Fuels and Heats of Reaction

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Exp: Preparation of ethene and examine its properties

Ethene is produced by dehydrating ethanol using aluminium oxide as a catalyst.

This is an elimination reaction where H_2O is removed from ethanol.

Procedure	Observations	Explanation
Some ethanol is poured into a test tube and glass wool is added. The test tube is clamped horizontally.		Glass wool soaks up the ethanol and holds it in place at the end of the horizontal test tube.
Aluminium oxide is placed in the middle of the horizontal test tube.		
The Al_2O_3 is heated gently	Bubbles of gas are seen collecting in the test tube	As the tube is heated the ethanol turns into a vapour and passes over the hot Al_2O_3. The ethanol is dehydrated to ethene. If the ethanol was heated directly it would evaporate too quickly and pass too fast over the Al_2O_3 and some ethanol would not be converted to ethene.

Procedure	Observations	Explanation
The ethene is captured; 5 test tubes and 1 gas jar are filled.		First test tube is discarded as it mostly contains air.
Once the samples have been collected the delivery tube is lifted out of the water. After this the Bunsen burner is turned off.		*If this step was not taken ‘suck back’ would occur. Suck back occurs when the vapours in the boiling tube cool and create a vacuum sucking the water into boiling tube. The cold water entering the hot boiling tube would cause the boiling tube to break.*

Testing the properties of Ethene

Procedure	Observations	Explanation
Physical Properties:	Ethene is a colourless gas with a sweetish smell. Insoluble in water (polar) Soluble in organic solvents (non-polar)	
Combustion: A lighted taper is brought to the mouth of a sample test tube.	Gas burns with a yellow luminous flame that is slightly smoky	$C_2H_4 + O_2 \longrightarrow 2CO_2 + 2H_2O$
Limewater is added to the test tube and shaken.	Limewater turns milky	Carbon dioxide was formed when ethene burned in air $Ca(OH)_2 + CO_2 \longrightarrow CaCO_3 + H_2O$

Testing the properties of Ethene

Procedure	Observations	Explanation
Addition of bromine: Bromine water is added to a test tube of ethene and shaken.	Colour change from red to colourless.	Bromine (red) reacts to form 1,2 dibromoethane (colourless)
Addition of acidified $KMnO_4$: Acidified $KMnO_4$ is added to a test tube of ethene and shaken.	Colour change from purple to colourless.	Mn^{7+} (red) is reduced to Mn^{2+} (colourless)

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Exp: Preparation of ethyne and examine its properties

Safety precautions: ethyne forms an explosive mixture with air so no naked flame should be anywhere near the equipment.

Procedure	Observations	Explanation
Calcium carbide is placed in a Buchner flask.	Calcium carbide is a grey-black solid	Glass wool soaks up the ethanol and holds it in place at the end of the horizontal test tube.
Water is slowly added to the calcium carbide using a dropping funnel.	Fizzing takes place in the Buchner flask. A white solid is formed. The Buchner flask gets warm.	Ethyne gas is formed. Calcium hydroxide (white) is formed. The reaction is exothermic (gives out heat). $CaC_2 + 2H_2O \longrightarrow Ca(OH)_2 + C_2H_2$

Testing the properties of Ethyne

Procedure	Observations	Explanation
Physical Properties:	Ethyne is a colourless gas with a sweetish smell. Insoluble in water (polar) Soluble in organic solvents (non-polar)	
Combustion: A lighted taper is brought to the mouth of a sample test tube.	Gas burns with a yellow luminous flame and a lot of soot is formed	$2C_2H_2 + 5O_2 \longrightarrow 4CO_2 + 2H_2O$ Soot is formed due to unburnt carbon.

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Testing the properties of Ethyne

Procedure	Observations	Explanation
Addition of bromine: Bromine water is added to a test tube of ethyne and shaken.	Colour change from red to colourless.	Bromine (red) reacts to form colourless compounds.
Addition of acidified $KMnO_4$: Acidified $KMnO_4$ is added to a test tube of ethene and shaken.	Colour change from purple to colourless.	Mn^{7+} (red) is reduced to Mn^{2+} (colourless)

Oil Refining and its Products

Crude oil is a fossil fuel, formed of decomposed animals. It is pumped up from underground and consists of a mixture of hydrocarbons.

Crude oil is itself is not useful and needs to be separated into its components.

Fractional distillation

Fractional distillation is the process used to separate crude oil into useful parts.

This is done by heating the crude oil and separating groups with similar boiling points.

These groups are called fractions.

Process of Fraction Distillation

1. Crude oil is heated in a furnace (600^{o}C)
2. The hot mixture enters the bottom of the fractionating column (tall tower with many trays to collect the different fractions).
3. The fractionating column is hotter at the bottom.
4. Heavier fractions with higher boiling points are collected at the lower levels.
5. Lighter fractions with low boiling points are collected at the higher levels.

Really Great and Noble Kings Don’t Leave Families Begging

Name of fraction	Carbons	Uses
Refinery Gas (petroleum gas) B.P. 25^{o}C to 40^{o}C	C_1-C_4	Liquified Petrolium Gas (LPG)
Light Gasoline (petrol) B.P. 40^{o}C to 75^{o}C	C_5-C_{10}	Petrol for cars
Naptha B.P. 75^{o}C to 150^{o}C	C_7-C_{10}	Chemicals for petrochemical industry
Kerosene B.P. 150^{o}C to 240^{o}C	C_{10}-C_{14}	Fuel for planes
Diesel Oil B.P. 240^{o}C to 500^{o}C	C_{14}-C_{19}	Diesel for cars/truck/etc
Lubricating Oil (residue fractions) B.P. 400^{o}C	C_{19}-C_{35}	Lubricant for engines
Fuel Oil (residue fractions) B.P. 450^{o}C	C_{30}-C_{40}	Fuel for ships/power stations/heating plants
Bitumen (residue fractions) B.P. 500^{o}C	$>C_{35}$	Used for tar on roads

Octane Number

Octane number of a fuel is a measure of the tendency of the fuel to resist knocking.

Knocking is also known as auto-ignition

Auto-ignition is the premature ignition of the petrol/air mixture before normal ignition of the mixture by a spark takes place.

Octane Number

2,2,4 –trimethylpentane (iso-octane) has an octane number of 100 (low tendency to auto-ignite).

Heptane has an octane number of 0 (high tendency to auto-ignite).

2,2,4 –trimethylpentane and heptane are reference hydrocarbons for the octane number scale.

Octane Number

The octane number of a fuel can be measure by comparison with the reference hydrocarbons or by chemical analysis.

A mixture of 10% 2,2,4 –trimethylpentane and 90% heptane has an octane number of 10.

Factors Affecting Octane Number

1. Length of the chain:

The shorter the alkane chain, the higher the octane number.

2. Degree of branching:

The more branched the chain, the higher the octane number.

3. Straight-chain versus cyclic structure:

Cyclic structures have higher octane numbers than straight-chain molecules

Anti-knocking additive

It was found in 1920s that added tetraethyl lead helped to reduce the knocking in engines.

However leaded petrol has been phased out since 2000 due to the poisonous lead pollution caused.

Also lead compounds poison the metal catalysts in catalytic converters of cars.

Methods to increase octane number of petrol

1. **<u>Isomerisation</u>**

This involves changing straight chained alkanes into their isomers.

- The alkanes are heated in the presence of a catalyst, causing the chain to break.
- The chain fragments are allowed to join back together when they do so they are more likely to formed branched-chain alkanes.

Example: pentane $\longrightarrow$ 2-methylbutane

octane number = 62 octane number = 93

Methods to increase octane number of petrol

2. Catalytic Cracking

Catalytic cracking is the breaking down of long chain hydrocarbon molecules by the action of heat and catalysts onto short chain molecules for which there are greater demand.

Example: $C_{12}H_{26} \longrightarrow$ Propene + 2-methylbutane + But-1-ene

Note: The total number of carbons and hydrogens must be equal on both sides. At least one product must be unsaturated. You can be asked to figure out a missing product given the others.

Secondary benefit of catalytic cracking

A second benefit of catalytic cracking is that the alkenes produced are important as feedstock for the petrochemical industry.

Methods to increase octane number of petrol

3. Dehydrocyclisation

This involves the use of catalysts to form ring compounds.

When dehydrocylisation occurs straight chain compounds are converted to cycloalkanes. Cycloalkanes are then converted to aromatic compounds.

Hexane $\longrightarrow$ Cyclohexane $\longrightarrow$ Benzene

Methods to increase octane number of petrol

4. Adding oxygenates

This involves adding fuels with oxygen in them.

The three commonly used oxygenates are: methanol, ethanol, and MTBE (methyl tertiary-butyl ether).

These are commonly added to petrol.

Secondary benefit: oxygenates reduce pollution as the fuels burn ‘cleaner’.

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Hydrogen

Hydrogen gas (H_2) is a non hydrocarbon fuel.

<u>Manufacture of Hydrogen:</u>

1. Steam reforming of natural gas

$$CH_4 + H_2O \longrightarrow 3H_2 + CO$$

2. Electrolysis of water

$$H_2O \longrightarrow H_2 + \frac{1}{2}O_2$$

Important use of hydrogen

One of hydrogen gas' most important uses is in the manufacture of ammonia.

$$N_2 + 3H_2 \longrightarrow 2NH_3$$

Thermochemistry

Thermochemistry is the study of heat changes during reactions.

Exothermic reactions give out heat to the surroundings (feels hot).

Endothermic reactions take in heat from the surroundings (feels cold).

Heat of reaction

Heat of reaction is the heat change when the number of moles of reactants indicated in the balanced equation for the reaction react completely.

Unit: kJ mol^{-1}

Heat of reaction is shown using ΔH (‘delta H’).

Exothermic reactions have a negative ΔH ($\Delta H = -242$ kJ mol^{-1})

Endothermic reactions have a positive ΔH ($\Delta H = +242$ kJ mol^{-1})

Heat of Combustion

Combustion reactions occur when a substance is burned in oxygen.

Heat of combustion of a substance is the heat change when one mole of the substance is completely burned in excess oxygen.

Heat of Combustion (common errors)

$$C + \frac{1}{2}O_2 \longrightarrow CO \qquad \Delta H = -111 kJ\ mol^{-1}$$

The ΔH for this reaction is not the heat of combustion as when carbon is burned in excess oxygen the product is carbon dioxide not carbon monoxide

$$2C_4H_{10} + 13O_2 \longrightarrow 8CO_2 + 10H_2O \qquad \Delta H = -5754 kJ\ mol^{-1}$$

In this equation 2 moles of C_4H_{10} are burned, heat of combustion is for one mole. So heat of combustion = $\frac{-5754}{2}$ = -2877kJ mol^{-1}

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Bomb Calorimeter

A bomb calorimeter is used to measure heat of combustion.

Steps:

1. A known mass of the substance is placed in the bomb
2. The bomb is filled with oxygen under pressure (ensures excess)
3. The bomb is placed into a known quantity of water in the calorimeter.
4. The substance is ignited. The temperature change in the water is measured.
5. The formula below is used to find the heat produced

Heat produced = mass x specific heat capacity x temperature change.

Kilogram calorific value

Kilogram calorific value of a fuel is the heat energy produced when 1 kg of the fuel is completely burned on oxygen.

Kilogram calorific value = $\frac{heat\ of\ combustion}{relative\ molecular\ mass}\ x\ 1000$

Bond energy

Bond energy is the average energy required to break one mole of a particular covalent bond and to separate the neutral atoms completely from each other.

Single bonds are more easily separated than double bonds, and double bonds are more easily separated than triple bonds.

Also the more polarised the covalent bond the easier it is to break.

Heat of Neutralisation

Heat of neutralisation is the heat change when one mole of H^+ ions from an acid reacts with one mole of OH^- ions from a base.

e.g. $HCl + NaOH \longrightarrow NaCl + H_2O \qquad \Delta H = -57.1\ kJ\ mol^{-1}$

Exp: Determine the heat of reaction of hydrochloric acid and sodium hydroxide

Procedure	Observations	Explanation
Equal volumes of HCl and NaOH are placed into two separate polystyrene cups. The volumes and concentrations are recorded.		The rise in temperature will be proportional to the concentration of acid and base used.
Once both liquids are at the same temperature the NaOH is quickly added to the HCl. The lid is placed on the cup.	A rise in temperature is observed	The reaction is exothermic, heat is given out during the neutralisation reaction.
The maximum temperature reached is recorded.		

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Steps to ensure/improve accuracy

Procedure	Observations	Explanation
Digital thermometer is used to give a reading to 0.1°C		This gives a more accurate reading.
A burette could be used to measure the two liquids before placing them in separate cups.		This gives a more accurate reading.
A lid is useful as it prevents heat loss to the surroundings.		Ensures all heat produced in the reaction is recorded.
Ensure no splashing occurs when adding the two liquids together.		Prevents loss of liquid i.e. loss of reactants.

Calculations

The formula below is used to calculate the heat produced in the reaction.

$$Heat\ given\ out = mass\ x\ specific\ heat\ capacity\ x\ rise\ in\ temperature$$

$$Heat\ given\ out = m\ x\ c\ x\ (t_2 - t_1)$$

*Mass must be in kg

*Specific heat capacity must be in J kg^{-1} K^{-1}

*Remember when calculating the heat of neutralisation refers to one mole of H^+ ions/OH^- ions.

*Diprotic acids (H_2SO_4) give off two moles of H^+ ions per one mole.

*Triprotic acids (H_3PO_4) give off thee moles of H^+ ions per one mole.

Calculations

Sometimes you will be given heat capacity rather than specific heat capacity. In this case use the formula below.

$$Heat\ given\ out = heat\ capacity\ x\ rise\ in\ temperature$$

$$Heat\ given\ out = C\ x\ (t_2 - t_1)$$

*Specific heat capacity must be in J kg^{-1} K^{-1}

*Remember when calculating the heat of neutralisation refers to one mole of H^+ ions/OH^- ions.

*Diprotic acids (H_2SO_4) give off two moles of H^+ ions per one mole.

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Heat of Formation

Heat of formation of a compound is the heat change that takes place when one mole of a compound in its standard state is formed from its elements in their standard states.

$$2H_{2(g)} + \frac{1}{2}O_{2(g)} \longrightarrow 2H_2O_{(l)} \qquad \Delta H = -285.8 \text{ kJ mol}^{-1}$$

Note that hydrogen and oxygen are gases and water is a liquid, they are in their standard state.

(s) = solid (l) = liquid (g) = gas (aq) = aqueous (dissolved in water)

Hess’s Law

Hess’s Law states that if a chemical reaction takes place in a number of stages, the sum of the heat changes in the separate stags is equal to the heat change if the reaction is carried out in one stage.

$$A \xrightarrow{\Delta H = +50\ \mathrm{kJ\ mol^{-1}}} B \xrightarrow{\Delta H = +100\ \mathrm{kJ\ mol^{-1}}} C \xrightarrow{\Delta H = +50\ \mathrm{kJ\ mol^{-1}}} D$$

$$A \xrightarrow[\Delta H = +200\ \mathrm{kJ\ mol^{-1}}]{} D$$

Law of Conservation of Energy

Law of Conservation of Energy states that energy cannot be created or destroyed but can only be converted from one form of energy into another.