AQA AS level Unit 2 Chemistry notes by Luna Hu

Energetics

Enthalpy: measures the total heat content of a system under constant pressure Standard enthalpy change: change in enthalpy at constant pressure and temperature. (298 K and 100kPa) Standard state: State of substance under standard conditions. Bond dissociation energy: Energy required to break a covalent bond with all species at gaseous state. Mean bond enthalpy: Average value of the bond dissociation enthalpy for a type of covalent bond taken from a

Mean bond enthalpy: Average value of the bond dissociation enthalpy for a type of covalent bond taken from a range of different compounds.

Standard enthalpy of reaction: Enthalpy change when 1 mole of a substance is transformed by a chemical reaction with all reactants and products at standard states, under standard conditions.

Standard enthalpy of formation: Enthalpy required to form 1 mole of a substance from its constituent elements with all reactants and products in standard states under standard conditions

Standard enthalpy of combustion: Enthalpy change when 1 mole of a substance is completely combusted in oxygen with all reactants and products in standard states under standard conditions.

The enthalpies of all elements in their standard states are taken as 0. (By definition)

Hess' law: The enthalpy change of a reaction is the same regardless of the route taken from reactants to products. * Always include state symbols

Endothermic: When the amount of energy required to break the bonds is greater than the amount of energy generated in the making of bonds. E.g. Photosynthesis, decomposition

Exothermic: When the amount of energy required to break the bonds is less than the amount of energy generated in the making of bonds. E.g. Combustion, neutralization



Exothermic products are more stable as it has lower energy Remember to draw single-headed arrows!! NOT DOUBLE HEADED

It is important to measure the enthalpy because:

- We can measure the energy of fuels
- Calculate energy requirements
- Predict whether or not a reaction will take place

Measuring the enthalpy change of reaction:

- Mass of substance BEING heated
- Temperature change of substance being heated
- Specific heat capacity of the substance (The specific heat is the amount of heat required to change a unit mass of a substance by one degree in temperature.)





Use polystyrene cups (except for

Combustion is less accurate

because more heat is lost to

surroundings.

surroundings.

combustion) because they are good insulators so less heat is lost to



Intersection of 2 blue lines shows the extrapolated but more accurate ΔT , because some heat is still lost to the surroundings immediately when the reactants are added together.

Characteristics of good fuel:

- High calorific content
- Energy dense
- Easy to store, transport, and cheap



Thermochemical cycles can also be used to represent the enthalpy change of a reaction. 0 is represented by the constituent elements. These diagrams clearly show and compare the differences in enthalpies of reactants and products.

Kinetics

In order for a reaction to occur: particles must collide with E>Ea (activation energy) and at the correct orientation

Rate of reaction: The change in concentration of a substance over a specified amount of time

To increase rate of reaction:

- Increase the temperature: Increases the speed of the molecules as well as their energy, meaning the frequency of collision is increased and the proportion of successful collisions per unit time is increased. (+10k =~ double rate of reaction)
- Increase concentration (solution): Increases the number of particles per unit volume, thus the frequency of collisions per unit time increases, though the proportion of successful collisions remains the same.
- Increase pressure (gas): Increases the number of gas particles per unit volume, thus the frequency of collisions per unit time increases, though the proportion of successful collisions remains the same. (for the direction of the reaction of higher # moles of gas to smaller.)
- Increase surface area (solid): Increases the number of particles exposed/able to be reacted, thus the frequency of collision per unit time increases, but the proportion of successful collisions remains unchanged.
- Use a catalyst: lowers the activation energy thus the number of particles with E > Ea increases, thus the number of successful collisions increases.

Represented on a graph:

- + Temperature: steeper, levels off the same.
- + Concentration: steeper, eventually levels off higher (extent depends on concentration)
- + Pressure: Steeper, levels off the same.
- + Surface area: steeper, levels off the same
- + Catalyst: steeper, levels off the same

• Why graph levels off & why gradient decreases: over time, number of reactants/volume decreases, collisions/time decreases, rate of reaction decreases. (eventually the limiting reactant is used up)



- No particle have 0 energy
- The peak is the most probable energy
- Slightly right of the peak is the mean energy
- There is no upper limit to the curve
- Area under the curve remains the same as the number of particles remains constant
- For a reaction to happen, the E > Ea.

• A small increase in temperature will result in a much larger increase in the number of particles with E > Ea.

• Number of collisions in a given time increases as the temperature increases, but this is not as important to the rate of reaction as the increase in the number of effective collisions.

Activation energy is the minimum energy a particle/molecule requires for a reaction to occur. - Molecules pass on energy as they collide. (Some lose, some gain)

<u>Catalysts</u>: Increases rate of reaction without getting used up.

• Provides an alternative route of lower activation energy.

Catalysts don't affect the enthalpy change of a reaction; they only lower the activation energy of forward reaction.

(Nor do they change position of equilibrium)

Types of catalysts:

Heterogeneous- Catalyst is in a different phase to reactants

Homogeneous- Catalyst is in the same phase as reactants

Different phases are separated by distinct boundaries: e.g. water and oil, solid and solution.

How solid catalysts actually work:

Adsorption: reactants form weak bonds with catalyst – to hold them in place to be reacted Desorption: products break away from metal atoms so more can be reacted on catalyst surface.

Equilibrium – can be reached from either direction but can only be reached in a closed system – evinced when the macroscopic properties of the system do not change with time.

Dynamic equilibrium: When the rate of the forward and backward reaction are equal, and the concentration of reactants and products remain constant in a closed system.

Shifting the position of the equilibrium by changing the conditions can alter the proportion of the reactants and products.

La Châtelier's principle: If a system at equilibrium is disturbed, the equilibrium will shift in the direction that counters the disruption. (But it can't tell how far the equilibrium shifts)

To change conditions of an equilibrium reaction:

• Changing concentrations: Equilibrium will shift to the direction that reduces the concentration of that reactant/product.

• Changing overall pressure: (only works in gas phase) Equilibrium will shift to the direction countering the increase/decrease in pressure

• Changing temperature: Equilibrium will shift to the direction to counter increase/decrease in temperature.

• Catalyst: doesn't shift equilibrium as it increases the rate of forward and backward reaction equally.

Applications:

Haber process: N₂ (g) + 3H₂ (g) $\leftarrow \rightarrow$ 2NH₃ (g) Δ H^{*} = -92KJ mol⁻¹ Conditions: 400°C, 20000kPa, iron catalyst

(Important liquid fuel/chemical feedstock)

Ethanol: (hydration of ethene) H₂C=CH₂ (g) + H₂O (g) $\leftarrow \rightarrow$ CH₃CH₂OH (g) Δ H* + -46KJ mol⁻¹ Conditions: 300°C, 6500 kPa

• High pressure (too high) will polymerize the ethane

• Too much steam will dilute catalyst

Methanol: CO (g) + 2H₂ (g) $\leftarrow \rightarrow$ CH₃OH (g) Δ H* = -91 KJmol⁻¹ Conditions: 500K, 10000kPa

Temperature: Costs money to reach and maintain high temperature Pressure: costs money to reach and maintain high pressure. Equipment! Explosion! ^ Cost may outweigh benefit.

A compromise temperature: high enough to ensure rapid reaction, low enough for decent yield. (Because high temperature results in increased rate of reaction <u>but</u> decreases yield; vice versa)

Redox: reduction-oxidation

Oxidation: gain of oxygen, loss of electron(s) Reduction: loss of oxygen, gain of electron(s), reduction in charge, gain in hydrogen

Oxidizing agent: accepts electrons (and is reduced) Reducing agent: donates electrons (and is oxidized) (ALWAYS REMEMBER TO IDENTIFY THE <u>SPECIES</u> NOT JUST THE SINGLE ION!)

Oxidation state:

Shows distribution of electrons in a compound/molecule. Charge of element/ion/atom in a compound. Ionic: number of electrons lost or gained.

*Every element has oxidation state of 0 when uncombined

ElementOxidation stateHydrogen+1 (except metal hydrides)G1+1G2+2Aluminium+3Oxygen-2 (except in peroxide and with F)Chlorine-1 (except with F or O)

Half equation: an ionic equation used to describe the gain or loss of electrons during a redox process. 2 half equations combine to form balanced equation for redox reaction. Simplest half equation: no spectator ions

Group 7 Halogen Atomic number Electronegativity Atomic radius Melting point State Fluorine Highest Pale yellow gas 9 17 Chlorine Green gas Bromine 35 Reddish liquid 53 Grey solid (purple gas) Iodine Highest Largest Electronegativity decreases down group Bond enthalpies Increased shielding 300 • Increased distance bond enthalpy • Attraction between bonding electrons and nuclei is decreased. (kJ mol⁻¹) Atomic radius: 200 • Increased number of main level shells • Weaker attraction between e in shells More diffuse 100 Melting point: VDW forces * electron #, area, shape, shells Bond enthalpy: 0 F-F |-| CI-CI Br-Br Fluorine is unexpectedly weak because it is very small, thus the non-bonding electrons are too close so they repel each other.

Oxidizing ability increases up the group. (Better at attracting electrons) Evinced in displacement reactions. (G7 in G1+G7 compound displaced by more reactive G7)

Reducing ability of halide ions increase down the group. Further away + more shielding so easier to lose electron. All **solid** sodium halides can react with **CONC** sulfuric acid. Product reflects reducing powers of halide ions.

NaCl (s) + H_2SO_4 (l) \rightarrow NaHSO₄ (s) + HCl (g)

NaBr (s) + H₂SO₄ (l) \rightarrow NaHSO₄ (s) + HBr (g) H₂SO₄ (l) + 2Br⁻ + 2H⁺ \rightarrow 2H₂O + Br₂ (l) + SO₂ (g)

NaI (s) + H₂SO₄ (l) → NaHSO₄ (s) + HI (g) H₂SO₄ (l) + 2I⁺ + 2H⁺ → 2H₂O + I₂ (l) + SO₂ (g) H₂SO₄ (l) + 6I⁺ + 6H⁺ → 4H₂O (l) + 3I₂ (s) + S (s) H₂SO₄ (l) + 8I⁻ + 8H⁺ → 4H₂O (l) + 4I₂ (s) + H₂S (g) Neutralization: not redox. Observe: white fumes (HCl) blue litmus turns red

Observe: Choking gas SO₂ Respective liquids/vaporized.

Observe: Yellow solid sulfur

Observe: rotten egg smell

Identification of group 7 halides:

- 1. Add dilute nitric acid to get rid of CO₃²⁻ and OH⁻ impurities
- 2. Add silver nitrate solution into solutions
- 3. Precipitate forms

Halide	AgF	AgCl	AgBr	AgI
Color	colourless	white	cream	Pale yellow
Further test		Dissolves in dilute	Dissolves in conc	Doesn't redissolve.
		ammonia	ammonia	

Uses of chlorine: kill bacteria and sterilize water.

Disproportionation: oxidation state increases and decreases simultaneously.

Reaction with water: (chlorine is soluble)

Cl₂ (g) + H₂O (l) \rightleftharpoons HClO (aq) + HCl (aq) [in cold water] 2Cl₂ (g) + 2H₂O (l) → 4HCl (aq) + O₂ (g) [UNDER SUN] NaClO (s) + H₂O (l) \rightleftharpoons HClO (aq) + NaOH (aq) [DIRECT CHLORINATION] (HClO: Chloric (I) acid) Cl₂ (g) + 2NaOH (aq) \rightleftharpoons NaCl (aq) + NaClO (aq) + H₂O (l)[making of NaClO w/cold, dilute NaOH] NaClO (Sodium Chlorate (I)): Making bleach and water disinfection

Group 2 – alkaline earth metals

Element	Atomic number	Metallic radius	MP/BP	Ionization energy
Magnesium	12		v	Highest
Calcium	20		Highest	
Strontium	38		٨	
Barium	56	Largest	^	

Size increases: extra filled main level of electrons

MP/BP decreases: sea of delocalized electrons further away from nuclei, weaker attraction.

[Exception: magnesium: lattice structure is different.]

Ionization energy decreases: more shielding and distance from nuclei thus easier to remove

Reaction with water and steam (more reactive down the group)

Water: $M(s) + 2H_2O(l) \rightarrow M(OH)_2(aq) + H_2(g)$ Steam: $M(s) + H_2O(g) \rightarrow MO(s) + H_2(g)$ (M = metal)

Uses of group 2 compounds:

*Calcium hydroxide used to treat acidic soil.

*Magnesium sulfate is used as a laxative.

*Barium sulphate is used as x-ray lining (your body doesn't absorb it since its very insoluble)

*Barium chloride is used to test for sulfates because it forms white precipitate with it.

Anion	Trend
Hydroxide	More soluble down
Carbonate	Less soluble down
Sulfate	Less soluble down

Extraction of metals:

Metals combine with sulfur and oxygen Roast sulfide in air → oxide (SO₂ produced. Collected → sulfuric acid) ^ with water and oxygen Gangue: clay and rock impurities Sometimes temperature required for metal to react with Carbon is too high (uneconomic) Ideal reducing agent: Cheap, readily available, don't cause pollution, no harmful byproduct.

Iron (haematite) [continuous] $C + O_2 \rightarrow CO_2$ [Exothermic 2000k] $CO_2 + C \rightarrow 2CO$ [reducing agent] $Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$ Byproduct: SiO ₂	Recycling: reduces scrap in landfill No CO ₂ produced (energy used to melt produced CO ₂) Easily separable: magnetic
Manganese: reduction with coke (impure carbon) or carbon	arbon monoxide
Copper (malachite): reduction with coke (old method) $CuCO_3 \rightarrow CuO + CO_2$ [Thermal decompositio $2CuO + C \rightarrow 2Cu + CO_2$	or carbon monoxide n]
New method: • Spray Cu <u>low-grade ore</u> with dilute acid in the preser • Cu extracted from solution with scrap iron + Scrap iron is cheap + No CO ₂ produced & less energy use than reduction w	nce of thiobacillus ferrooxidans. rith carbon
Aluminium (bauxite) [continuous] Al ₂ O ₃ dissolve in molten cryolite: Na ₃ AlF ₆ Pass through current of 300000A (VERY HIGH COST)	[melting point 1240 k] 1000 k less!
Cathode: $Al^{3+} + 3e^{-} \rightarrow Al$ Anode: $O^{2-} \rightarrow \frac{1}{2}O_2 + 2e^{-}$ ^ @ high temp, O_2 reacts with carbon anode (CO ₂) Recycling: uses 5% of energy required to make them +less CO ₂ Increased transportation costs (CO ₂ emitted in the pro	cess)
Titanium (Rutile) [batch] Strong, low density, resistant to corrosion $TiO_2 + 2Cl_2 + C \rightarrow TiCl_4 + CO_2$ [TiCl distilled off. Temp $TiCl_4 + 4Na \rightarrow Ti + 4 NaCl$ [inert argon atm • Can't use carbon as reducing agent, as @ high temp, n EXPENSIVE: • Using a more reactive metal as reducing agent • Batch process (heat back up) • 3 step process	: 1173 k] nosphere: stop metals reacting w/0&N 1300k] netal react w/Carbon → carbide (brittle)
Tungsten → filament lamps • Can't use carbon as reducing agent as @ high temp, n WO ₃ + 3H ₂ → 3H ₂ O + W (H ₂ highly flammable)	netal react w/Carbon → carbide (brittle)

Haloalkanes have polar bonds with the carbon it is bonded to, as they are all more electronegative than carbon.

- Polarity decreases down the group as difference in electronegativity decreases.
- The polarity is not sufficient to make them soluble in water.
- Increased branching decreases melting/boiling point: (decreased surface area therefore less vdw)

The reactivity of the haloalkane depends on :

Bond enthalpy and polarity, but the effects of bond enthalpy is greater than that of polarity. The stronger/higher the bond enthalpy, the less reactive/harder it is for the halogen to leave.



Tertiary Haloalkanes are more reactive than primary Haloalkanes

Nucleophilic substitution: to introduce new functional groups into organic compounds.

The carbon is electron deficient, it can be attacked by reagents that are electron rich or have electron rich areas. 1. The nucleophile provides the electrons for a new bond (using its lone pair)

2. Carbon can only have 8 outermost electrons thus the Halide ion is displaced (lowest bond enthalpy with C)

Nucleophile: electron pair donor

• Has a lone, unshared pair of electron on electronegative atom. (to form a covalent bond)

• OH-, CN-, and NH3 (neutral)

•Bond between C – Halogen breaks (heterolytic fission) resulting in production of ions.

Substitution: Chemical changes which replace atoms/groups of atoms by another atom/groups of atoms. Hydrolysis: compound split in a reaction by water.

Unimolecular nucleophilic subsitution - sN1



- Ammonia as nucleophile
- Organic compound formed is a primary amine. Meth**yl**amine, Eth**yl**amine, Prop**y**lamine etc.

Note: with CN-, nitriles are formed. Ethanenitrile, Propanenitrile (the C in CN must be taken into account) Elimination: Hydrogen halide is eliminated from the molecule, leaving a double bond. (Alkene) A.K.A. hydrolysis

Under different conditions (No water present, only G1 hydroxide dissolved in ethanol, and heated) the OH- will act as a base, removing the H+ ion from the haloalkane.



Formation of Haloalkanes – Free radical substitution reaction (chain reaction) $CH_4 + Cl_2CH_3Cl + HCl$



Initiation – The formation of free radicals (from non-free radicals) Initiated by UV light. eg. $Cl_2 \rightarrow Cl_{\bullet} + Cl_{\bullet}$

Propagation – 'Recycling' free radicals (free radical to free radical and back to initial free radical) 2 stages Eg. Cl•+ CH₄ \rightarrow HCl+•CH₃ •CH₃ + Cl₂ \rightarrow CH₃Cl+•Cl

Termination – Free radicals removed (free radical with free radical \rightarrow no radical) Eg. Cl• + Cl• \rightarrow Cl₂ •CH₃ + •CH₃ \rightarrow C₂H₆ Cl• + CH₃ \rightarrow CH₃Cl

CFCs

• Very unreactive in normal conditions

• Goes high up in the atmosphere before decomposed by UV light. Uses:

• Short chain – Aerosol, refrigerants, propellants

• Long chain - solvent, dry cleaning

Ozone: shields earth from excess UV radiation which causes blindness and skin cancer in humans Ozone at ground level causes lung irritation, degradation of plastics and paints.

Deterioration of ozone layer: $Cl \bullet + O_3 \rightarrow ClO \bullet + O_2$ $ClO \bullet + O_3 \rightarrow 2O_2 + Cl \bullet$

Overall equation: $20_3 \rightarrow 30_2$

Alkenes

- Unsaturated hydrocarbons (1 or more c-c double bond) decolorizes bromine water
- Planar molecule
- Restricted rotation (overlapping p orbital $\rightarrow \pi$ orbital)
- More reactive than alkanes as it's very susceptible to electrophilic attacks (the double bond)

Position isomers: (difference in position of double bond)



CH2=CH-CH2-CH3 but-1-ene



CH3-CH=CH-CH3

but-2-ene

Stereoisomerism: Same structural formula, bonds arranged differently in space (due to lack of free rotation about double bond)





cis-1,2-dichloroethene

If the higher priority groups are on \underline{z} he \underline{z} ame \underline{z} ide: \underline{z} isomer If the higher priority groups are on the eppesite side: e isomer

Determining higher priority: Highest atomic number.

Electrophilic addition

bans-1,2-dichloroethene

- the double bond is a high electron density area

- Electrophile is attracted to the double bond

- Positively charged (area or ion)
- Accepts pair of electrons
- Carbocation formed
- now negative ion forms a bond

Electrophilic addition of sulfuric acid to an alkene



- 1. δ + Hydrogen in H₂SO₄ is attracted to electron dense area (double bond)
- 2. Accepts an electron, forming a carbocation
- 3. Now negative ion attracted to + carbocation

Note: the electrophile can be a neutral molecule eg. Br – Br. Negative charge area in double bond induces a temporary charge on both Br



Note: Tertiary carbocation is much more stable than primary as alkyl groups have a tendency to release electrons (positive inductive effect) which stabilizes the positive charge of the carbocation. Thus the more the C + is attached to alkyl groups, the more likely it will be the main intermediate carbocation.

Polymerization of alkenes

Polymers: long chain molecules formed when many small molecules (monomers) join up in long chains



(Addition polymerization of propene) - not additional!

Repeating unit: smallest group of atoms that produce the polymer. (basically the monomer)
low density: free radical substitution (branching, don't pack together)

Polymer + name	Uses
Polyethene (CH ₂ =CH ₂)	Plastic bags, bottles
Polypropene (CH ₃ -CH=CH ₂)	Rope, milk crates
Polychloroethene (Cl-CH=CH ₂)	Vinyl records
Polypropenitrile (CN-CH=CH ₂)	Clothing
Poly 1,1,2,2-tetrafluroethene (CF ₂ =CF ₂)	cookware

Plastic problems:

- not biodegradable
- Landfill sites
- Problem for animals when ingested

Solutions: reduce plastic usage or recycle

Mechanical recycling	Feedstock recycling
- separate different types of plastic	- Heat plastic
- wash once	- Break polymer into monomer
- ground up into small pellets	- make new plastics
- Melted and remoulded	
	- can only be done limited amount of times:
	plastic's properties degrades each time heated
	(chains break)



- OH = hydrogen bonding (thus higher mp bp than alkanes with similar RMM)

- Shorter chain alcohols soluble in water

Making alcohol:

• Fermentation

1. Anaerobic respiration: $C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$ [using YEAST]

2. comprimise temperature : 35°C

- anaerobic to prevent oxidation

Biofuel: fuels produced from vegetable matter and organic waste

+ carbon neutral: an activity that has no net annual carbon (greenhouse gas) emissions to the atmosphere

+ idea of carbon sink; recycling CO2

• Hydration of ethene (covered in previous chapter)

Comparing the 2 methods of manufacturing ethanol:

	1 0	
	Fermentation	Hydration
+	Renewable	Continuous
	Carbon neutral	High purity, yield, atom economy, fast
	Sugar canes cheap to grow	
	Low temperature (35)	
-	Batch	Non-renewable
	Low purity	High energy and pressure (energy use)
	Low yield & slow	
	Low atom economy	
	Fermentation stops at 15%	
	Labour intensive	

Oxidation of alcohols:

Excess alcohol, dilute acid, K₂Cr₂O₇, heat and distill



Elimination reaction: When a small molecule leaves parent molecule

Dehydration of alcohols: pass through hot concentrated sulfuric acid or Al₂O₃



Analytical techniques

Infrared spectroscopy: Identify functional groups in organic molecules

- Most compounds absorb infrared radiation
- Wavelendths absorbed corresponds to natural frequenc for vibration of bonds
- IR re-emitted from sample of decreased intensity (transmittance)

Fingerprint region (below 1500cm⁻¹)

- complex vibrations of whole molecule
- unique to particular molecule

(identify isomers by superimposing with IR spectrums in database)

Greenhouse gases have large IR absorbtion ranges.

EXAM TECHNIQUES

General:

- FORMS acid rain
- Making plastic
- Making bleach
- State effects (rather than just naming)
- Don't just write p/d orbital: specify shell number

Why is a process used:

- See product (pollution? Harmful?)
- See reactant (Harmful? Expensive? Explosive? Recycling?)
- Time and energy considerations (conditions)
- Atom economy
- Identifying species: the whole thing, not just the ion!
- Simplest ionic equation: write out whole equation and rid spectator ions.
- Mechanisms: use <u>curly arrow</u>.

Calculations:

- Look back at equation to check (moles)
- Enthalpy of formation/reaction/combustion: divide by # moles!
 - Do plenty of past papers
 - Read the syllabus
 - Mark papers carefully, use the mark scheme to streamline answers
 - Make note of mistakes and review them
 - Read examiner reports if necessary

Good luck and don't leave revision to the last minute!