

Reactivity 1.1

IB CHEMISTRY SL

25 Mn Manganese 54.938045	16 S Sulfur 32.065	J	6 C Carbon 12.0107	2 He Helium 4.002602	25 Mn Manganese 54.938045
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Reactivity 1.1.1

Understandings:

- Chemical reactions involve a transfer of energy between the system and the surroundings, while total energy is conserved.

Learning outcomes:

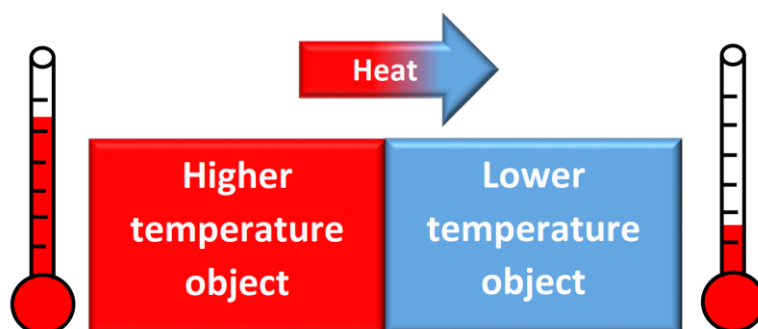
- Understand the difference between heat and temperature.

Linking questions:

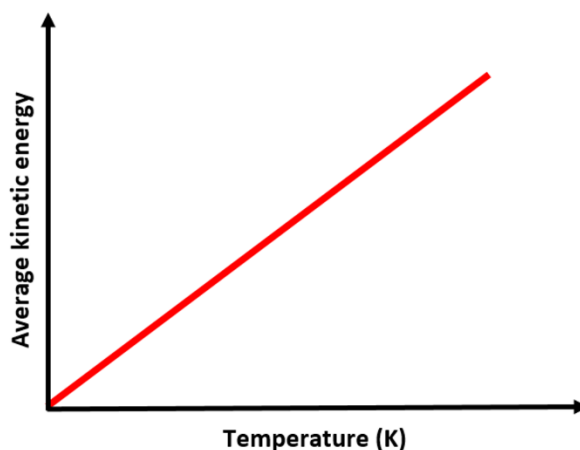
- Structure 1.1 What is the relationship between temperature and kinetic energy of particles?

Heat and temperature

- Heat is the transfer of energy from a higher temperature object to a lower temperature object (measured in joules, J).
- The direction of heat flow is from hot (higher temperature) to cold (lower temperature).



- Absolute temperature is the measure of the average kinetic energy of the particles in a substance.
- Absolute temperature in kelvin (K) is directly proportional to the average kinetic energy of the particles in a substance.



Converting between kelvin (K) and °C

- To convert between °C and K, add or subtract 273 (273.15).
- The kelvin scale does not have a negative value.

Examples:

- $100\text{ }^{\circ}\text{C} = 373\text{ K}$
- $0\text{ }^{\circ}\text{C} = 273\text{ K}$
- $0\text{ K} = -273\text{ }^{\circ}\text{C}$ (absolute zero)

Exercises:

1. Distinguish between the terms heat and absolute temperature.

Absolute temperature (in kelvin, K) is a measure of the average kinetic energy of the particles in a substance. Heat is the transfer of energy from an area of higher temperature to lower temperature.

2. Convert the following temperatures from °C to K ($0\text{ }^{\circ}\text{C} = 273\text{ K}$)

a) 298 K b) 351 K c) 373 K d) 0 K e) 260 K

3. Two samples of chlorine gas (both containing the same number of molecules) are at 350 K and 550 K respectively. Which sample has the higher average kinetic energy?

The sample of gas at 550 K has the highest average kinetic energy.

4. Two beakers of water, one containing 250 cm³ and the other 500 cm³ of water, are at the same temperature (298 K). Compare the average kinetic energy and the heat content of the two beakers of water.

Both beakers of water are at the same temperature, therefore they have the same average kinetic energy. The beaker with 500 cm³ of water has more heat than the other beaker.

5. A hot piece of iron with a temperature of 500 K is put into a beaker of water at 298 K. Describe the direction of heat flow and what will happen to the temperature of the iron and the water after one hour.

The heat will flow from the block of iron to the water (from higher temperature to lower temperature). After one hour, the temperature of the iron and the water will be the same – they will have reached thermal equilibrium.

Reactivity 1.1.2 and 1.1.3

Understandings:

- Reactions are described as endothermic or exothermic, depending on the direction of energy transfer between the system and the surroundings (1.1.2).
- The relative stability of reactants and products determines whether reactions are endothermic or exothermic (1.1.3).

Learning outcomes:

- Understand the temperature change (decrease or increase) that accompanies endothermic and exothermic reactions, respectively (1.1.2).
- Sketch and interpret potential energy profiles for endothermic and exothermic reactions (1.1.3).

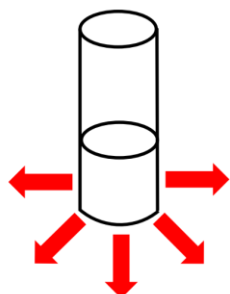
Additional notes:

- Axes for energy profiles should be labelled as reaction coordinate (x), potential energy (y).

Exothermic and endothermic reactions

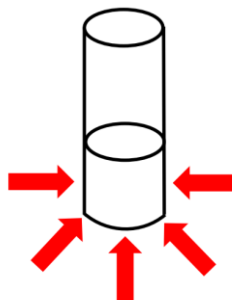
- Chemical reactions can be classified as exothermic or endothermic depending on whether heat is absorbed or released by the system or surroundings.

Exothermic reaction



Heat flows from
the system to the
surroundings

Endothermic reaction



Heat flows from
surroundings into
the system

- The system is the reactants and products (the chemical reaction).
- The surroundings consist of everything else outside of the system (including the reaction mixture).

Exothermic reactions

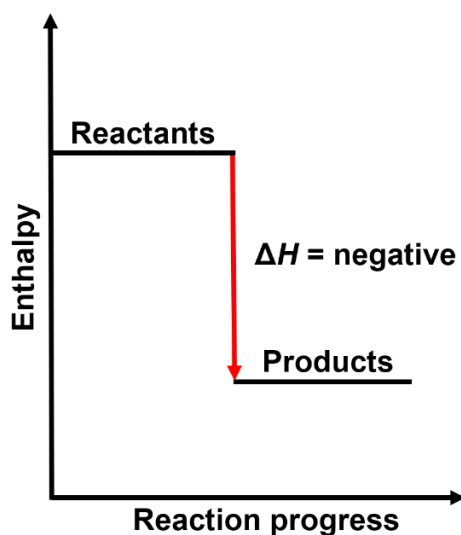
- In an exothermic reaction, heat flows from the system to the surroundings.
- The temperature of the reaction mixture and the surroundings increases as heat is released by the system.
- Examples of exothermic reactions include combustion and neutralisation.

Endothermic reactions

- In an endothermic reaction, heat flows from the surroundings to the system.
- The temperature of the reaction mixture and the surroundings decreases as heat is absorbed by the system.
- Examples of endothermic reactions include photosynthesis and thermal decomposition reactions.

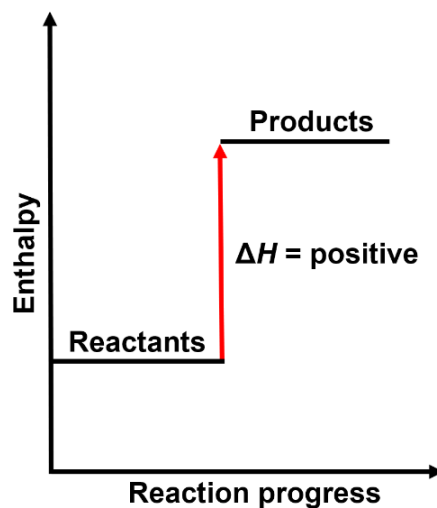
Energy level profiles

Energy level profile for an exothermic reaction (note that the y-axis can be labelled as potential energy and the x-axis as reaction coordinate).



- $\Delta H = \text{negative}$ (< 0).
- Products have lower enthalpy than reactants.
- Products are more energetically stable than reactants.

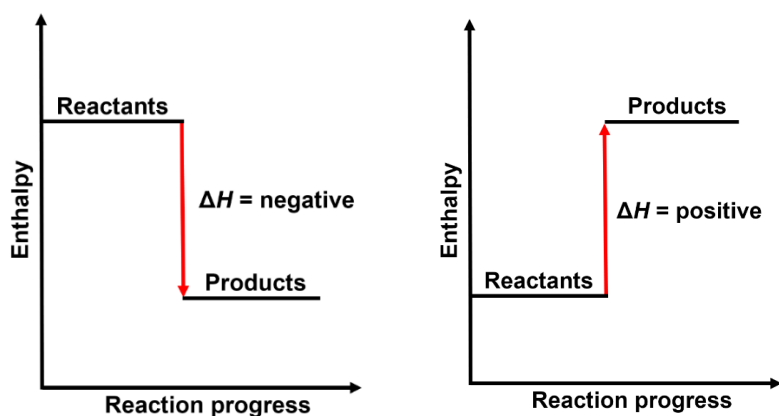
Energy level profile for an endothermic reaction.



- $\Delta H = \text{positive}$ (> 0).
- Products have higher enthalpy than reactants.
- Products are less energetically stable than reactants.

Exercises:

1. Sketch energy level profiles for an exothermic reaction and an endothermic reaction.



2. Complete the table summarising exothermic and endothermic reactions.

	Exothermic reaction	Endothermic reaction
Sign of enthalpy change (ΔH)	negative	positive
Which has lower enthalpy, reactants or products?	products	reactants
Which is more energetically stable?	products	reactants
Is heat absorbed or released by the system?	released	absorbed

3. Classify the following reactions as endothermic or exothermic:
 - a. Propane burns in excess oxygen releasing heat. **Exothermic**
 - b. The reading on the thermometer increases when sodium hydroxide and hydrochloric acid are mixed together in a beaker. **Exothermic**
 - c. When ammonium nitrate and water are mixed together in a cold pack, the temperature decreases. **Endothermic**

Reactivity 1.1.4

Understandings:

- The standard enthalpy change for a chemical reaction, ΔH^\ominus , refers to the heat transferred at constant pressure under standard conditions and states. It can be determined from the change in temperature of a pure substance.

Learning outcomes:

- Apply the equations $Q = mc\Delta T$ and $\Delta H = -Q/n$ in the calculation of the enthalpy change of a reaction.

Additional notes:

- The units of ΔH^\ominus are kJ mol^{-1} .
- The equation $Q = mc\Delta T$ and the value of c , the specific heat capacity of water, are given in the data booklet.

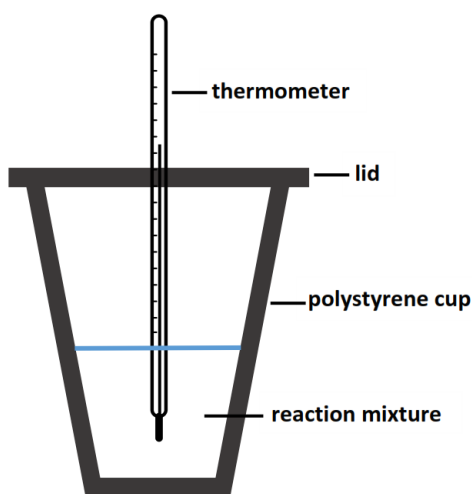
Enthalpy change (ΔH)

- Enthalpy, H , is the heat content of a substance.
- Enthalpy is the sum of the internal energy (U) and the product of pressure and volume (PV):

$$H = U + PV$$

- Enthalpy change (ΔH) is the amount of heat absorbed or released in a chemical reaction.
- If a process occurs at constant pressure, the heat released or absorbed is equal to the change in enthalpy ($q = \Delta H$).
- The standard enthalpy change of reaction (ΔH^\ominus) is the enthalpy change measured under standard conditions (100 kPa and usually 298 K).

Calculating enthalpy changes from experimental data



Enthalpy changes can be measured using a simple calorimeter (shown opposite).

The heat absorbed or released in the reaction increases or decreases the temperature of a known mass of water (or solution).

The amount of heat absorbed or released can be calculated using the equation

$$q = mc\Delta T$$

$$q = mc\Delta T$$

q - heat (J)

m - mass of water (or solution)

c - specific heat capacity ($\text{J g}^{-1} \text{ }^\circ\text{C}^{-1}$)

ΔT - change in temperature

Specific heat capacity

- Specific heat capacity, c , is defined as the amount of heat required to raise the temperature of 1 kg of a substance by 1 K (or °C).
- The units are $\text{J kg}^{-1} \text{K}^{-1}$ or $\text{J g}^{-1} \text{K}^{-1}$ (or °C).

$$c = \frac{q}{m\Delta T}$$

- Substances with higher specific heat capacity values require more heat to change their temperature than substances with lower specific heat capacity values.
- The specific heat capacity of water is $4.18 \text{ J g}^{-1} \text{ }^\circ\text{C}^{-1}$

Exercise: The same amount of heat is added to equal masses of each of the substances in the table below. List the substances in order of the smallest temperature change to the largest temperature change when the heat is added.

Substance	Specific heat capacity / $\text{J g}^{-1} \text{ }^\circ\text{C}^{-1}$
Aluminium	0.903
Ethanol	2.42
Copper	0.385
Silver	0.235
Iron	0.449

Smallest temperature change				Largest temperature change
Ethanol	Aluminium	Iron	Copper	Silver

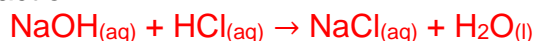
The higher the specific heat capacity, the smaller the temperature change.

Exercises:

1. Outline what is meant by standard enthalpy change of reaction (ΔH^\ominus).
Standard enthalpy change of reaction is the enthalpy change of a reaction carried out under standard conditions (100 kPa, 298 K).
2. Calculate the enthalpy change for the following reactions.

For examples (a) and (b) the enthalpy change is known as the standard enthalpy change of neutralisation (ΔH^\ominus_n), which is the enthalpy change when an acid and base are reacted together to form one mole of water under standard conditions.

- a. 200.0 cm³ of 0.400 mol dm⁻³ HCl is added to the same volume and concentration of NaOH solution inside a coffee-cup calorimeter. The initial temperature was 25.1 °C, and the maximum temperature was 27.7 °C. Calculate the enthalpy change of the reaction.



$$n(\text{NaOH}) = 0.400 \times (200.0 \div 1000) = 0.0800 \text{ mol}$$

$$n(\text{HCl}) = 0.400 \times (200.0 \div 1000) = 0.0800 \text{ mol}$$

$$q = mc\Delta T$$

$$q = 400.0 \times 4.18 \times (27.7 - 25.1)$$

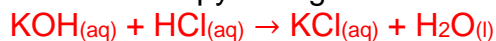
$$q = 4347.2 \text{ J}$$

For one mole of water produced:

$$\Delta H = 4347.2 \div 0.0800 = -54340 \text{ J mol}^{-1} = -54.3 \text{ kJ mol}^{-1}$$

Reaction is exothermic so a negative sign is used for the ΔH .

- b. 400.0 cm³ of 0.500 mol dm⁻³ hydrochloric acid was reacted with 400.0 cm³ of 1.00 mol dm⁻³ potassium hydroxide and the temperature increased by 3.20 °C. Calculate the enthalpy change of the reaction.



$$n(\text{KOH}) = 1.00 \times (400.0 \div 1000) = 0.400 \text{ mol}$$

$$n(\text{HCl}) = 0.500 \times (400.0 \div 1000) = 0.200 \text{ mol}$$

HCl is the limiting reactant – ratio of HCl to H₂O is 1:1

$$q = mc\Delta T$$

$$q = 800.0 \times 4.18 \times 3.20$$

$$q = 10700.8 \text{ J}$$

For one mole of water produced:

$10700.8 \div 0.200 = -53504 \text{ J mol}^{-1} = -53.5 \text{ kJ mol}^{-1}$ (note the negative sign because reaction is exothermic).

- c. The literature value for the standard enthalpy change of neutralisation is $-57.0 \text{ kJ mol}^{-1}$. For each of the above examples, calculate the percentage error and suggest possible sources of error.

$$\% \text{ error} = \frac{\text{experimental value} - \text{theoretical value}}{\text{theoretical value}} \times 100$$

Percentage error for a:

$$\% \text{ error} = \frac{(-54.3) - (-57.0)}{(-57.0)} \times 100 = 5\%$$

Percentage error for b:

$$\% \text{ error} = \frac{(-53.5) - (-57.0)}{(-57.0)} \times 100 = 6\%$$

Sources of error include heat loss to the surroundings and some heat absorbed by the calorimeter.

Assumptions: the solution has the same density and specific heat capacity as water ($1 \text{ g cm}^{-3} / 4.18 \text{ J g}^{-1} \text{ }^\circ\text{C}^{-1}$).

- d. A 1.00 g sample of octane (C_8H_{18}) is burned in a calorimeter containing 1200.0 cm^3 of water at an initial temperature of $25.0 \text{ }^\circ\text{C}$. After the reaction, the final temperature of the water is $33.0 \text{ }^\circ\text{C}$. Calculate the enthalpy change, in kJ mol^{-1} .

$$n(\text{C}_8\text{H}_{18}) = m \div M = 1.00 \div 114.26 = 8.75 \times 10^{-3} \text{ mol}$$

$$q = mc\Delta T$$

$$q = 1200.0 \times 4.18 \times (33.0 - 25.0)$$

$$q = 40128 \text{ J}$$

For one mole of C_8H_{18} :

$$40128 \div 8.75 \times 10^{-3} = -4586057.143 \text{ J mol}^{-1} = -4.59 \times 10^3 \text{ kJ mol}^{-1}$$

(note the negative sign because reaction is exothermic)

- e. In an experiment to measure the enthalpy change of combustion of ethanol ($\text{C}_2\text{H}_5\text{OH}$), a student heated a copper calorimeter containing 100.0 cm^3 of water with a spirit lamp and collected the following data.

Initial temperature of water:	20.0 °C
Final temperature of water:	55.0 °C
Mass of ethanol burned:	1.78 g

Calculate the enthalpy change of combustion of ethanol in kJ mol^{-1} .

$$n(\text{C}_2\text{H}_5\text{OH}) = m \div M = 1.78 \div 46.08 = 0.0386 \text{ mol}$$

$$q = mc\Delta T$$

$$q = 100.0 \times 4.18 \times (55.0 - 20.0)$$

$$q = 14630 \text{ J}$$

For one mole of $\text{C}_2\text{H}_5\text{OH}$:

$$14630 \div 0.0386 = -379015.544 \text{ J mol}^{-1} = -379 \text{ kJ mol}^{-1}$$

(note the negative sign because reaction is exothermic)

- f. Use the values in the table below to calculate the percentage error for each example and suggest possible sources of error.

Compound	ΔH_c^\ominus (kJ mol^{-1})
C_8H_{18}	-5483
$\text{C}_2\text{H}_5\text{OH}$	-1058

$$\% \text{ error} = \frac{\text{experimental value} - \text{theoretical value}}{\text{theoretical value}} \times 100$$

Percentage error for d:

$$\% \text{ error} = \frac{(-4590) - (-5483)}{(-5483)} \times 100 = 16\%$$

Percentage error for e:

$$\% \text{ error} = \frac{(-379) - (-1058)}{(-1058)} \times 100 = 64\%$$

Possible sources of error include heat loss to the surroundings /incomplete combustion/heat absorbed by the calorimeter.