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 ΔT**
- **m is the mass of water being heated (we assume 1 gcm^{-3} even if it is not pure water)**
- **c is the specific heat capacity (we assume 4.2 J K^{-1} 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 **ad**sorbed 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.
- CO_2 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 <u>only</u> 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

C_2H_5OH ethanol

$CH_3CH(OH)CH_3$

propan-2-ol

$CH_3CH(CH_3)CH_2CH_3$

2-methylbutane

Organic reactions

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

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$C_2H_5OH + 3O_2 \rightarrow 2CO_2 + 3H_2O$$

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 $CH_3CH(OH)CH_3$
- 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^o eg ethyne C_2H_2
  - 3 electron groups: trigonal planar 120^o eg ethene
  - 4 electron groups: tetrahedral 109^o 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.**