

SL HL Paper 3 Section A Data Response (7) **with worked answers**

Compound **X** is a crystalline solid that occurs naturally in some fruits.

Analysis of pure Compound **X** shows that it contains 68.84% carbon, 4.96% hydrogen and 26.20% oxygen by mass.

The mass spectrum of Compound **X** shows a molecular ion peak with $m/z = 122$.

The low resolution ^1H NMR spectrum of Compound **X** shows two signals with an integration trace ratio of 5:1.

The infrared spectrum of Compound **X** shows a broad strong peak between 2500 and 3000 cm^{-1} and a sharp peak at 1700 cm^{-1} .

(a) (i) Show that the molecular formula of Compound **X** is $\text{C}_7\text{H}_6\text{O}_2$. **[2]**

From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	$68.84/12.01 = 5.73$	7
Hydrogen	$4.96 / 1.01 = 4.91$	6
Oxygen	$26.2 / 16.00 = 1.64$	2

The empirical formula is $\text{C}_7\text{H}_6\text{O}_2$ **[1]**

The molecular ion peak gives M as 122 g mol^{-1} so the molecular formula is $\text{C}_7\text{H}_6\text{O}_2$ **[1]**

(Underlying chemistry concepts can be found in 1.2 The mole & Avogadro's constant.)

(ii) State the information that can be deduced about the structure of Compound **X** from its ^1H NMR spectrum. **[2]**

The hydrogen atoms in the molecule exist in two different chemical environments. **[1]**

Five H atoms are in the same environment and one is in a different environment. **[1]**

(Underlying chemistry concepts can be found in 11.3 Spectroscopic identification of organic compounds.)

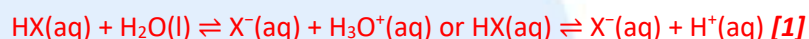
(iii) Deduce the molecular structure of Compound X. [1]

C_6H_5COOH . [1]

(C_6H_5COOH fits the mass spectral and 1H NMR data. The IR data confirms this structure as the broad strong peak between 2500 and 3000 cm^{-1} is due to $-OH$ and the sharp peak at 1700 cm^{-1} is due to $C=O$.)

Underlying chemistry concepts can be found in 11.3 Spectroscopic identification of organic compounds.)

(b) The value for the acid dissociation constant of Compound X is 6.31×10^{-5} . Using HX to represent Compound X, state the equation for the reaction of Compound X with water. [1]



(Note that to gain the mark the equation must have reversible arrows as the value for the equilibrium constant shows that it is a weak acid.)

(Underlying chemistry concepts can be found in 8.4 Strong & weak acids & bases.)

(c) The following table shows the solubility of Compound X in water at different temperatures:

Temperature / $^{\circ}C$	Solubility / $g\text{ dm}^{-3}$
0	1.7
18	2.7
25	3.4
40	5.5
75	21.5
100	56.3

Suggest how an impure sample of Compound X could be purified in a school laboratory. [1]

Recrystallise Compound X from distilled water. [1]

(Dissolve in boiling water, filter to remove any insoluble impurities, leave to cool then filter off the crystals and wash with a little cold distilled water before drying.)

(Underlying chemistry concepts can be found in 4.4 Intermolecular forces.)

(d) Compound X reacts with propan-1-ol when warmed in the presence of a sulfuric acid catalyst. The inorganic product obtained in this reaction is water.

(i) State the name of the type of reaction that is taking place. [1]

Condensation or esterification [1]

(Underlying chemistry concepts can be found in 10.2 Alcohols.)

(ii) Deduce the molecular formula of the organic product. [1]

$C_7H_6O_2 + C_3H_8O \rightarrow H_2O + C_{10}H_{12}O_2$ so the molecular formula is $C_{10}H_{12}O_2$ [1]

(Underlying chemistry concepts can be found in 10.2 Alcohols.)