An Extended Problem Using Enthalpy Changes from Y12

ANSWERS

Introduction

This problem will involve the use of ***Enthalpies of Combustion,*** $\Delta_c H$, to obtain ***Enthalpies of Formation,*** $\Delta_f H$.

The Enthalpies of Formation will then be used to calculate the $\Delta_r H$ for an esterification reaction.

The problem is associated with a simple **esterification reaction**. Many of you will be familiar with this reaction from GCSE. Esters are organic molecules made by the reaction of a carboxylic acid with an alcohol. A common example is shown in the box below:

ethanoic acid	+	ethanol	→	ethyl ethanoate	+	water
$CH_3COOH_{(l)}$	+	$CH_3CH_2OH_{(l)}$	→	$CH_3COOCH_2CH_{3(l)}$	+	$H_2O_{(l)}$

Enthalpies of Combustion are typically quite straight forward to obtain directly by experiment in a simple **combustion calorimeter** or a more accurate **bomb calorimeter**.

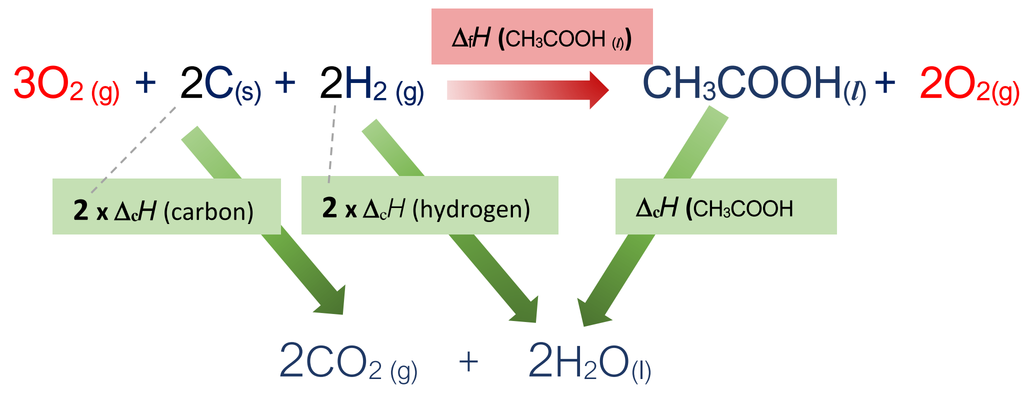
Enthalpies of combustion of these molecules are presented in the table below. Enthalpies of combustion of carbon and hydrogen are also given.

Chemical	Enthalpy of Combustion $\Delta_c H$ / $kJmol^{-1}$
$C_{(s)}$	-394
$H_{2(g)}$	-286
$CH_3COOH_{(l)}$	-874
$CH_3CH_2OH_{(l)}$	-1368
$CH_3COOCH_2CH_{3(l)}$	-2238

Task 1

Draw **Hess Cycles** involving the **enthalpies of combustion** $\Delta_c H$ that will allow you to calculate the **enthalpies of formation** $\Delta_f H$ for the following compounds:

a) ethanoic acid, $CH_3COOH_{(l)}$



Note that only one mole (of the 3 moles) of $O_{2\,(g)}$ is consumed in the reaction for the enthalpy of formation of ethanoic acid, CH_3COOH.
The other 2 moles $O_{2\,(g)}$ are required for the combustion reactions.

Layout

$\Delta_f H(CH_3COOH_{(l)})$ $= (+\,2 \times \Delta_c H(C)) + (+\,2 \times \Delta_c H(H_2)) + (-\,\Delta_c H(CH_3COOH_{(l)}))$

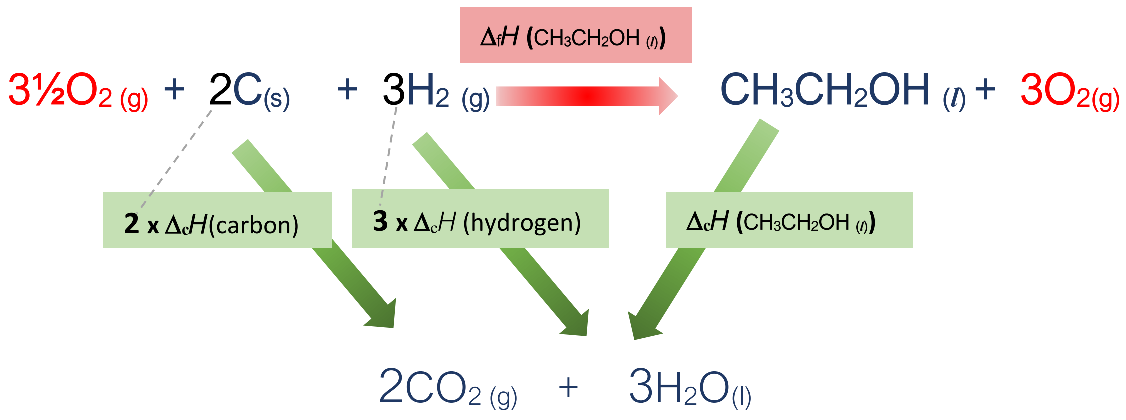
ROUTE 1 = ROUTE 2

Adding Values

$\Delta_f H(CH_3COOH_{(l)})$ $= (+\,2 \times -394) + (+\,2 \times -286) + (-\,-874) = -486$ kJ mol^{-1}

$\Delta_f H\ (CH_3COOH) = -486$ kJ mol^{-1}

b) ethanol, $CH_3CH_2OH_{(l)}$



Note that only ½ mole (of the 3½ moles) of $O_{2\,(g)}$ is consumed in the reaction for the enthalpy of formation of ethanoic acid, CH_3COOH.
The other 3 moles $O_{2\,(g)}$ are required for the combustion reactions.

Layout

$\Delta_f H(CH_3CH_2OH_{(l)})$ =(+ 2 x $\Delta_c H$(C)) + (+ 3 x $\Delta_c H(H_2)$) + (- $\Delta_c H(CH_3CH_2OH_{(l)})$)

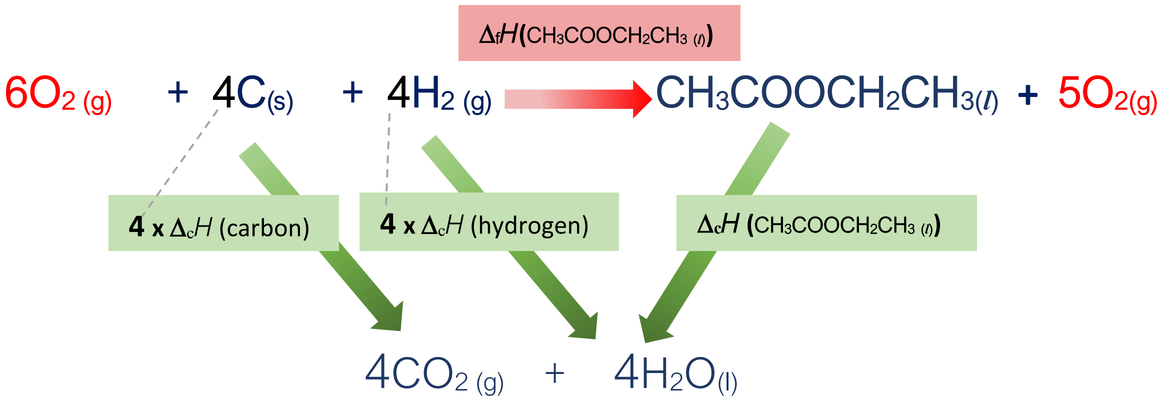
ROUTE 1 = ROUTE 2

Adding Values

$\Delta_f H(CH_3CH_2OH_{(l)})$ = (+ 2 x -394) + (+ 3 x -286) + (- - 1368) = -278 kJ mol^{-1}

$\Delta_f H (CH_3CH_2OH)$= -278 kJ mol^{-1}

c) ethyl ethanoate, $CH_3COOCH_2CH_{3(l)}$



Note that only one mole (of the 6 moles) of $O_{2\,(g)}$ is consumed in the reaction for the enthalpy of formation of ethyl ethanoate, $CH_3COOCH_2CH_3$.
The other 5 moles $O_{2\,(g)}$ are required for the combustion reactions of C and H_2.

Layout

$\Delta_f H(CH_3COOH_{(l)})$ =(+ 4 x $\Delta_c H$(C)) + (+ 4 x $\Delta_c H(H_2)$) + (- $\Delta_c H(CH_3CH_2OH_{(l)})$)

ROUTE 1 = ROUTE 2

Adding Values

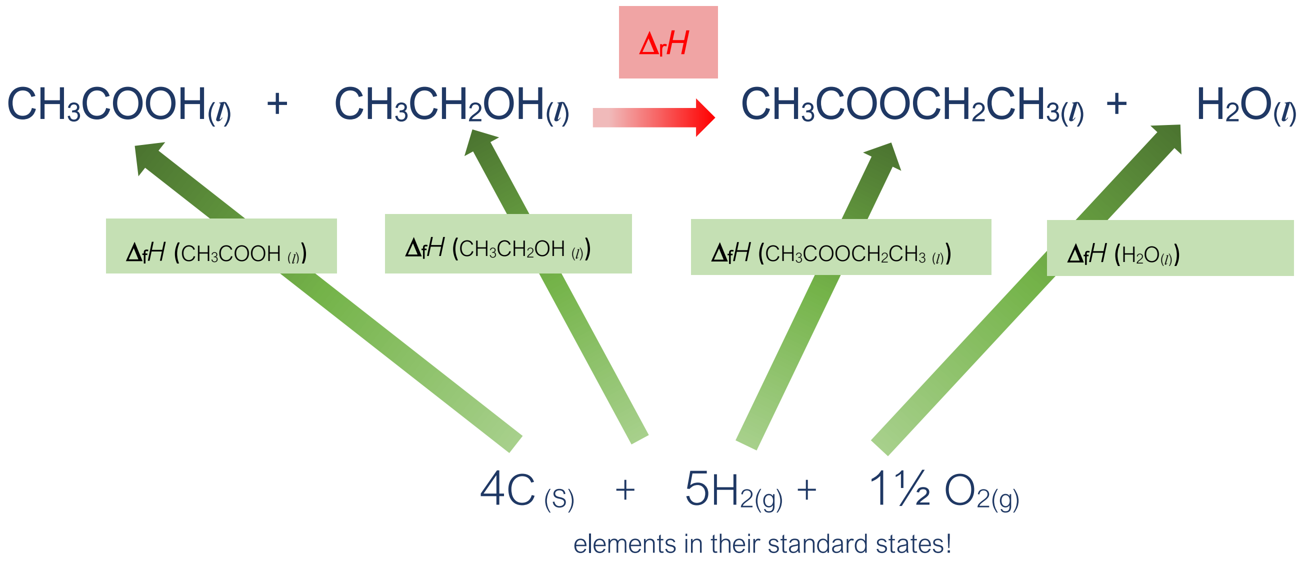
$\Delta_f H(CH_3COOH_{(l)})$ = (+ 4 x -394) + (+ 4 x -286) + (- - 2238) = -482 kJ mol^{-1}

$\Delta_f H\ (CH_3COOCH_2CH_3)$ = -482 kJ mol^{-1}

Task 2

Using the **enthalpies of formation,** $\Delta_f H$, calculated in Task 1, draw a Hess Cycle and calculate the enthalpy of reaction $\Delta_r H$ for the esterification reaction between ethanoic acid and alcohol. You may be thinking that you haven't been given a value for $\Delta_f H$ (H_2O). But, if you think about it carefully, the value for $\Delta_f H$ (H_2O) is shown somewhere in the data that you have been given.

Clue: In the case of hydrogen and carbon (and a few others) the value of ΔHf is also the same value as another enthalpy change.



$\Delta_r H$ = (- $\Delta_f H(CH_3COOH_{(l)})$) + (- $\Delta_f H(CH_3CH_2OH_{(l)})$) + (+ $\Delta_f H(CH_3COOCH_2CH_{3(l)})$) +(- $\Delta_f H(H_2O_{(l)})$)

ROUTE 1 = ROUTE 2

$\Delta_r H$ = (- -486) + (- -278) + (+ -482) + (+ -286) = -4 kJ mol^{-1}

For this esterification reaction, $\Delta_r H$ = -4 kJ mol^{-1}