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 $^2$H isotopes (deuterium /D) formula can be written D$_2$O. 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$_2^-$, hydrogen carbonate HCO$_3^-$, manganate (VII) (permanganate) MnO$_4^-$
  - Carbonate CO$_3^{2-}$, sulfate SO$_4^{2-}$, sulfite SO$_3^{3-}$, dichromate (VI) Cr$_2$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 6.02x10$^{23}$ 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. CuSO₄·5H₂O (s) (blue) -> CuSO₄ (s) (white) + 5H₂O (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 dm³ sol contains 1 mol of solute dissolved in each 1 dm³ solution
- mol=conc x 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), mol dm⁻³ → mass dm⁻³: x Mr
- Molar gas volume \( V_m \): the volume per mole of gas molecules a stated temperature and pressure (24 dm³ 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 x 10³)
  - \( V= \) vol m³ (cm³ to m³ x 10⁻⁶ // dm³ to m³ x 10⁻³)
  - \( n= \) mol of gas
  - \( R= \) ideal gas constant 8.314 J mol⁻¹ 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 = actual yield/theoretical yield × 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 = (sum molar masses desired product)/(sum molar masses all products) × 100

High atom economy: large proportion desired products, few waste products, important for sustainability - makes 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: H⁺ + OH⁻ → H₂O

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 cm³ +/- 0.2 cm³, 250 cm³ +/- 0.3 cm³

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 cm³ +/- 0.04 cm³, 25 cm³ +/- 0.06. Burette: 50 cm³ +/- 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 cm³)

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 Pₓ, Pᵧ, Pₗ

● 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 toothy 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$_6$, CIF, CIF$_3$, CIF$_5$, CIF$_7$.
- Different numbers unpaired electrons → different possibilities of compounds (e.g. sulfur)

![Diagrams of sulfur molecules with varying unpaired electrons]

- 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
CH₄= tetrahedral 109.5°, NH₃ pyramidal 107°, H₂O nonlinear 104.5°
Multiple bonds treated as a bonding region
Different shapes/bond angles:*  
 2: 180°, linear e.g. CO₂  
3: 120°, trigonal planar e.g. BF₃  
4: 109.5°, tetrahedral e.g. CH₄  
6: 90°, octahedral e.g. SF₆  
Ammonium ion has 4 bonding pairs so tetrahedral  
CO₃²⁻ and NO₃⁻ ions are trigonal planar*  
SO₄²⁻ 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 δ+/- 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:
  ○ \( \text{H}_2\text{O} \): polar- \( \text{OH} \) bonds have permanent dipole, act in opposite directions but don't exactly oppose each other, overall O end is \( \delta^- \) and H end is \( \delta^+ \)
  ○ \( \text{CO}_2 \): nonpolar- \( \text{C} = \text{O} \) 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 \( \delta^- \) oxygen of water & - ions attracted to \( \delta^+ \) 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 → larger instantaneous + induced dipoles → greater induced dipole-dipole interactions → 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