

SI III Paper 3 Section A Data Response (7)

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 C₇H₆O₂. [2]

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

(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]

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

Temperature / °C	Solubility / g 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]

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

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