

# Solving structures with mass, IR and NMR spectra

Chemistry grades 11-12 (A Level · IB · Class 11-12) · Lab answers

These answers use the sample observations. Your colours and timings may differ slightly, so base your conclusions on the pattern of positive and negative results, and check predicted spectra against the reference tables.

**Level:** Chemistry grades 11-12 (A Level · IB · Class 11-12) · **Curriculum:** IB S3.2

## Question 1 Identify the liquids

A turns the dichromate from orange to green, so it is an oxidisable alcohol: **ethanol**. B gives an orange precipitate with 2,4-DNPH and no oxidation, so it is a ketone: **propanone**. C releases a gas with carbonate, so it is an acid: **ethanoic acid**.

## Question 2 Write the carbonate equation

$2\text{CH}_3\text{COOH} + \text{Na}_2\text{CO}_3 \rightarrow 2\text{CH}_3\text{COONa} + \text{H}_2\text{O} + \text{CO}_2$ . Atoms: C 4, H 8, O 6, Na 2 on both sides. The gas is **carbon dioxide**.

## Question 3 Predict the IR spectra

Ethanol (A): broad **O-H near  $3300\text{ cm}^{-1}$** . Propanone (B): strong **C=O near  $1715\text{ cm}^{-1}$**  and no O-H. Ethanoic acid (C): very broad **O-H from  $2500$  to  $3300\text{ cm}^{-1}$**  plus strong C=O near  $1710\text{ cm}^{-1}$ .

## Question 4 Predict the molecular ions

Ethanol  $\text{C}_2\text{H}_6\text{O}$ :  $24 + 6 + 16 = \mathbf{46}$ . Propanone  $\text{C}_3\text{H}_6\text{O}$ :  $36 + 6 + 16 = \mathbf{58}$ . Ethanoic acid  $\text{C}_2\text{H}_4\text{O}_2$ :  $24 + 4 + 32 = \mathbf{60}$ .

## Question 5 Predict proton NMR

Ethanol: **3 signals** (triplet 3H, quartet 2H, singlet 1H). Propanone: **1 signal**, a singlet of 6H. Ethanoic acid: **2 signals**, both singlets, 3H and 1H.

## Question 6 Predict $^{13}\text{C}$ NMR

Each liquid has **2 signals**. The C=O carbon is highest: about 205 ppm in propanone and about 178 ppm in ethanoic acid. In ethanol the highest is the C-O carbon, near 58 ppm.

### Question 7 Evaluate the method

2,4-DNPH reacts with **both aldehydes and ketones**, so it cannot tell them apart. A further test (Tollens' reagent) or an IR/NMR spectrum is needed. Running a known sample alongside as a control also improves reliability.