EDUCATION

85

CHEMISTRY

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 $5^{TH}/6^{TH}$ YEAR

HIGHER LEVEL

2024/2025

HEATS OF REACTION (THERMOCHEMISTRY)

STUDENT NAME:



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1112

CONTENTS



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Some chemical reactions can result in changes in temperature, for example heat can be given out or heat can be taken in. In this section of our course we are going to examine these heat changes and some reaction types in which this happens.

HEAT OF REACTION (ΔH)

The heat of reaction is the heat change that occurs when a reaction takes place according to a given balanced chemical equation.

EXOTHERMIC REACTION

In an exothermic reaction heat is given out from the reaction to the surroundings as the reaction loses heat. The heat of reaction is negative ($\Delta H = -$)

Examples – all combustion reactions are exothermic, the Haber Process for the manufacture of ammonia is exothermic, the reaction that occurs when conc. sulfuric acid is mixed with water.

ENDOTHERMIC REACTION In an endothermic reaction heat is taken in from the surroundings as the reaction gains heat. The heat of reaction is positive ($\Delta H = +$)

Examples – the reaction of ammonium nitrate with water and the formation of ethyne gas.

Different names can be given to heats of reactions depending on what happens in the reaction. For example the heat change that occurs when a substance is burned in oxygen is called the combustion, the heat change that occurs when an acid and base neutralise each other is called neutralisation etc. We are going to examine

- 1. Heat of combustion
- 2. Heat of formation
- 3. Heat of neutralisation

HEAT OF COMBUSTION

The heat of combustion of a substance is the heat change that occurs when 1<u>MOLE</u> of that substance is burned in an <u>excess</u> of oxygen. The units are expressed in kJ/mol.

As we can see from the definition each substance will have only <u>one</u> heat of combustion as the definition specifically refers to a <u>particular quantity</u> of the substance which is **1 MOLE**. If we burn more than or less than one mole, then the heat produced is not the heat of combustion. We can always adjust it to give the heat produced by one mole, to get the heat of combustion!!

It is important to remember that we can express 1 mole of a substance in different ways i.e. its molecular or atomic mass in grams or 22.4 I at s.t.p.

So for example we can get the heat of combustion of ethene, C_2H_4 , if we burn 1 mole of it or 28g of it or 22.4 litres of it at s.t.p



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WRITING EQUATIONS FOR HEATS OF COMBUSTION

The substance undergoing combustion is written on the **left-hand side** of the equation as it is a **reactant** in the reaction. As we are writing an equation for the 'heat of combustion' – 1 mole of the substance must be burned.

Examples - Write an equation to show the heat combustion of hydrogen

$$H_{2(g)} + \frac{1}{2}O_{2(g)} \rightarrow H_2O_{(l)}$$

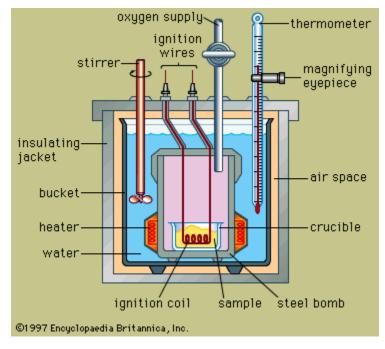
Write an equation to show the heat of combustion of ethene

Write an equation to show the heat of combustion of ethanol

THE BOMB CALORIMETER

We can <u>accurately</u> measure the heat of combustion of a substance using a piece of apparatus called the bomb calorimeter. If we examine the structure of a bomb calorimeter we see that it contains a **crucible** to hold the substance being burned, **wires** that can be electrically heated to ignite the sample, an **inlet tube** to provide an excess of oxygen and a **screw-on lid**. The bomb is then placed in a container of water that contains a **thermometer** to measure the heat change in the water and a **stirrer** so that the heat is evenly distributed throughout the water to get an accurate temperature reading.





By knowing (a) the amount of substance (SAMPLE) burned,

(b) the initial and final temperature of the water,

(c) the specific heat capacity of the water,

(d) the heat capacity of the calorimeter (STEEL IN THIS CASE) and

(e) the mass of the water in KG (EXPECT TO BE GIVEN DENSITY OF WATER)

it is then possible to measure the heat of combustion of the substance. (This calculation is not examined on this course but how a bomb calorimeter works is examined!)

Scientists also use the bomb calorimeter to measure the **kilogram calorific value** of fuels and food. When finding the kilogram calorific value we burn **1 kg** of the substance and see how much energy is given out (exothermic). In this way we can **compare the efficiency of various fuels** as we can see how much heat is produced when we burn 1kg of coal and compare it to burning 1kg of peat! However remember that the cost of the fuel is also a deciding factor.

Burning fuels that have a definite chemical formula will always give the same result but burning substances like coal or peat or petrol will vary as the composition of these substances vary due to quality.

KILOGRAM CALORIFIC VALUE The kilogram calorific value of a fuel is the heat that is produced when 1 kg of the fuel is burned in an excess of oxygen. The units are expressed in kJ/kg.

If given the heat of combustion of a substance, we can easily find the kilogram calorific value and vice versa.





Question – Given the heat of combustion of ethane is -1560 kJ/mol, calculate the kilogram calorific value.

Answer – $M_r(C_2H_6) = 2(12) + 6(1) = 30$

1 mole = 30g

30g = -1560kJ

1000g = x

x = -52,000 kJ/kg

SAMPLE QUESTIONS

- 1. Given that the heat of combustion of butane is -2877 kJ/mol, calculate the kilogram calorific value of butane.
- 2. If the kilogram calorific value of propane is -50,454 kJ/kg, calculate the heat of combustion of propane.

HEAT OF FORMATION The heat of formation is the heat change that occurs when 1 MOLE of a substance is formed from its elements in their standard states. The units are expressed in kJ/mol.

Again we see that we only get the heat of formation if we make 1 MOLE of the substance, or its molecular mass in grams or 22.4 I of it at s.t.p. We can also see from the definition that we form the substance 'from its elements in their standard states'. The standard state of an element or a compound is its form at 25 C at 1 atm. Just remember that substances like carbon, sodium, iron are monatomic and solid in their standard states and hydrogen, oxygen, nitrogen are diatomic and gaseous in their standard states.

WRITING EQUATIONS FOR HEATS OF FORMATION

The substance to be formed is written on the **right-hand side** of the equation, as it is the only **product. As we are writing an equation for the 'heat of formation' – 1 mole must be formed!** Example – write an equation for the formation of ethene.

$$2C_{(s)} + 2H_{2(g)} \rightarrow C_2H_{4(g)}$$

Write an equation for the heat of formation of ethanol.

Write an equation for the heat of formation of nitrogen dioxide.



It is more **difficult to measure the heats of formation** of substances than to measure the heats of combustion of substances, **as other products along with the main product will be formed also**.

However, a Russian scientist made this problem much easier! Hess (his name!) examined heat changes in many reactions and saw that the heat change that occurred in going from one substance to another was the same whether one single route was taken or several routes. This is now called **Hess's Law**. (every year except 2007!!!!)

HESS'S LAW

Hess's Law states that if a chemical reaction takes place in several stages, then the <u>sum</u> of the individual stages equals the heat change if the reaction had been carried out in one single stage.

We can use this law to work out the heats of formation of substances given other information.

Example – The heats of formation of carbon dioxide and water were found by experiment to be -394 kJ/mol and -286 kJ/mol respectively. The heat of combustion of ethanoic acid was found to be -876 kJ/mol. Use this information to calculate the heat of formation of ethanoic acid.

Step 1 - Write an equation to show the heat of formation of ethanoic acid (required)

Step 2 – Write equations to show the other information given in the question (given)

Step 3 – Rearrange these given equations so that the substances in the given equations are on the correct sides, as in the required equation, and so that you have the correct amounts.

Step 4 – Cancel what you can in the given equations so that you are left with what you have in the required equation.

Step 5 – Add up the heats of reactions of the given equations to get the heat of formation of ethanoic acid.

Sample answer – Required -	$2C + 2H_2 + O_2 \rightarrow CH_3COOH$	$\Delta H = ?$
Given -	$C + O_2 \rightarrow CO_2$	$\Delta H = -395 kJ$
	$H_2 + \frac{1}{2}O_2 \to H_2O$	$\Delta H = -286 kJ$
	$CH_3COOH + 2O_2 \rightarrow 2CO_2 + 2H_2O \Delta H = -876kJ$	
(×2)	$2C + 2O_2 \rightarrow 2CO_2$	$\Delta H = -788 kJ$
(×2)	$2C + 2O_2 \rightarrow 2CO_2$ $2H_2 + O_2 \rightarrow 2H_2O$	$\Delta H = -572 kJ$
(reverse)	$2CO_2 + 2H_2O \rightarrow CH_3COOH + 2O_2 \frown \Delta H = +876kJ$	

 $2C + 2H_2 + O_2 \rightarrow CH_3COOH$





Hess's Law is really the Law of Conservation of Energy applied to heat changes in chemical reactions.

LAW OF CONSERVATION OF ENERGY

Defn – this law states that energy cannot be created or destroyed but can only be converted from one form of energy into another.

Explain why the heats of neutralisation of hydrochloric acid, nitric acid and sulfuric acid are roughly the same, i.e. –57 kJ /mol.

The heats of neutralisation of all strong acids by strong bases will be the same (-57 kJ/mol), because essentially the same reaction is happening in all. The hydrogen ion from the acid reacts with the hydroxide ion from the base to form water.

With weak acids e.g ethanoic acid, the heat of neutralisation will be less than -57 kJ/mol as extra heat is needed to get the acid to fully dissociate first and then this extra heat must be subtracted from -57 kJ/mol at the end.



EXPERIMENT – DETERMINATION OF THE HEAT OF REACTION OF HYDROCHLORIC ACID WITH SODIUM HYDROXIDE. (monobasic acid)

Theory behind the experiment – a **known number of moles of standard acid** is mixed with a **known number of moles of base** in an insulated container. The initial temperature of each is taken and then the final steady temperature of the two together. We then use the specific heat capacity of the resulting solution to get the heat produced by the reaction and then can adjust (if necessary) to get the heat of neutralisation.

The heat change in this is very small so very concentrated solutions need to be used to get an appreciable temperature change.

(The specific heat capacity is the heat needed to raise 1 kg of the solution by 1 degree).

Apparatus - two polystyrene cups with lids, thermometer (reading to 0.1 C accuracy), stirrer.

Materials – 100 cm^3 1M HCl, 100 cm^3 1M NaOH.

Method -

- 1. 100 cm^3 of 1M HCl were placed in a polystyrene cup and its temperature was noted. (N.B. known volume and known molarity)
- 2. 100 *cm*³ of 1M NaOH were placed in the other polystyrene cup and its temperature was noted. (Again known volume and known molarity)
- 3. The base was then added to the acid (a) <u>very quickly</u> to ensure heat was not lost to the surroundings, and (b) <u>stirring briefly</u> to ensure uniform heat distribution throughout the solution so that an accurate temperature reading can be obtained and (c) a thermometer that is sensitive to very small temperature changes is used.
- 4. The maximum steady temperature was noted.

Results –

Initial temperature of the acid – 15.6 C Initial temperature of the base – 15.6 C Average initial temperature of the solution – 15.6 C Final temperature of the solution – 22.1 C **Rise in temperature – 6.5 C** Specific heat capacity of the solution – 4.2 kJ/kg/C (given in question if its needed) Density of the solution – 1g/ cm^3 (given in question) Total volume of solution – 200 cm^3 (you may have to add to get this)

Calculations -

We will fill into the formula $E = mc\theta$ E= the amount of heat **produced by the amount used**.

m = the mass of the solution in KG (N.B. you must convert into KG) c = the specific heat capacity of the solution (given) θ = the rise in temperature.

Firstly we find the mass of the solution in KG. We use the total volume and density to find this.

$$density = \frac{mass}{volume}$$
$$1g / cm^{3} = \frac{x}{200cm^{3}}$$
$$x = 200g$$
so $x = 0.2kg$



Now fill all the information into the formula $E = mc\theta$ $E = 0.2kg \times 4.2kJ/kg/C \times 6.5C$ E = -5.46kJ heat produced by the 100 cm^3 of 1M acid used in experiment.

Moles of acid used - $\frac{100 \times 1}{1000}$ = 0.1 moles of HCl

-5.46kJ is the amount of heat produced by 0.1 moles of HCl, we now need to find how many moles of H^+ ions are in this amount of HCl.

 $HCl \rightarrow H^+ + Cl^-$ 0.1 mole 0.1 mole

so 0.1 moles of H^+ ion produces –5.46kJ of heat so 1 mole of H^+ ions will produce?

$$0.1 = -5.46 kJ$$

$$1 = x$$

x = -54.6 kJ/mol

What are the sources of possible error in this experiment?

SAMPLE QUESTION

When 200 cm^3 of a sodium hydroxide solution were added to 200 cm^3 of a 0.4 mol/l solution of sulfuric acid in a plastic container, a neutral solution was produced and the temperature rose by 5.5 C. The density and specific heat capacity of the neutral solution are 1g/ cm^3 and 4.2 kJ/kg/C respectively.

(i) Why was a plastic container used?

- (ii) What steps would you take to ensure an accurate measurement of the temperature rise?
- (iii) Calculate the heat of neutralisation of one mole of sulfuric acid by sodium hydroxide.



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BOND ENERGY

When bonds are broken it requires energy (endothermic) and when bonds are made energy is released (exothermic).

If we examine the bond energies in the combustion of methane we see the following: I suggest you draw out each of the molecules to see exactly how many bonds are being broken and how many are being formed.

4 C-H bonds must be broken, along with 2 O=O bonds. This is an endothermic process.

2 C=O bonds must be made, along with 4 O-H bonds. This is an exothermic process.

BOND ENERGY

Defn – bond energy is the energy required to break 1 MOLE of covalent bonds and to separate the neutral atoms completely from each other.

Bond energy values were used by Pauling to draw up the electronegativity table. They are **average values** as the bond energy value is **different for each bond that is broken**. For example in methane as each C-H bond is broken different amounts of energy are needed so an average of these four energy values is taken for the C-H bond.





ENERGY PROFILE DIAGRAMS

In an endothermic reaction, the products have more energy than the reactants, hence energy is taken in from the surroundings.

ENDOTHERMIC

In an exothermic reaction, the products have less energy than the reactants, so heat is lost to the surroundings.

EXOTHERMIC



WORK SHEET

LEAVING CERT QUESTION 2002

The following hydrocarbons can all be used as fuels. Methane (CH_4) butane (C_4H_{10}) 2,2,4-trimethylpentane (C_8H_{18})

- (a) Butane is a major component of LPG. What do the letters LPG stand for? Draw two structural isomers of butane.
- (b) Methane is a major component of natural gas.
 Why are mercaptans often added to natural gas?
 What environmental change or effect is associated with the release of methane to the atmosphere? Apart from leaking pipes, name a major source from which methane is released to the atmosphere.
- (c) What structural feature of 2,2,4-trimethylpentane results in it having a high octane rating? Give one other structural feature which increases the octane number of a hydrocarbon.
- (d) Define heat of combustion of a compound.
- (e) The combustion of butane is described by the following equation. $2C_4H_{10(g)} + 13O_{2(g)} \rightarrow 8CO_{2(g)} + 10H_2O_{(l)}$

Calculate the heat of combustion of butane given that the heats of formation of butane, carbon dioxide and water are –125, -394 and –286 kj/mol , respectively.

LEAVING CERT 2003 Define heat of combustion. (7)

Propane may be used in gas cylinders for cooking appliances. Propane burns according to the equation

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

- (I) The heats of formation of propane, carbon dioxide and water are -104, -394 and -286kj/mol respectively. Calculate the heat of combustion of propane. (12)
- (II) If 500 kJ of energy are needed to boil a kettle of water what mass of propane gas must be burned to generate this amount of heat? Express your answer to the nearest gram. (6)



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LEAVING CERT 2004

- (a) Define (I) heat of formation of a substance, (ii) octane number of a fuel. (11)
- (b) The combustion of methane is described by the following balanced equation.

 $CH_{4(g)} + 2O_{2(g)} \rightarrow CO_{2(g)} + 2H_2O_{(l)}$ $\Delta H = -890.4kJ / mol$

The standard heats of formation of carbon dioxide and water are –394 and –286 kJ/mol respectively. Calculate the heat of formation of methane. (12)

- (c) Methane is an excellent fuel. Give **two** properties of methane which account for its usefulness as a fuel. Natural gas is a rich source of methane. Why are mercaptans often added to natural gas? (9)
- (d) Methane is often found in gas fields which occur in association with crude oil deposits. Crude oil is fractionated in order to obtain more useful products. Outline clearly how the fractionation process is carried out. (12)
- (e) Identify two structural features of a hydrocarbon fuel which affect its octane number. (6)

LEAVING CERT 2005

The combustion of liquid benzene is described by the following equation:

$$2C_6H_{6(l)} + 15O_{2(g)} \rightarrow 12CO_{2(g)} + 6H_2O_{(l)}$$

Given that the heats of formation of carbon dioxide gas, liquid water and liquid benzene are -394, -286 and 49 kJ per mole respectively. Calculate the heat of combustion of liquid benzene. (12)



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LEAVING CERT 2006

(a) The table shows the octane numbers of four hydrocarbons.

- (i) What is meant by the octane number of a fuel? (8)
- (ii) Hexane has the lowest octane number of the four compounds listed. What structural feature of the molecule contributes to this? (3)
- (iii) In the case of each of the other three compounds, identify the structural feature of its molecules which contributes to it having a high octane number. (9)
- (iv) Name the process carried out in an oil refinery that converts hexane to compounds such as cyclohexane and benzene. Why is the use of benzene in petrol strictly controlled? (6)

NAME	FORMULA	OCTANE NUMBER
Hexane	$C_{6}H_{14}$	25
Cyclohexane	$C_{6}H_{12}$	83
Benzene	C_6H_6	100
2,2,4-trimethylpentane	$C_{8}H_{18}$	100

- (b) (i) Give two reasons why oxygenates such as MTBE are added to petrol.
 (ii) Give two reasons why the addition of lead to petrol has been discontinued. (12)
- (c) The combustion of cyclohexane may be described by the following balanced equation.

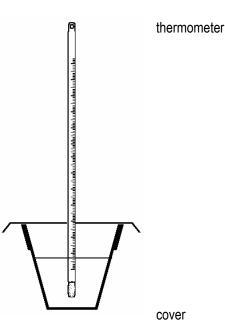
$$C_6H_{12(l)} + 9O_{2(g)} \rightarrow 6CO_{2(g)} + 6H_2O_{(l)}$$

Given that the heats of formation of cyclohexane, carbon dioxide and water are -156, -394 and -286 kJ per mole respectively, calculate the heat of combustion of cyclohexane. (12)



LEAVING CERT 2007 Q3

In an experiment to examine the heat of reaction for the reaction between sodium hydroxide with hydrochloric acid, a student added 50 cm^3 of 1.0 M HCl solution to the same volume of 1.0M NaOH solution in a polystyrene foam cup.



polystyrene cup

reaction mixture

(a) To achieve an appreciable temperature rise during the reaction, quite

concentrated solutions of acid and base, carrying the label illustrated, were used.

What word describes the chemical hazard illustrated in this label?

State one precaution the student should take when using these solutions. (8)



(b) The student had a choice of using either a graduated cylinder or a burette to measure out the solutions used in this experiment.

Which piece of apparatus should have been used to achieve the more accurate result? (3)

(c) If the hydrochloric acid and sodium hydroxide solutions had been stored at slightly different temperatures, explain how the initial temperature of the reaction mixture could have been obtained. (6)





(d) List three precautions which should have been taken in order to obtain an accurate value for the highest temperature reached by the reaction mixture. (9)

(e) What was the advantage of mixing the solutions in a polystyrene foam cup rather than in a glass beaker or in a metal calorimeter? (3)

(f) Calculate the number of moles of acid neutralised in this experiment.

Taking the total heat capacity of the reaction mixture used in this experiment as 420 J K–1, calculate the heat released in the experiment if a temperature rise of 6.7 °C was recorded.

Hence calculate the heat of reaction for

NaOH + HCI \rightarrow NaCl + H₂O (18)

(g) Name the piece of apparatus used in industry to accurately measure the heats of combustion of foods and fuels. (3)

LEAVING CERT 2008

Write a balanced chemical equation for the combustion of ethanol, C_2H_5OH .

Given that the heats of formation of ethanol, carbon dioxide and water are -278, -394 and -286 kJ/mol, respectively, calculate the heat of combustion of ethanol. (18)

LEAVING CERT 2009

The combustion of one of the C4H8 isomers is described by the following balanced equation.

C4H8 + 6O2 \rightarrow 4CO2 + 4H2O Δ H = -2710 kJ mol

The standard heats of formation of water and carbon dioxide are –286 and –394 kJ mol, respectively. Calculate the heat of formation of this C4H8 isomer. (12)

LEAVING CERT 2010

(d) Define heat of combustion.

Outline how the heat of combustion of X (heptane) could be measured using a bomb calorimeter. (15) (e) In order to increase its octane rating, compound X is converted to compound Z(methyl benzene) in oil refineries by the following reforming (dehydrocyclisation) process:

$$C_7H_{16}~(\mathrm{I}) \quad \rightarrow \quad C_7H_8~(\mathrm{I}) \quad + \quad 4\,H_2~(\mathrm{g})$$

Calculate the heat change for this reaction given that the heats of formation of $C_7 H_{16}$ (I), and

 $C_{\rm 7}H_{\rm 8}\,$ (I) are –224.2 and 12.4 Kj/ mol, respectively.

State one important industrial use for the hydrogen produced in this reaction. (12)



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LEAVING CERT 2011

Steam reforming takes place according to the following balanced equation:

$CH_{4\,(g)}+H_{2}O_{\,(g)} \ \longrightarrow \ CO_{\,(g)}+3H_{2\,(g)}$

Calculate the heat of this steam reforming reaction given that the heats of formation of methane, steam and carbon monoxide are -74.6, -242 and -111 kJ mol₋₁ respectively. (12)

LEAVING CERT 2012

(d) Define heat of combustion.

Name the laboratory apparatus used to measure the heats of combustion of fuels and foodstuffs. (9)

(d) Calculate the heat of formation of the hydrocarbon (**C8H18**) produced in process (*iii*), given that its heat of combustion value has been measured to be –5502 kJ mol–1 and that the heats of formation of carbon dioxide and water are –394 and –286 kJ mol–1, respectively. (12)

LEAVING CERT 2013

Ethyne is produced from calcium carbide and water according to the following balanced equation:

$\label{eq:caC2(s) + 2H_2O(l)} \mathsf{CaC}_2(\mathsf{g}) + \mathsf{Ca(OH)}_2(\mathsf{g})^{\text{CaC}}_{\text{SEP}} + \mathsf{Ca(OH)}_2(\mathsf{g})^{\text{CaC}}_{\text{SEP}}$

Calculate the heat change for this reaction given that the heats of formation of calcium carbide, water, ethyne and calcium hydroxide are -59.8, -285.8, 227.4 and -985.2 kJ mol⁻¹ respectively. (15)



LEAVING CERT 2014

(e) Define heat of combustion. [sep]

Write the balanced equation for the complete combustion of butane in an adequate supply of oxygen. Calculate the heat of combustion of butane, given that the heats of formation of carbon dioxide, water and butane are -393.5, -285.8 and -125.7 kJ mol⁻¹, respectively. (24) [see]

LEAVING CERT 2015

(a) Each fraction separated in the refining of crude oil is a mixture of hydrocarbons. Identify a property of a hydrocarbon that results in its presence in a particular fraction.

(b) (i) Name the fraction, obtained from crude oil, that is used as fuel for jet aircraft. [ii] What process is used to convert molecules in this fraction to smaller molecules that are in greater demand? [ii]

- (c) What are the two reference hydrocarbons used to assign octane numbers to fuels? $\frac{1}{250}$
- (d) Give two advantages of adding oxygenates, such as ethanol, to petrol. []
- (e) Ethanol can also be used as a fuel. [1]

Each fraction separated in the refining of crude oil is a mixture of hydrocarbons. Identify a property of a hydrocarbon that results in its presence in a particular $\frac{1}{3EE}$ fraction. (5)

Calculate the heat of formation of ethanol given that the heat of combustion of $\frac{1}{350}$ ethanol is -1370.7 kJ mol⁻¹ and that the heats of formation of carbon dioxide and $\frac{1}{350}$ water are -393.5 and -285.8 kJ mol⁻¹ respectively. (12)



(f) The NASA Space Shuttle programme flew 135 missions between 1981 and 2011 using hydrogen as the fuel.

- . (i) Give two properties of hydrogen that made it the fuel of choice for the Space Shuttle.
- . (ii) State one disadvantage of hydrogen as a fuel.
- (*iii*) Give two ways that hydrogen gas is produced sepindustrially. (15)



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LEAVING CERT 2016

Name the oil refining process that converts octane into 2,2,4-trimethylpentane.

Name the oil refining process that converts octane into ethylbenzene according to the following balanced equation.

C8H18 (/) □→C8H10 (/) + 4H2 (g)

Explain why these conversions are desirable.

Calculate the heat of reaction for the conversion of octane to ethylbenzene above, given that the heats of formation of octane and ethylbenzene are -250.1 and -12.5 kJ mol⁻¹ respectively. (18)

LEAVING CERT 2017

(a) Identify the hydrocarbon gas produced by anaerobic bacterial decomposition of either animal waste or vegetation.

Give a major use of this gas. Why is the concentration of this gas in the atmosphere a cause of concern? (11)

(b) The boiling points of propane (C_3H_8) and dodecane ($C_{12}H_{26}$) are -42 °C and 216 °C respectively. Explain why high molecular mass alkanes have high boiling points. (6)

c) (i) Write a balanced equation for the dehydrocyclisation reaction in which heptane is converted into methylbenzene and hydrogen. (ii) What is the purpose of dehydrocyclisation in oil refining? (9)

(d) But-2-ene, 2-methylbutane and a second alkene (X) were the products of catalytic cracking of a dodecane ($C_{12}H_{26}$) molecule.

- (i) Draw a structural formula for each named product.
- (ii) Deduce the molecular formula of the third product (X). (9)

(e) State Hess's law. The heats of formation of dodecane, but-2-ene, 2-methylbutane and X are -350.9, -9.3, -178.4 and 20.0 kJ mol⁻¹ respectively. Use the data to calculate the heat change for the cracking reaction:



C12H26 (l) \rightarrow but-2-ene (g) + 2-methylbutane (l) + X (g) (15)

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LEAVING CERT 2018

3. The cardboard cup with plastic lid in the diagram contained 150 cm^3 of 1.0 M hydrochloric acid solution at room temperature. A volume of 160 cm³ of 1.0 M sodium hydroxide solution – also at room temperature – was added quickly and the mixture was stirred. The temperature of the mixture rose rapidly by 6.4 K and then began to fall gradually. The equation for the neutralisation reaction that took place is: HCI $(aq) + \text{NaOH}(aq) \rightarrow \text{NaCI}(aq) + \text{H2O}(l)$

(a) Is this reaction exothermic or endothermic? Justify your answer. (5)

(b) (i) (ii) Suggest a reason why the temperature, having risen, then began to fall gradually.



Why should the mixture be stirred before taking temperature readings?

(*iii*) The thermometer used was accurate to 0.1 K. What temperature rise would have been recorded if the thermometer used was accurate to 1 K? (9)

(*c*) (*i*) (*ii*) Draw *or* describe the hazard warning pictogram that should be displayed on a container used to store 1.0 M **NaOH**. (12)

Why is it advantageous to use moderately concentrated solutions instead of dilute solutions in this experiment?

- (d) Calculate
 - (i) the number of moles of HCI neutralised in the cardboard cup,
 - (*ii*) the heat produced by the reaction mixture that had a total mass of 310 g, taking the specific heat capacity of the mixture as that of water, 4.2 kJ kg⁻¹ K⁻¹,
 - (*iii*) to one decimal place, the heat of reaction (*IH*) for the neutralisation of hydrochloric acid by sodium hydroxide according to the equation above. (18)
- . (e) The result obtained in this experiment was about 3% below the expected value. State and explain a modification to the method described that would give a more accurate result. (6)



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LEAVING CERT 2018

Refinery gas, naphtha, kerosene and gas oil are products of the <u>fractionation of crude oil.</u> (*a*) Explain the underlined term. (5)

- (b) (i) Name the two major components of liquid petroleum gas (LPG), a fuel obtained from refinery gas.
- . (ii) Why is methanethiol (CH3SH), a mercaptan, added to natural gas and to LPG?
- . (*iii*) Calculate the heat of combustion of methanethiol according to the equation: $CH3SH(g) + 3O2 (g) \longrightarrow CO2 (g) + 2H2O (l) + SO2 (g)$
- . The heats of formation of methanethiol, carbon dioxide, water, and sulfur dioxide are -22.8, -393.5, -285.8 and -296.8 kJ mol⁻¹ respectively. (21)



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ATOMIC THEORY DEFINITIONS

ATOMIC NUMBER

Defn - the atomic number of an atom is the number of protons present in the nucleus of an atom, (this equals the number of electrons in an atom).

MASS NUMBER

Defn - the mass number is the number of protons plus neutrons in the nucleus of an atom.

ISOTOPES

Defn - isotopes are atoms of the same element that have the same atomic number but different mass numbers due to the different numbers of neutrons present in the nucleus.

RELATIVE ATOMIC MASS

Defn- the average mass of <u>an atom</u> of an element compared to 1/12 the mass of the carbon -12 isotope, taking relative abundances of isotopes into account.

RELATIVE MOLECULAR MASS

Defn – the average mass of $\overline{a \text{ molecule}}$ of a compound compared to 1/12 the mass of the carbon – 12 isotope, taking relative abundances of isotopes into account.

RADIOACTIVITY

Defn – is the spontaneous disintegration of the nucleus with the emission of α , β or γ radiation.

NUCLEAR REACTION

Defn – a nuclear reaction involves a change in the nucleus of an atom and a new element is usually formed as a result.

CHEMICAL REACTION

Defn – a chemical reaction involves electrons being shared or transferred from on atom to another – the nucleus of the atom remains the same.

HALF-LIFE

Defn - this is the time taken for half the nuclei in a given sample to decay.

HEISENBERG'S UNCERTAINTY PRINCIPLE

Defn - This states that it is impossible to know <u>both</u> the position and the speed of an electron <u>at the same time</u> as electrons move in a wave motion.

ATOMIC ORBITAL

Defn – an atomic orbital is a region in space around the nucleus of an atom in which there is a high probability of finding an electron.

ENERGY LEVEL

Defn - is the discrete amount of energy an electron has when it is in an atom

TRANSITION ELEMENT

Defn – an element that forms at least one ion with a partially filled d- sublevel.

D-BLOCK ELEMENT

Defn- an element whose highest energy electron occupies a d- sublevel.

AUFBAU PRINCIPLE

Defn - electrons occupy the lowest available energy level.

HUNDS RULE OF MAXIMUM MULTIPLICITY

Defn - when two or more orbitals of <u>equal energy</u> are available (i.e. 2px 2py 2pz), electrons fill them singly before filling them in pairs

PAULI EXCLUSION PRINCIPLE

Defn - no more than two electrons can occupy an orbital and this they can only do if they have opposite spin.

FIRST IONISATION ENERGY

Defn - this is the minimum amount of energy required to remove the first most loosely bound electron from a mole of <u>isolated</u> atoms of an element in its <u>neutral</u> gaseous ground state.

 $X_{(g)} \rightarrow X^{+}_{(g)} + e^{-}$

STOICHIOMETRY DEFINITIONS

A MOLE

Defn - a mole of a substance is that amount of it which contains the Avogadro's constant number of particles.

AVOGADRO'S CONSTANT

Defn – is the number of carbon atoms in exactly 12 grams of the C-12 isotope. This equals 6×10^{23} particles.

AVOGADRO'S LAW

Defn - equal volumes of all gases at the same temperature and pressure contain equal numbers of molecules.

MOLAR MASS

Defn – the molar mass of a substance is its atomic mass (or its molecular mass) expressed in grams.

MOLAR VOLUME

Defn – at s.t.p. the molar volume of any gas occupies a volume of 22.4 litres (22,400 cm^3).

LIMITING REACTANT

Defn- the limiting reactant is the reactant that is <u>fully consumed</u> when a reaction goes to completion.

THEORETICAL YIELD

Defn- the theoretical yield of a reaction is the quantity of product that should form when all of the limiting reactant reacts. To get the theoretical yield use the molar ratio from the balanced equation between the limiting reactant and product.

ACIDS AND BASES DEFINITIONS

ACIDS- Arhenius' theory

Defn - An acid produces H^+ ions in water.

MONOBASIC ACID

Defn – A monobasic acid produces one H^+ ion in solution e.g. HCl and HNO_3 .

DIBASIC ACID

Defn – A dibasic acid produces two H^+ ions in solution e.g. H_2SO_4 .

TRIBASIC ACID

Defn – A tribasic acid produces three H^+ ions in solution e.g. H_3PO_4 .

<u>BASES- Arhenius' theory</u> Defn - A base produces OH^- ions in water.

Deni - A base produces O11 Ions in water

<u>ACID- Bronsted-Lowry threory</u> Defn - an acid is a proton (H^+) donor.

<u>BASE- Bronsted-Lowry theory</u> Defn - a base is a proton (H^+) acceptor.

AMPHOTERIC

Defn - a substance that can act as both an acid and a base.

DEFINITIONS

CONJUGATE PAIRS

Defn - Two species that differ by one proton.

<u>SALTS</u>

Defn - A salt is formed when the H^+ of the acid is replaced by a metal ion or NH_4^+ (ammonium ion).

STRONG ACID Defn –a strong acid is a good proton donor.

WEAK ACID Defn – is a poor proton donor.

<u>CONJUGATE ACID</u> Defn – a base plus a proton.

<u>CONJUGATE BASE</u> Defn – an acid minus a proton.

BONDING DEFINITIONS

COMPOUND

Defn- a compound is a substance that is made up of two or more elements combined together chemically.

THE OCTET RULE

Defn- This rule states that when atoms bond, most atoms tend to want an electron arrangement of eight electrons in their outermost shell.

VALENCY

Defn- the valency of an atom tells us the number of chemical bonds an atom can form.

IONIC BOND

Defn – an ionic bond is formed due to the electrostatic attraction between oppositely charged ions caused by the complete transfer of electrons from one atom to another.

SIGMA BONDING

Defn - When orbitals overlap 'head-on'/ end on. This can occur between two s orbitals, an 's' and a 'p' orbital or two 'p' orbitals. (draw diagrams)

PI BONDING

Defn - When orbitals overlap 'side-ways'. This can occur between two 'p' orbitals only. (draw diagram)

<u>PURE COVALENT BONDING</u> Defn – a pure covalent bond occurs when electrons are shared equally.

POLAR COVALENT BONDING

Defn – a polar covalent bond occurs when electrons are shared unequally.

DATIVE COVALENT BONDING

Defn - only one atom supplies the electrons needed to make a covalent bond. In a dative covalent bond one atom supplies both the electrons being shared in the bond.

POLAR MOLECULE

Defn - This term means that the slight positive and slight negative poles of a molecule are separated by a distance, they do not coincide.

ELECTRONEGATIVITY

Defn – the relative power of <u>attraction</u> of an atom of an element <u>for the shared pair of electrons in a covalent</u> <u>bond.</u>

HYDROGEN BONDING (intermolecular force of attraction)

Defn – a hydrogen bond is an intermolecular force of attraction that occurs <u>when</u> hydrogen is bonded to a small more electronegative element such as O, F or N.

OXIDATION AND REDUCTION DEFINITIONS

OXIDATION IN TERMS OF ELECTRONS Defn- oxidation is the loss of electrons.

REDUCTION IN TERMS OF ELECTRONS

Defn- reduction is the gain of electrons.

OXIDATION NUMBER

Defn- the charge an element has or appears to have when in a molecule when certain rules are applied.

OXIDATION IN TERMS OF CHANGE IN OXIDATION NUMBER

Defn- oxidation is an increase in oxidation number.

REDUCTION IN TERMS OF CHANGE IN OXIDATION NUMBER Defn- reduction in a decrease in oxidation number.

VOLUMETRIC ANALYSIS DEFINITIONS STANDARD SOLUTION

Defn – a standard solution is a solution of known concentration.

PRIMARY STANDARD

Defn - A primary standard is a <u>substance</u> that is available in 100% purity, is stable in air, has a high molar mass for accuracy and dissolves easily in water and can be made up to a standard solution directly.

SECONDARY STANDARD

Defn – a secondary standard is a substance that is not available in 100% purity, is not stable in air, has a low molecular mass and does not dissolve readily in water and cannot be made up to a standard solution directly.

STANDARDISE

Defn – to standardise is to find out the concentration of a solution by titration or colorimetry.

SHAPES OF MOLECULES DEFINITIONS

VALENCE SHELL ELECTRON PAIR REPULSION THEORY

Defn –Pairs of electrons in the outer shell of an atom arrange themselves to be as far away from each other as possible so as to minimise the repulsions between them.

LONE PAIRS OF ELECTRONS

Defn - Pairs of electrons in the outer shell of the atom that do not take part in bonding.

BONDING PAIRS OF ELECRONS

Defn - Pairs of electrons in the outer shell that are shared between atoms.

THERMOCHEMISTRY DEFINITIONS

HEAT OF REACTION

Defn- The heat change that occurs when a reaction takes place according to a given balanced chemical equation.

EXOTHERMIC REATION Defn- A reaction where heat is lost from the reaction to the surroundings. $\Delta H = -$

ENDOTHERMIC REACTION

Defn- A reaction where heat is taken in by the reaction from the surroundings. $\Delta H = +$

HEAT OF COMBUSTION

Defn- The heat change that occurs when <u>1 mole</u> of a substance is burned in an excess of oxygen.

KILOGRAM CALORIFIC VALUE

Defn- The heat that is produce when <u>1 kilogram</u> of a fuel is burned in an excess of oxygen.

HEAT OF FORMATION

Defn- The heat change that occurs when <u>1 mole</u> of a substance is formed from its elements in their standard states.

HESS' LAW

Defn – when a reaction takes place in stages the sum of the heat changes of the individual stages equals the heat change if the reaction were to take place in one stage.

ORGANIC CHEMISTRY DEFINITONS

HYDROCARBON

Defn- A compound that consists of the elements carbon and hydrogen only.

SATURATED

Defn- Single bonds around the carbon atoms.

UNSATURATED

Defn- A multiple bond present between two carbon atoms.

AROMATIC

Defn - Contains a benzene ring in the structure.

ALIPHATIC

Defn- Straight or branched chained molecule.

IONIC ADDITION REACTION

Defn - Two reactants react to form one main product.

FREE RADICAL SUBSTITUTION REACTION

Defn - An atom or group of atoms is replaced by an atom or group of atoms to form two main products.

CONDENSATION REACTION

Defn - Two <u>different</u> molecules combine to form a more complex molecule with the production of a smaller molecule such as water.

DEFINITIONS

ESTERIFICATION REACTION

Defn - An alcohol and a carboxylic acid react reversibly to form an ester and water. This is an example of a condensation reaction.

ELIMINATION REACTION

Defn - A smaller molecule is removed from a larger molecule. A double bond is formed in one of the product molecules.

DEHYDRATION REACTION

Defn - Removal of water from a molecule. This is an elimination reaction.

HYDROGENATION REATION

Defn - Addition of hydrogen to an alkene molecule involving a nickel catalyst and 200 ° C.

HETROLYTIC FISSION

Defn - A molecule splits to form two different ions.

HOMOLYTIC FISSION

A molecule splits to form two identical atoms using u.v light.

POLYMERISATION REACTION

Defn – a reaction where many small molecules called monomers combine together to form a very large molecule called a polymer.

CHEMICAL EQUILIBRIUM DEFINITONS

CHEMICAL EQUILIBRIUM

Defn – a system is said to have reached a state of equilibrium when the <u>rate of</u> the forward reaction equals the <u>rate of</u> the reverse reaction.

DYNAMIC EQUILIBRIUM

Defn – the forward and reverse reactions occur at the same time.

LE CHATELIER'S PRINCIPLE

Defn – when a system <u>at equilibrium</u> is subjected to a stress such as a change in temperature, pressure or concentration the system will alter to oppose the effect of the stress.

REVERSIBLE REACTION

Defn – both forward and reverse reactions happen at the same time.

GAS LAWS DEFINITONS

BOYLES LAW

Defn- at a constant temperature, the volume of a fixed mass of any gas is inversely proportional to the pressure of the gas.

CHARLES LAW

Defn- at a constant pressure, the volume of a fixed mass of any gas is directly proportional to the absolute temperature. (Kelvin)

DEFINITIONS

IDEAL GAS

Defn – a gas that obeys all the gas laws under all conditions of temperature and pressure.

AVOGADRO'S LAW

Defn- equal volumes of all gases under the same conditions of temperature and pressure contain equal numbers of molecules.

GAY-LUSSAC'S LAW OF COMBINING VOLUMES

Defn- when gases react, the volumes consumed in the reaction bear a simple whole number ratio to each other, and to the volumes of any gaseous product of the reaction, all volumes measured under the same conditions of temperature and pressure.

ELECTROCHEMISTRY DEFINITONS

ELECTROLYTE

Defn- a substance that in the molten or dissolved state can conduct electricity.

ELECTROCHEMICAL SERIES

Defn- a list of elements arranged in order of their tendency to lose electrons.

DISPLACEMENT REACTION

Defn- a reaction where a metal will take the place of a less reactive metal from a solution of its salts.

ELECTROLYSIS

Defn – a process that uses electricity to bring about a chemical reaction.

RATES OF REACTION DEFINITONS

RATE OF REACTION

Defn- the change in concentration, per unit time of any one reactant or product.

CATALYST

Defn- a substance that alters the rate of a reaction without itself being used up in the reaction.

HETEROGENOUS CATALYSIS

Defn – the catalyst and the reactants are in different phases.

HOMOGENOUS CATALYSIS

Defn- the catalyst and the reactants are in the same phase.

<u>AUTOCATALYSIS</u>

Defn- the catalyst is a product of the reaction.

ACTIVATION ENERGY

Defn- the minimum amount of energy colliding molecules must have in order for a reaction to take place.

pH AND INDICATORS

pН

Defn – minus the log to base 10 of the hydrogen ion concentration (where the hydrogen ion concentration is expressed in mol per litre).

INDICATOR

Defn – a substance that changes colour depending on the pH of the solution in which it is placed.

WATER DEFINITIONS

HARD WATER

Water that does not form a lather easily with soap.

TEMPORARY HARDNESS

Hardness that can be removed by boiling. Caused by calcium and magnesium hydrogencarbonates.

PERMANENT HARDNESS

Hardness that cannot be removed by boiling. Caused by calcium and magnesium sulfates.

BIOCHEMICAL OXYGEN DEMAND

The amount of dissolved oxygen consumed by biochemical action when a sample of water was kept in the dark for 5 days at 20 deg Celsius.

PRINCIPLES

MASS SPECTROMETER

Separation of ions based on them having different masses when moving in an magnetic field.

FRACTIONAL DISTILLATION

Separation of components of crude oil based on them having different boiling points.

STEAM DISTILLATION

Two immiscible liquids together have a lower boiling point than either of the liquids on their own.

<u>CHROMATOGRAPHY</u>

A mobile phase carries a dissolved mixture through a stationary phase. Separation happens because some of the components of the mixture are attracted to significantly different extents to the mobile or stationary phase.

RECRYSTALLISATION

More solute is soluble in a hot solvent than in a cold one.

COLORIMETRY

Concentration of solute is proportional to colour intensity of solution.

Note- these may not include all terms but will be a good start! BE SURE TO ADD ANY OTHER TERMS YOU MEET DURING THE YEAR.