms within molecules bonded strongly with covalent bonds
- Simple molecular substances have low mpt/bpt: only weak intermolecular forces break, not strong covalent bonds
- Nonpolar simple molecules tend to be soluble in nonpolar solvents (hexane): intermolecular forces form between molecules and solvent, weakening intermolecular forces in simple lattice, so they break & compound dissolves
- Tend to be insoluble in polar solvents (water): little interaction between molecules in lattice & solvent molecules, intermolecular bonding in solvent too strong to be broken
- Solubility of polar simple molecular substances is hard to predict: depends on strength of dipole. May dissolve because polar solute/solvent molecules can attract each other (similar to ionic dissolving). Some with part polar part nonpolar dissolve
- Simple molecular structures don't conduct electricity: no mobile charged particles within structure, so nothing to complete an electrical circuit

6.4 hydrogen bonding

- Found in molecules containing: electronegative atom w/ lone pair electrons (O,N,F) attached to a hydrogen atom





- Shape around hydrogen atom involved in bond is linear, bond shown by dashed line
- Solid is less dense than liquid: hydrogen bonds hold water molecules apart in open lattice structure, water molecules in ice further apart than in water, so ice is less dense than liquid water & floats. 2 lone pairs on oxygen and 2 hydrogens, so each molecule can form 4 bonds → open tetrahedral lattice full of holes. Bond angle H involved 180°
- Relatively high mpt/bpt: hydrogen bonds & london forces, large quantity of energy is needed to break hydrogen bonds. When ice lattice breaks, arrangement hydrogen bonds is broken & when boils hydrogen bonds break completely
- Other anomalous properties: relatively high surface tension + viscosity
- DNA is held together by hydrogen bonds: AT pair form 2 hydrogen bonds, CG pair forms 3. Pairs match up correctly because bases must fit together so hydrogen atom one molecule and O/N from other align correctly

