

Energetics SL

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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5.1 Measuring energy changes

Understandings:

- Heat is a form of energy.
- Temperature is a measure of the average kinetic energy of the particles.
- Total energy is conserved in chemical reactions.
- Chemical reactions that involve transfer of heat between the system and the surroundings are described as endothermic or exothermic.
- The enthalpy change (ΔH) for chemical reactions is indicated in kJ mol^{-1}
- ΔH values are usually expressed under standard conditions, given by ΔH^\ominus , including standard states.

Applications and skills:

- Calculation of the heat change when the temperature of a pure substance is changed using $q = mc\Delta T$
- A calorimetry experiment for an enthalpy of reaction should be covered and the results evaluated.

Guidance:

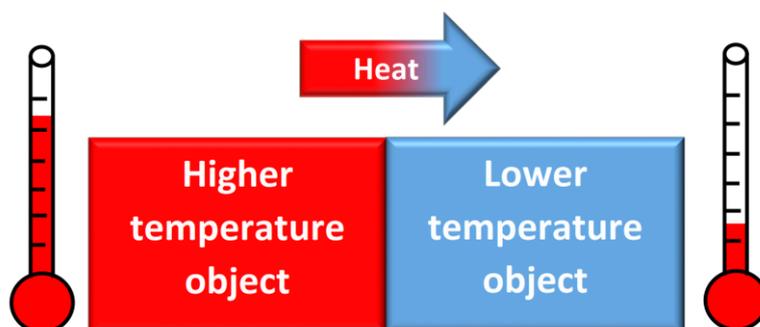
- Enthalpy changes of combustion (ΔH_c^\ominus) and formation (ΔH_f^\ominus) should be covered.
- Consider reactions in aqueous solution and combustion reactions.
- Standard state refers to the normal, most pure stable state of a substance measured at 100 kPa. Temperature is not a part of the definition of standard state, but 298 K is commonly given as the temperature of interest.
- The specific heat capacity of water is provided in the data booklet in section 2.
- Students can assume the density and specific heat capacities of aqueous solutions are equal to those of water but should be aware of this limitation.
- Heat losses to the environment and the heat capacity of the calorimeter in experiments should be considered, but the use of a bomb calorimeter is not required.

Syllabus checklist

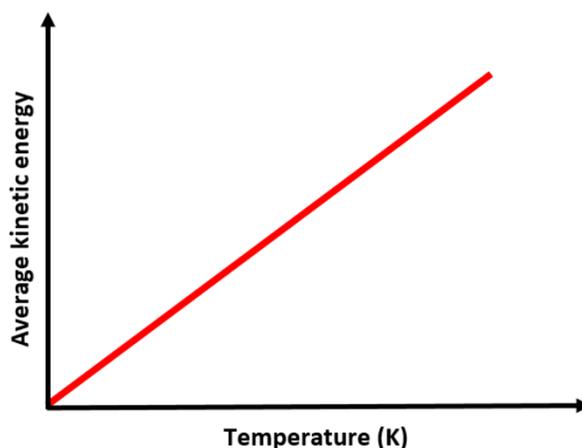
Objective	I am confident with this	I need to review this	I need help with this
Outline the difference between heat and temperature			
State the conditions for the standard enthalpy change (ΔH^\ominus)			
Describe the characteristics of exothermic and endothermic reactions			
Sketch enthalpy level diagrams for exothermic and endothermic reactions			
Calculate enthalpy changes using the equation $q=mc\Delta T$			
Describe possible errors and limitations in experiments to calculate enthalpy change			

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
- 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.

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

- a) 25°C b) 78°C c) 100°C d) -273°C e) -13°C

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?

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.

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.

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):

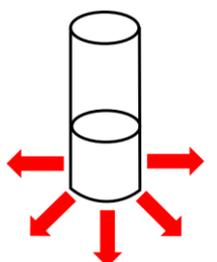
$$H = U + PV$$

- 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).

Exothermic and endothermic reactions

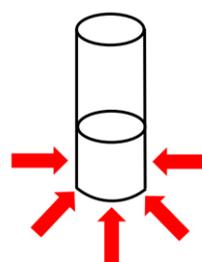
- Chemical reactions can be classified as exothermic or endothermic depending on whether heat is absorbed or released by the system or surroundings.

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

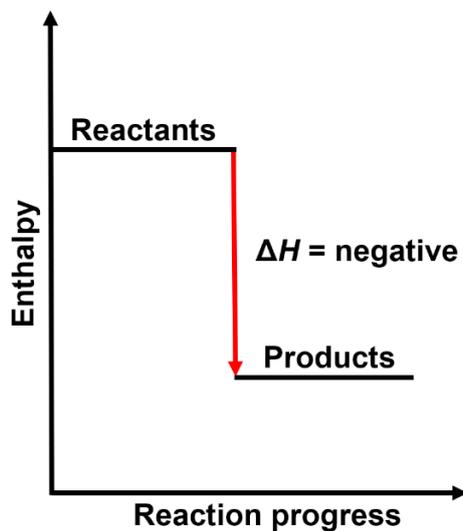
- In an exothermic reaction, heat flows from the system to the surroundings.
- The temperature of the reaction mixture and the surroundings increases as heat is released by the system.
- Examples of exothermic reactions include combustion and neutralisation.

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.

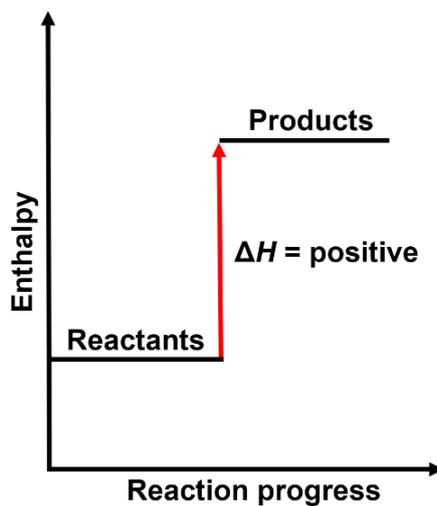
Enthalpy level diagrams

Enthalpy level diagram an exothermic reaction



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

Enthalpy level diagram an endothermic reaction



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

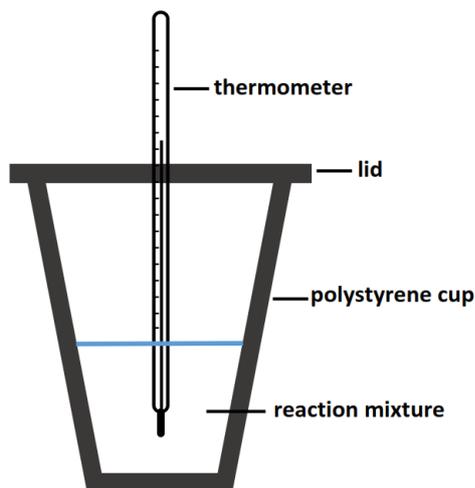
Exercises:

1. Define the term *standard enthalpy change of reaction* (ΔH^\ominus).
2. Sketch enthalpy level diagrams for an exothermic reaction and an endothermic reaction.
3. Complete the table summarising exothermic and endothermic reactions.

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

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

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 $^\circ\text{C}$).
- The units are $\text{J kg}^{-1} \text{ K}^{-1}$ or $\text{J g}^{-1} \text{ K}^{-1}$ (or $^\circ\text{C}$).

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

- 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

Exercises:

1. 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_n^\ominus), 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 cm^3 of $0.400 \text{ mol dm}^{-3}$ HCl is added to the same volume and concentration of NaOH solution inside a coffee-cup calorimeter. The initial temperature was $25.1 \text{ } ^\circ\text{C}$, and the maximum temperature was $27.7 \text{ } ^\circ\text{C}$. Calculate the enthalpy change of the reaction.

- b. 400.0 cm^3 of $0.500 \text{ mol dm}^{-3}$ hydrochloric acid was reacted with 400.0 cm^3 of 1.00 mol dm^{-3} potassium hydroxide and the temperature increased by $3.20 \text{ } ^\circ\text{C}$. Calculate the enthalpy change of the reaction.

- 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.

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

- 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} .

- 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:	$20.0 \text{ }^\circ\text{C}$
Final temperature of water:	$55.0 \text{ }^\circ\text{C}$
Mass of ethanol burned:	1.78 g

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

- 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 ₈ H ₁₈	-5483
C ₂ H ₅ OH	-1058

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

5.2 Hess's law

Understandings:

- The enthalpy change (ΔH) for a reaction that is carried out in a series of steps is equal to the sum of the enthalpy changes for the individual steps.

Applications and skills:

- Application of Hess's Law to calculate enthalpy changes.
- Calculation of ΔH values using ΔH_f^\ominus data
- Determination of the enthalpy change of a reaction that is the sum of multiple reactions with known enthalpy changes.

Guidance:

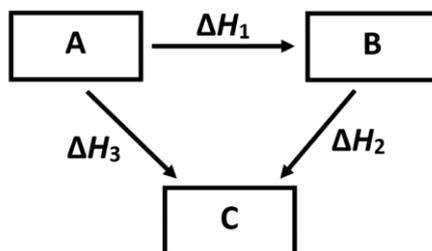
- Enthalpy of formation data can be found in the data booklet in section 12.
- An application of Hess's Law is $\Delta H^\ominus = \sum \Delta H_f^\ominus \text{ products} - \sum \Delta H_f^\ominus \text{ reactants}$

Syllabus checklist

Objective	I am confident with this	I need to review this	I need help with this
Outline the meaning of the standard enthalpy change of formation (ΔH_f^\ominus)			
Calculate enthalpy changes using standard enthalpy change of formation values			
Determine the enthalpy change of a reaction that is the sum of multiple reactions with known enthalpy changes			
Interpret enthalpy cycles to calculate enthalpy changes			

Hess's law

- Hess's law states:
"The enthalpy change for a chemical reaction is independent of the route by which the chemical reaction occurs."
- This means that regardless of the route, if the starting point and end point are the same, the enthalpy change will also be the same.
- Enthalpy cycles are an application of Hess's law.
- Whichever route is taken to get to the products C, the enthalpy change is the same.

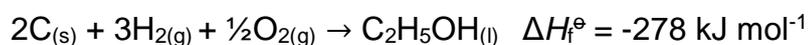


$$\Delta H_3 = \Delta H_1 + \Delta H_2$$

Standard enthalpy change of formation (ΔH_f^\ominus)

- The standard enthalpy change of formation (ΔH_f^\ominus) is the enthalpy change when one mole of a substance is formed from its elements in their standard states under standard conditions.
- Standard state is the normal, most pure stable state of a substance measured at a pressure of 100 kPa.

Examples:



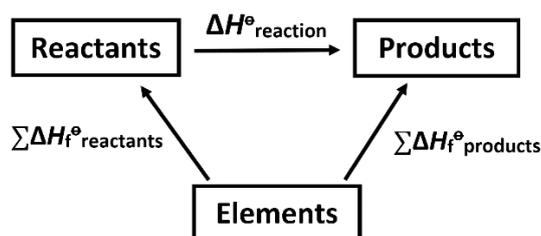
- Note that fractional coefficients are used because the equation is written for the formation of one mole of product.

Exercise: Write equations for the formation of one mole of the following compounds.

1. $\text{C}_3\text{H}_8(g)$
2. $\text{CH}_3\text{OH}(l)$
3. $\text{MgCl}_2(s)$

Calculating ΔH for a reaction using ΔH_f^\ominus values

- Using the enthalpy cycle below and applying Hess's law, we arrive at the following equation:

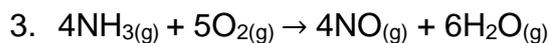
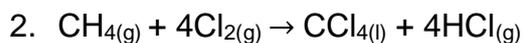
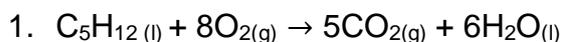


$$\Delta H^\ominus = \Sigma \Delta H_f^\ominus_{\text{products}} - \Sigma \Delta H_f^\ominus_{\text{reactants}}$$

- ΔH_f^\ominus values can be found in table 12 of the data booklet.
- Elements have a standard enthalpy change of formation of zero.

Exercise: Calculate the enthalpy change for each of the reactions below, given the data in the table.

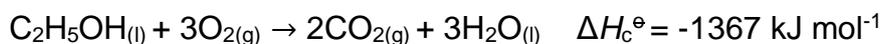
	ΔH_f^\ominus (kJ mol ⁻¹)
CO _{2(g)}	-394
CH _{4(g)}	-74.9
H ₂ O _(g)	-241.8
HCl _(g)	-92.3
C ₅ H _{12(l)}	-173
CCl _{4(l)}	-95.7
NH _{3(g)}	-45.9
NO _(g)	+90.3



Standard enthalpy change of combustion (ΔH_c^\ominus)

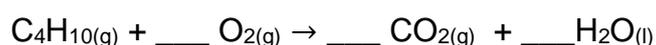
- The standard enthalpy change of combustion (ΔH_c^\ominus) is the enthalpy change when one mole of a substance is burned completely in oxygen under standard conditions.

Example:



- Note that the equation is balanced for one mole of reactant and the oxygen is assumed to be the excess reactant.

Write an equation for the complete combustion of one mole of butane, C_4H_{10} .

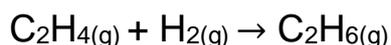


Calculating ΔH using ΔH_c^\ominus values

- The equation used to calculate the ΔH of a reaction using ΔH_c^\ominus values is given below.

$$\Delta H^\ominus = \sum \Delta H_c^\ominus \text{ reactants} - \sum \Delta H_c^\ominus \text{ products}$$

Example: Determine the ΔH of the following reaction using the values given in the table.

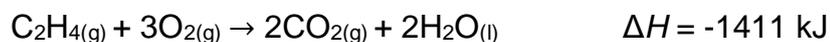
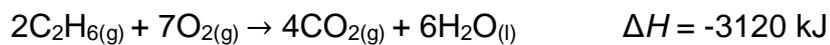


	ΔH_c^\ominus
C_2H_4	-1411
H_2	-286
C_2H_6	-1561

Calculating the enthalpy change of a reaction that is the sum of multiple reactions with known enthalpy changes

- Applying Hess's law, the enthalpy change for a reaction can be calculated using multiple reactions with known enthalpy changes.

Example:

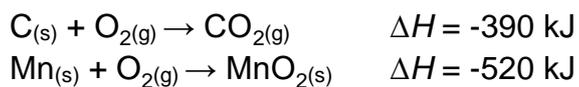


Calculate the enthalpy change for the following reaction:

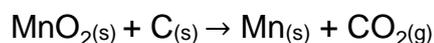


Exercises:

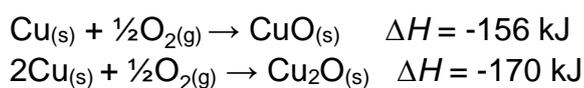
1. Using the equations below:



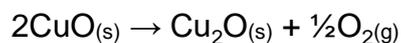
Determine the ΔH (in kJ) for the following reaction.



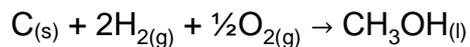
2. Using the equations below:



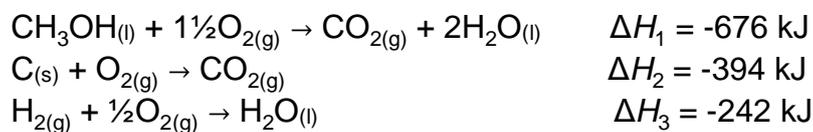
Determine the ΔH (in kJ) for the following reaction.



3. Calculate the enthalpy change, ΔH , for the reaction:

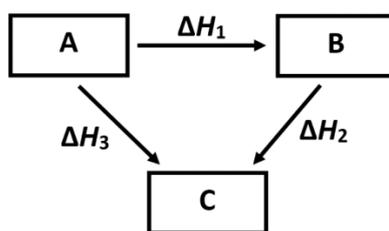


using Hess's Law and the following information.



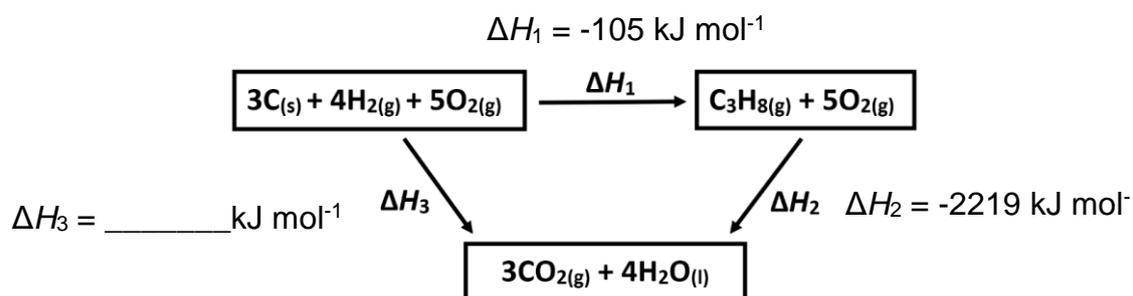
Enthalpy cycles

- Enthalpy cycles are an application of Hess's law.
- Whichever route is taken to get to C, the enthalpy change is the same.

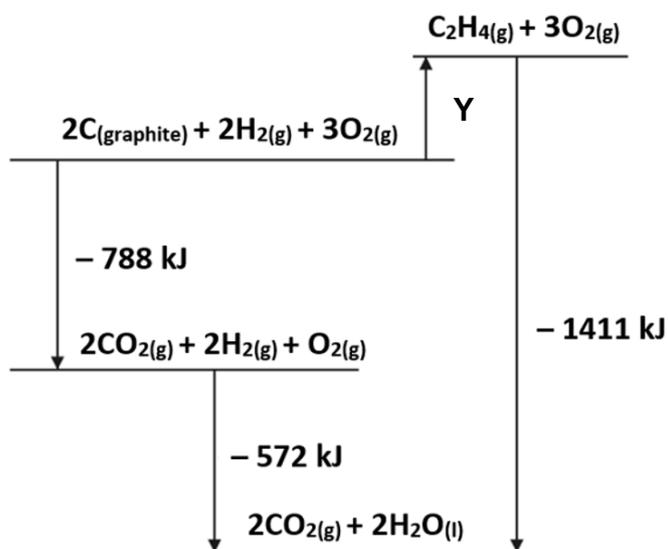


$$\Delta H_3 = \Delta H_1 + \Delta H_2$$

Example 1: Using the values below for ΔH_1 and ΔH_2 , calculate ΔH_3



Example 2: Calculate the value of Y using the values given in the enthalpy cycle.



5.3 Bond enthalpies

Understandings:

- Bond-forming releases energy and bond-breaking requires energy.
- Average bond enthalpy is the energy needed to break one mole of a bond in a gaseous molecule averaged over similar compounds.

Applications and skills:

- Calculation of the enthalpy changes from known bond enthalpy values and comparison of these to experimentally measured values.
- Sketching and evaluation of potential energy profiles in determining whether reactants or products are more stable and if the reaction is exothermic or endothermic.
- Discussion of the bond strength in ozone relative to oxygen in its importance to the atmosphere.

Guidance:

- Bond enthalpy values are given in the data booklet in section 11.
- Average bond enthalpies are only valid for gases and calculations involving bond enthalpies may be inaccurate because they do not take into account intermolecular forces.

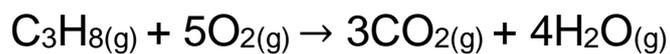
Objective	I am confident with this	I need to review this	I need help with this
Describe the energy changes involved in bond breaking and bond making			
Calculate enthalpy changes using average bond enthalpy values			
Outline why enthalpy change values calculated using average bond enthalpies differ from the actual value			
Describe the bonding in bonding and ozone			
Explain the importance of ozone in the atmosphere			
Explain the difference in the wavelength required to break the bonds in ozone and oxygen			

Average bond enthalpies

- Average bond enthalpy is the energy needed to break one mole of bonds in a gaseous molecule averaged over similar compounds.
- Bond breaking is endothermic (requires energy).
- Bond making is exothermic (releases energy).

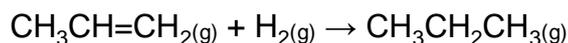
$$\Delta H = \sum (\text{bonds broken}) - \sum (\text{bonds formed})$$

Example calculate the enthalpy change for the following reaction:

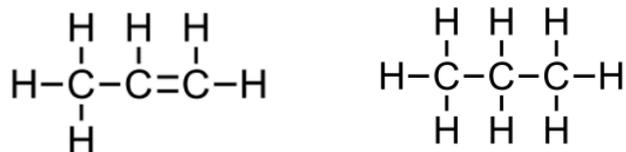


Exercises

1. Propane can be formed by the hydrogenation of propene.

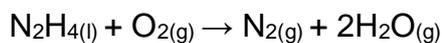


Structures of propene (left) and propane (right):



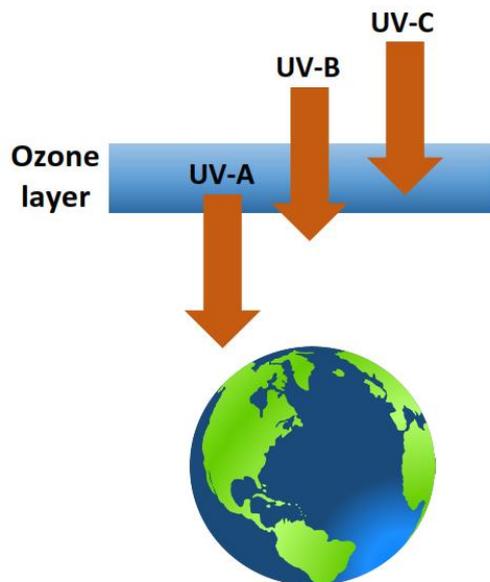
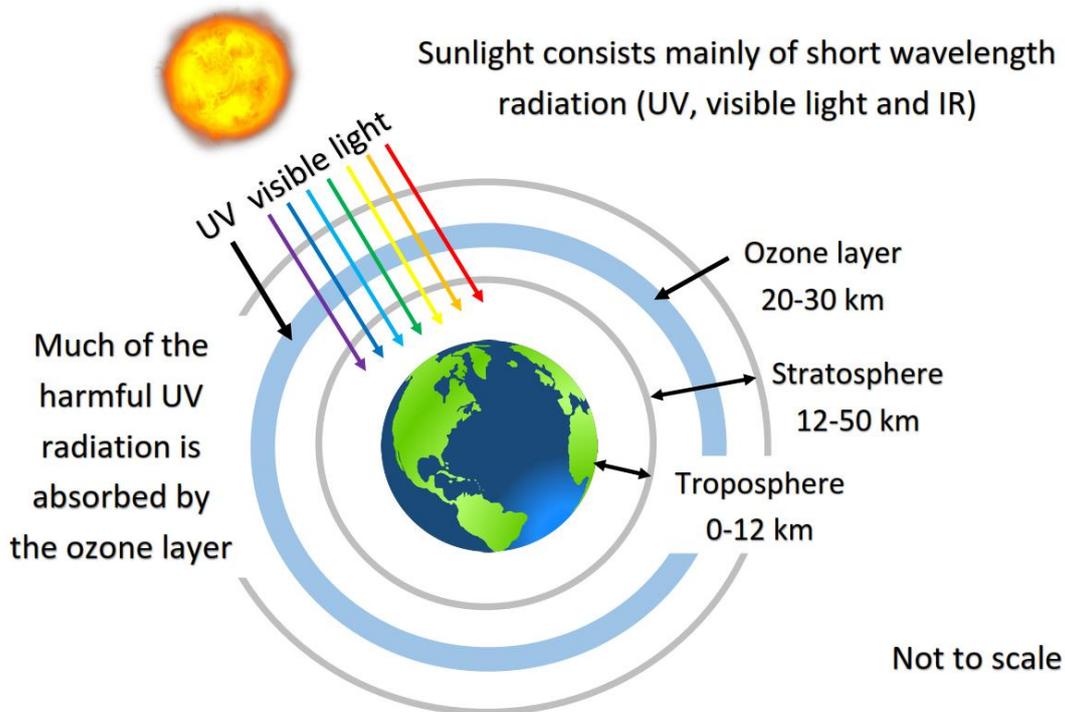
Determine a value for the hydrogenation of propene using information from Table 11 of the Data Booklet. State and explain if the reaction is exothermic or endothermic.

2. Use the information from Table 11 of the Data Booklet to calculate the enthalpy change for the following reaction.



3. State three reasons why enthalpy changes calculated using average bond enthalpies can be inaccurate.

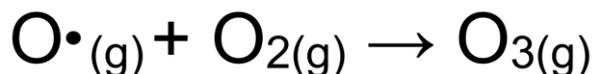
Ozone in the atmosphere



Ozone absorbs UV radiation in the range of 200 nm-315 nm. This corresponds to the higher energy UV radiation (UV-B and UV-C) which can cause damage to living tissue.

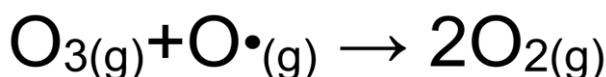
Formation of ozone

- The oxygen molecule dissociates in the presence of high energy UV radiation to form two oxygen free radicals.
- The free radicals then react with molecular oxygen to form ozone.



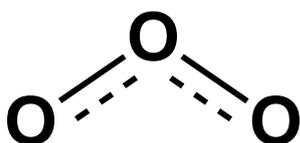
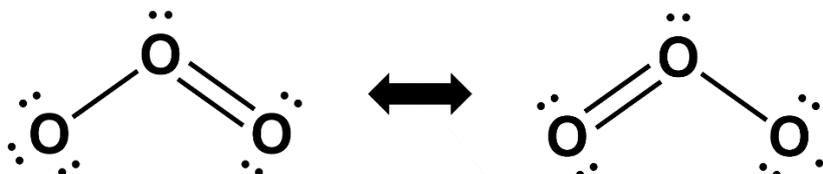
Destruction of ozone

- The ozone molecule dissociates in the presence of lower energy UV radiation to form O_2 and an oxygen free radical.
- The free radical reacts with ozone to form molecular oxygen.

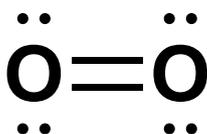


Bond strength in ozone and oxygen

- Ozone, O_3 , exists as two resonance structures.



The bonds in ozone are of equal length and strength; intermediate between a single and a double bond (bond order 1.5).



The oxygen molecule has a double covalent bond between the oxygen atoms (bond order 2).

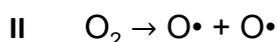
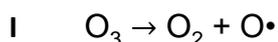
- The double bond in O₂ is stronger than the bonds in O₃ – it requires more energy to break the bond in O₂ than in O₃
- The double bond in O₂ is broken by UV radiation with a wavelength of <242 nm forming two oxygen free radicals.
- The bond in O₃ is broken by UV radiation with a wavelength of <330 nm forming an oxygen molecule and an oxygen free radical.

Molecule	Bond order	λ UV radiation (nm)
O ₂	2	<242
O ₃	1.5	<330

- Stronger double bond in O₂ requires higher energy UV radiation (shorter wavelength) to break.
- Weaker bond in O₃ requires lower energy (longer wavelength) to break.

Exercises:

1. The following reactions take place in the ozone layer by the absorption of ultraviolet light.



State and explain, by reference to the bonding, which of the reactions, **I** or **II**, requires a shorter wavelength of UV light.

2. Explain why UV radiation with a wavelength of between 300 and 330 nm contributes to photochemical decomposition of ozone but not to the formation of ozone from oxygen.