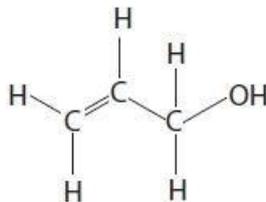## Questions

Q1.

Prop-2-en-1-ol is an unsaturated alcohol with the structure shown.

A student planned to use bond enthalpy data to calculate a value for the enthalpy change of combustion of prop-2-en-1-ol.

(i) When researching the bond enthalpy data, the student claimed that it was not necessary to find the value for the C=C
    bond as they could use the value for a C–C bond and multiply it by two.
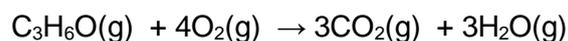   Explain why the student is **incorrect**.

(2)

....

....

....

....

(ii) Calculate a value for the enthalpy of combustion of prop-2-en-1-ol using the data shown.

$$C_3H_6O(g) + 4O_2(g) \rightarrow 3CO_2(g) + 3H_2O(g)$$

Bond	C–C	C=C	C–O	C=O	O–H	C–H	O=O
Bond enthalpy / kJ mol^{-1}	347	612	358	805	464	413	498

(3)

(iii) Explain, in terms of entropy, why the combustion of prop-2-en-1-ol is always feasible in the gaseous state.
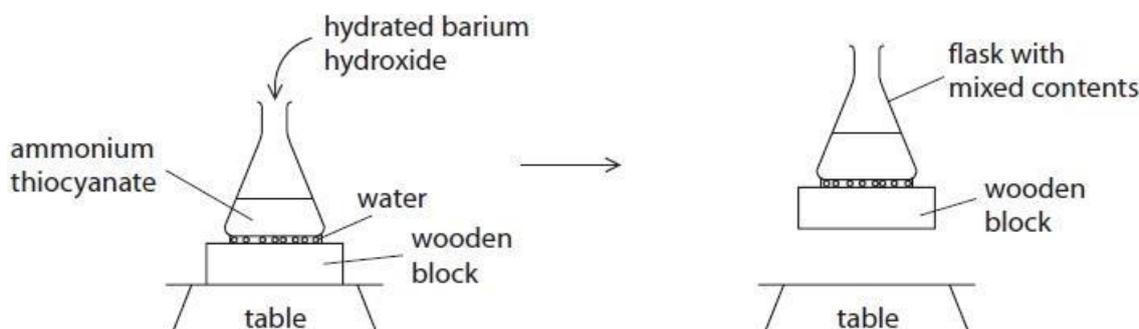
(2)

....

....

....

....
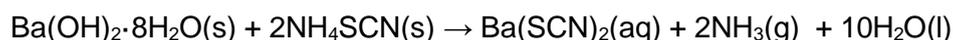
(Total for question = 7 marks)

Q2.

This question is about entropy.

Some hydrated barium hydroxide is added to ammonium thiocyanate in a flask which is placed on a few drops of water on a wooden block. After the addition, the contents are stirred and then the flask can be lifted up with the wooden block attached, as shown.

The equation for the reaction is

$$Ba(OH)_2 \cdot 8H_2O(s) + 2NH_4SCN(s) \rightarrow Ba(SCN)_2(aq) + 2NH_3(g) + 10H_2O(l)$$

(i) Give **two** reasons why you would expect $\Delta S_{system}^{\ominus}$ to be positive.

(2)

....

....

....

....

(ii) Explain why the wooden block is lifted up by the flask.

(2)

....

....

....

....
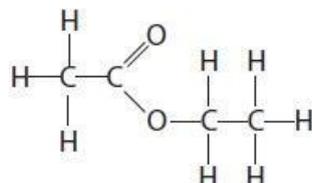
(Total for question = 4 marks)

Q3.

Ethyl ethanoate is an ester.
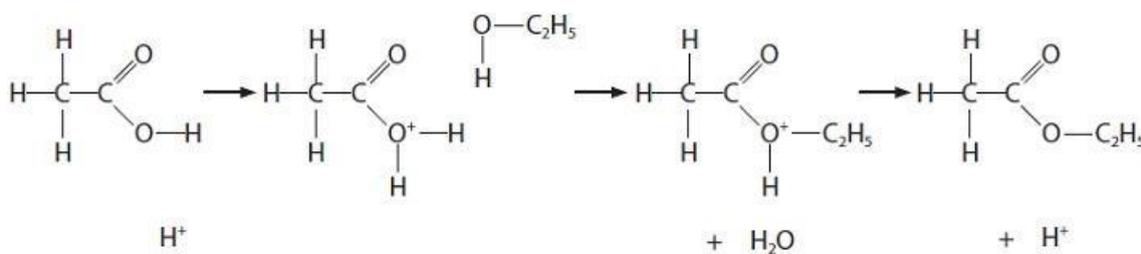

One method for the formation of ethyl ethanoate is the reaction between ethanol and ethanoic acid, which is catalysed by hydrogen ions.

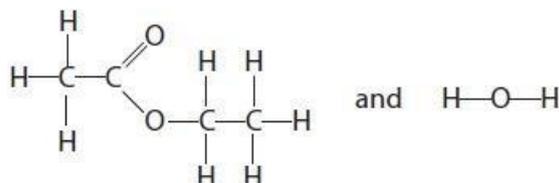$$CH_3COOH + C_2H_5OH \rightleftharpoons CH_3COOC_2H_5 + H_2O$$

An incomplete simplified mechanism for this reaction is shown.

(i) Add curly arrows and relevant lone pairs of electrons to complete the mechanism.

(4)

(ii) In an experiment, the oxygen atom in ethanol is replaced by the oxygen-18 isotope, ^{18}O. The products of the esterification are

Label the ^{18}O oxygen atom in one of the products.
Justify your answer.

(2)

....

....

....

....

(iii) Calculate the standard molar entropy of ethyl ethanoate using your knowledge of Gibbs free energy, ΔG, and the data in the table.

Include sign and units in your answer.
Use $\Delta G = -RT \ln K$ and other appropriate equations.

Quantity	Value
Gas constant, R	8.31 J mol^{-1} K^{-1}
Temperature, T	298 K
Equilibrium constant of esterification reaction, K	4.0
Enthalpy change of esterification reaction, ΔH	-6.0 kJ mol^{-1}
Standard molar entropy of ethanoic acid, S^O	159.8 J K^{-1} mol^{-1}
Standard molar entropy of ethanol, S^O	160.7 J K^{-1} mol^{-1}
Standard molar entropy of water, S^O	69.9 J K^{-1} mol^{-1}

(6)

(Total for question = 12 marks)

Q4.

This question is about enthalpy changes and entropy changes.

Calcium carbonate decomposes on heating.

$$CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$$

$\Delta_r H = +178 \text{ kJ mol}^{-1}$

$\Delta S_{system} = +165 \text{ J mol}^{-1} \text{ K}^{-1}$

Show, by calculating the value for the free energy change, ΔG, that this decomposition is not feasible at 298 K, and then calculate the minimum temperature to which calcium carbonate must be heated to make it decompose.
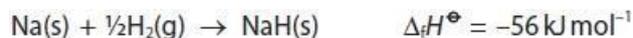
(3)

(Total for question = 3 marks)

Q5.

Sodium hydride, NaH, can be used to generate hydrogen for fuel cells.

The equation for the formation of sodium hydride is

$$Na(s) + \tfrac{1}{2}H_2(g) \rightarrow NaH(s) \qquad \Delta_f H^{\ominus} = -56 \text{ kJ mol}^{-1}$$

The standard entropy change of the system, $\Delta S^{\ominus}_{system}$, for this reaction is -76.5 J K^{-1} mol^{-1}.

(i) Deduce the feasibility of this reaction at 298 K by calculating the free energy change, ΔG.

(2)

....

....

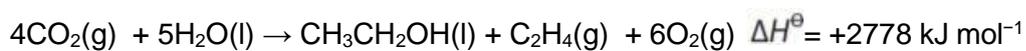(ii) Calculate the temperature at which $\Delta G = 0$.

(1)

(Total for question = 3 marks)

Q6.

Chemists are researching a process to make ethanol and ethene directly from carbon dioxide and water.

$4CO_2(g) + 5H_2O(l) \rightarrow CH_3CH_2OH(l) + C_2H_4(g) + 6O_2(g)$ $\Delta H^{\ominus} = +2778$ kJ mol^{-1}

	$CO_2(g)$	$H_2O(l)$	$CH_3CH_2OH(l)$	$C_2H_4(g)$	$O_2(g)$
$S^{\ominus}$ / J K^{-1} mol^{-1}	213.6	69.9	160.7	219.5	205.0

Calculate $\Delta S^{\ominus}_{total}$ for the reaction and hence determine whether the reaction is feasible under standard conditions.

(5)

(Total for question = 5 marks)

Q7.

This question is about entropy and free energy.

Complete the table by giving the sign of the entropy change of the system, ΔS_{system} , for each reaction.

(2)

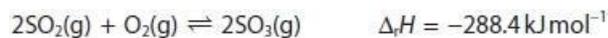| Reaction	Sign of ΔS_{system}
$CO_2(s) \rightarrow CO_2(g)$	
$NaCl(s) + aq \rightarrow NaCl(aq)$	
$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$	

(Total for question = 2 marks)

Q8.

This question is about entropy and free energy.

Sulfur dioxide reacts with oxygen to form sulfur trioxide.

$$2SO_2(g) + O_2(g) \rightleftharpoons 2SO_3(g) \qquad \Delta_r H = -288.4 \, kJ \, mol^{-1}$$

The standard molar entropy values at 298 K are given in the table.

	$SO_2(g)$	$O_2(g)$	$SO_3(g)$
$S^{\ominus} / JK^{-1}mol^{-1}$	+248.1	+205.0	+95.6

(i) Calculate the entropy change of the system, ΔS_{system} , for the forward reaction.

Include a sign and units in your answer.

$$2SO_2(g) + O_2(g) \rightarrow 2SO_3(g)$$
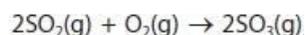
(2)

(ii) Calculate the free energy change, ΔG, at 298 K and hence deduce whether the reaction is feasible.

(3)

....

....

....

(iii) In industry, the reaction is carried out at about 700 K using a vanadium(V) oxide catalyst.

Calculate the value of the equilibrium constant, K, at 700 K.
ΔG at 700 K is –60 kJ mol^{-1}

(3)

(iv) The equilibrium constant has a larger value at 298 K than at 700 K.

Explain why the reaction is carried out at 700 K and not at 298 K.

(2)

....

....

....

....

....

....

....

....
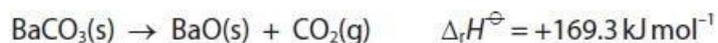
(Total for question = 10 marks)

Q9.

This question is about the white solid barium carbonate.

Barium carbonate decomposes under suitable conditions to form barium oxide and carbon dioxide.

$$BaCO_3(s) \rightarrow BaO(s) + CO_2(g) \qquad \Delta_r H^\ominus = +169.3 \, kJ \, mol^{-1}$$

Standard molar entropy data related to this reaction are shown.

Substance	Standard molar entropy, $S^\ominus$ /$J \, K^{-1} \, mol^{-1}$
$BaCO_3(s)$	112.1
$BaO(s)$	70.4
$CO_2(g)$	213.6

(i) Show that barium carbonate is thermally stable at 298 K, using the data in the equation and in the table.

(5)

(ii) Calculate the lowest temperature, in °C, at which it is thermodynamically

feasible for barium carbonate to decompose.
Give your answer to three significant figures.

(3)

(Total for question = 8 marks)

Q10.

* A student wrote:

Whether or not a reaction occurs depends only on the thermodynamic feasibility calculated using

$$\Delta G = \Delta H - T\Delta S_{system}$$

Discuss this statement.

Include reference to:

- changes in the values and signs of the terms in the equation for both endothermic and exothermic reactions
- circumstances where a reaction that is predicted to be thermodynamically feasible may not occur in practice.

(6)

(Total for question = 6 marks)

Q11.

This question is about entropy and free energy.

Calculate the total entropy change, ΔS_{total} , for the thermal decomposition of calcium carbonate at 298 K.

$$CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$$

[Data: $\Delta_r H = +178\,kJ\,mol^{-1}$ $\Delta S_{system} = +160\,J\,K^{-1}\,mol^{-1}$]

(3)

(Total for question = 3 marks)