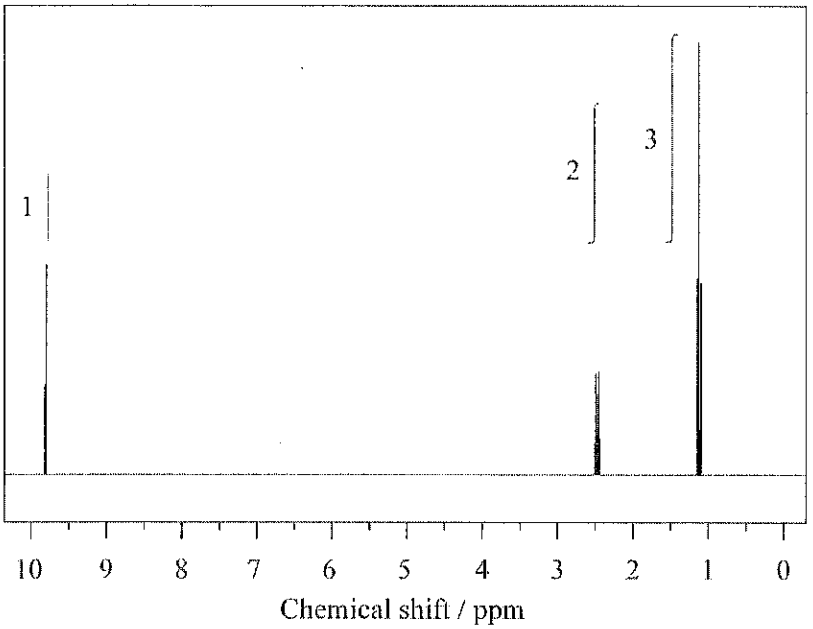
Topic 21 P2 Problems

A2. The ^{1}H NMR spectrum of **X** with molecular formula C_3H_6O is shown below.



(a) Deduce which of the following compounds is **X** and explain your answer. *[2]*

$CH_3–CO–CH_3$ $CH_3–CH_2–CHO$ $CH_2=CH–CH_2OH$

Compound:

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Explanation:

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(Question A2 continued)

(b) State and explain the splitting pattern you would expect in a high resolution spectrum for the peak at 1.1 ppm. *[2]*

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(c) The infrared and mass spectra for **X** were also recorded.

(i) Apart from absorptions due to C–C and C–H bonds, suggest **one** absorption, in wavenumbers, that would be present in the infrared spectrum. *[1]*

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(ii) Apart from absorptions due to C–C and C–H bonds, suggest **one** absorption, in wavenumbers, absent in this infrared spectrum but present in one of the other compounds shown in part (a). *[1]*

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(d) Suggest the formulas and m/z values of **two** species that would be detected in the mass spectrum. *[2]*

Species: . . . . . .

m/z: . . . . . .

Species: . . . . . .

m/z: . . . . . .

Option A — Modern analytical chemistry

A1. Butan-1-ol, butan-2-ol, 2-methylpropan-1-ol and 2-methylpropan-2-ol are four structural isomers with the molecular formula $C_4H_{10}O$.

(a) Details of the ^1H NMR spectra of two of these alcohols are given below.

Spectrum 1

Two peaks: A singlet at 1.3 ppm (relative to the TMS reference) with an integration trace of nine units, and another singlet at 2.0 ppm with an integration trace of one unit.

Spectrum 2

Four peaks: A doublet at 0.9 ppm with an integration trace of six units.
A complex pattern at 1.7 ppm with an integration trace of one unit.
A singlet at 2.1 ppm with an integration trace of one unit.
A doublet at 3.4 ppm with an integration trace of two units.

Consider the proton environments present in each of the alcohol molecules when answering the following questions.

(i) Identify which alcohol gives spectrum 1 and explain your answer by stating which hydrogen atoms in the molecule are responsible for each of the two peaks. *[3]*

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(ii) Deduce which alcohol gives spectrum 2. Explain which hydrogen atoms are responsible for the peaks at 0.9 ppm and 3.4 ppm and explain why both of these peaks are split into doublets. *[4]*

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(Question A1 continued)

(b) The mass spectrum of one of the alcohols shows peaks at *m/z* values of 74, 59 and 45.

(i) Deduce which **two** of the alcohols could produce this spectrum and identify the species responsible for the three peaks. *[4]*

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(ii) The spectrum also shows a significant peak at $m/z = 31$. Suggest which alcohol is responsible for this spectrum and deduce the species responsible for the peak at $m/z = 31$. *[2]*

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(c) Explain why the infrared spectra of all four alcohols are very similar. *[2]*

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