

Developing Fuels

Revision notes

Amount of substance

- A mole is the unit of 'amount of substance'.
- Moles of solid = mass / M_r
- 1 mole of any gas is 24dm^3 at r.t.p.

Energy changes in reactions

- Exothermic reactions release heat, causing a temperature rise, and ΔH is negative.
- Endothermic reactions take in heat, causing the temperature of the surroundings to fall, and ΔH is positive.
- ΔH_c is the enthalpy change when 1 mole of a substance is completely burned in oxygen under standard conditions.
- ΔH_f is the enthalpy change when 1 mole of a substance is formed from its elements in their standard states.

Energy changes in reactions

- **Limitations of simple calorimetry experiments include:**
 - Heat loss to the surroundings
 - Incomplete combustion/ incomplete reaction
 - Measurement uncertainties
- **$E = m c \Delta T$**
- **m is the mass of water being heated (we assume 1 g cm^{-3} even if it is not pure water)**
- **c is the specific heat capacity (we assume $4.2 \text{ J K}^{-1} \text{ g}^{-1}$ even if it is not pure water)**
- **ΔT is the temperature change**

Energy changes in reactions

- Using $E = m c \Delta T$ gives the energy change in J for this specific experiment.
- To work out kJ mol^{-1} you must divide your answer in J by the number of moles of fuel burnt. (Then divide by 1000 to convert to kJ.)

Hess's Law

- The enthalpy change for a reaction is the same regardless of the route taken, provided the start and finish conditions are the same.
- If you are calculating an enthalpy change using ΔH_c values from a data book, then $\Delta H_r = \Delta H_c(\text{reactants}) - \Delta H_c(\text{products})$.
- If you are calculating an enthalpy change using ΔH_f values from a data book, then $\Delta H_r = -\Delta H_f(\text{reactants}) + \Delta H_f(\text{products})$.
- Use the 'Hess cycle help guide' on Moodle.

Bond enthalpies

- **Bond enthalpy is the energy required to break 1 mole of a particular bond. It is often taken as the average value for that particular bond in a range of molecules (eg C-H in methane, ethane, methanol, ethanoic acid...)**
- **Short bonds are stronger than long bonds.**
- **Bond breaking is an endothermic process.**
- **Bond making is an exothermic process.**

Bond enthalpies

- **To calculate the enthalpy change of reaction:**
 - Add up all the bonds that need to be broken. These have + kJ mol⁻¹.
 - Add up all the bonds that need to be made. These have - kJ mol⁻¹.
 - Add the two numbers to work out the overall enthalpy change:
Bonds broken(+ve value) + Bonds made(-ve value)

Entropy

- Entropy is a measure of the number of ways that molecules/atoms can be arranged. (Ensure you use 'molecules' or 'atoms' correctly according to the context you are given.)
- A solid has a low entropy.
- A liquid has a higher entropy than a solid.
- A solution has a higher entropy than a pure liquid.
- A gas has the highest entropy.

Kinetics

- **A catalyst speeds up a reaction but can be recovered chemically unchanged at the end of the reaction.**
- **A catalyst poison bonds irreversibly to the catalyst surface.**
- **A heterogeneous catalyst is in a different phase to the reactants (generally a solid catalyst with gaseous reactants).**

Function of a heterogeneous catalyst

1. Reactants get **adsorbed** onto the catalyst surface. Bonds within the reactants are weakened.
2. Bonds break.
3. New bonds form to produce the product.
4. The product diffuses away from the catalyst surface.

A catalyst works by weakening the bonds, holding the reactants in an appropriate orientation and providing an alternative pathway with a lower activation energy.

Uses of catalysts

- **Catalytic converters are heterogeneous catalysts that change harmful pollutant gases into less dangerous ones.**
- **Zeolites are catalysts used as molecular sieves in isomerisation, reforming and cracking processes.**

Pollutants

- **CO from incomplete combustion. Toxic to humans.**
- **CO₂ from combustion. Contributes to the greenhouse effect.**
- **Particulates from incomplete combustion. Causes surfaces including lungs to blacken.**
- **Unburnt hydrocarbons from incomplete combustion. Contributes to photochemical smog and hazardous to human health.**

Pollutants

- NO_x from the reaction of nitrogen and oxygen from the atmosphere under conditions of high temperature. Dissolves in water to produce acid rain.
- SO_x from the combustion of sulphur impurities in fuels. Dissolves in water to produce acid rain.
- Reduce pollution by using cleaner fuels, by scrubbing exhaust gases, and by reducing fuel use.

Organic functional groups

- Crude oil consists of a mixture of compounds, mainly hydrocarbons.
- Hydrocarbons are compounds containing only hydrogen and carbon.
- Crude oil can be separated by fractional distillation.

Organic functional groups

- Alkanes – saturated hydrocarbons C_nH_{2n+2}
- Cycloalkanes – saturated hydrocarbons in a ring shape C_nH_{2n}
- Alkenes – unsaturated hydrocarbons C_nH_{2n}
- Arenes – hydrocarbons containing a benzene ring.
- Alcohols R-OH.
- Ethers R-O-R.

Organic functional groups

- **Aliphatic** – straight chain, not containing a benzene ring.
- **Aromatic** – containing a benzene ring.
- **Saturated** – containing single carbon-carbon bonds only.
- **Unsaturated** – containing at least one carbon-carbon double bond.

Organic functional groups

1 carbon = meth

2 carbons = eth

3 carbons = prop

4 carbons = but

5 carbons = pent

6 carbons = hex

7 carbons = hept

8 carbons = oct

CH_4 methane

$\text{C}_2\text{H}_5\text{OH}$ ethanol

$\text{CH}_3\text{CH}(\text{OH})\text{CH}_3$

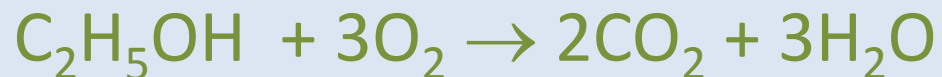
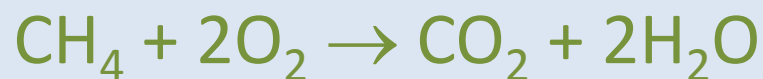
propan-2-ol

$\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$

2-methylbutane

Organic reactions

- **Complete combustion of alkanes and alcohols gives carbon dioxide and water.**



Isomerism

- Isomers have the same molecular formula but different structural formula.
- Full structural formula show all the bonds in the molecule.
- Shortened structural formula show information about the location of the atoms – eg $\text{CH}_3\text{CH}(\text{OH})\text{CH}_3$
- Skeletal formula show just the carbon skeleton and functional groups, using zigzags. Hydrogens are not shown.

Isomerism

- **The electron pair repulsion principle predicts the shapes of molecules:**
 - 2 electron groups: linear 180° eg ethyne C_2H_2
 - 3 electron groups: trigonal planar 120° eg ethene
 - 4 electron groups: tetrahedral 109° eg CH_4

Octane number

- Octane number of a petrol is the tendency of the petrol towards auto-ignition which causes 'knocking' in a car engine.
- The higher the octane number, the less knocking.
- Increasing chain length decreases (worsens) octane number. Butane 94, pentane 62, hexane 25, heptane 0.
- Increasing branching increases (improves) octane number.

Refining fuels

- **Fractional distillation:**
 - separating the components of crude oil on the basis of their different boiling points.
- **Isomerisation:**
 - the process of converting a straight chain alkane into a branched isomer.
 - This improves the octane number.
 - The catalyst is aluminium oxide / platinum.
 - Zeolites are used as molecular sieves to separate the isomers.

Refining fuels

- **Reforming:**

- the process of converting a straight chain alkane into cycloalkanes and aromatic compounds.
- This improves the octane number.
- The catalyst is platinum.
- During the process some of the hydrocarbons decompose to carbon, which decreases the efficiency of the catalyst. Excess hydrogen is added to suppress the formation of carbon.

Refining fuels

- **Cracking:**
 - the process of converting a long alkane into a shorter alkane (sometimes branched) and an alkene.
 - This improves the octane number and produces alkenes for polymerisation.
 - The catalysts used are zeolites.

Alternative fuels

- **Chemists improve fuels by:**
 - developing new blends.
 - adding oxygenates (generally ethers).
 - searching for and developing new fuels.
 - carrying out research for the hydrogen economy.
- **Alternative fuels include biofuels, hydrogen and nuclear.**
- **All fuels have benefits and risks associated with them. Choices have to be made about ensuring a sustainable energy supply.**