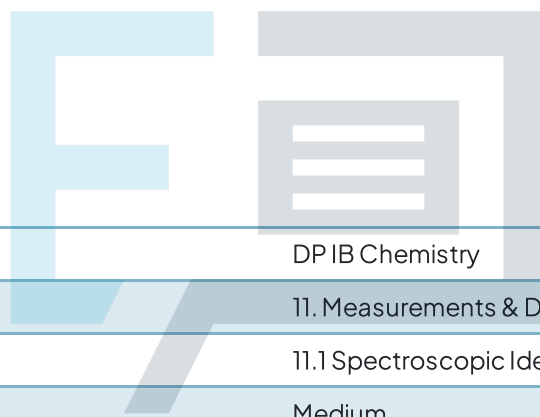




# 11.1 Spectroscopic Identification

## Mark Schemes



Course	DP IB Chemistry
Section	11. Measurements & Data Processes
Topic	11.1 Spectroscopic Identification
Difficulty	Medium

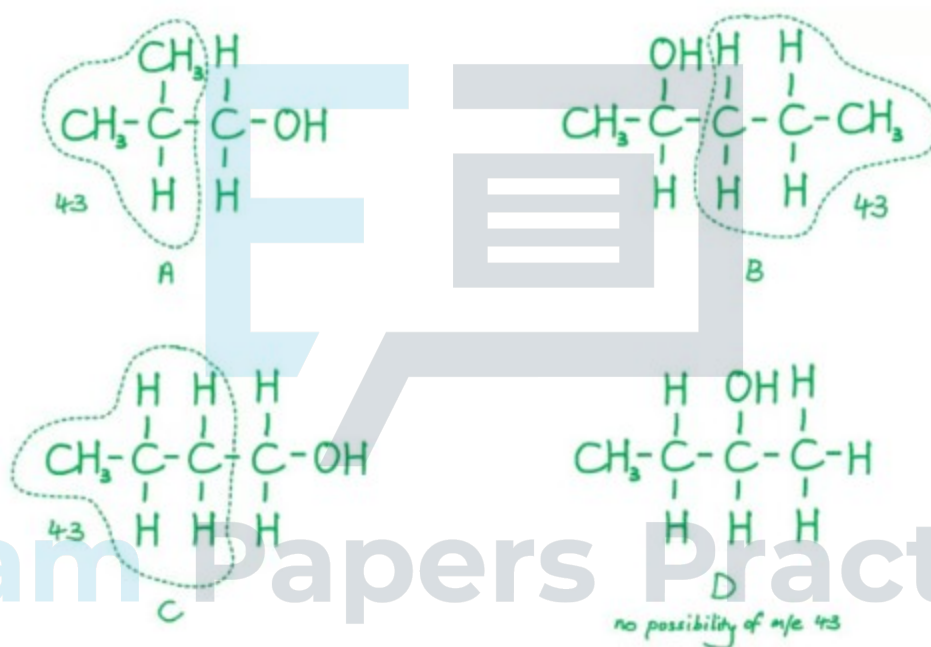
# Exam Papers Practice

To be used by all students preparing for DP IB Chemistry HL  
Students of other boards may also find this useful

1

The correct answer is **D** because:

- A line at  $m/e = 43$  corresponds to an ion with a mass of 43 for example; this is characteristic of a propyl or isopropyl fragment:
  - $[\text{CH}_3\text{CH}_2\text{CH}_2]^+$
  - $[(\text{CH}_3)_2\text{CH}]^+$
- Butan-2-ol cannot have a fragment at  $m/e = 43$  which can be seen when you draw the structures



**A** is incorrect because the fragment  $[(\text{CH}_3)_2\text{CH}]^+$  would produce an  $m/e$  peak at 43

**B** is incorrect because the fragment  $[\text{CH}_2\text{CH}_2\text{CH}_3]^+$  would produce an  $m/e$  peak at 43

**C** is incorrect because the fragment  $[\text{CH}_3\text{CH}_2\text{CH}_2]^+$  would produce an  $m/e$  peak at 43

**Exam tip:** always draw the displayed structures out and ring around likely fragments

2

The correct answer is **A** because:

- A line at  $m/e = 45$  corresponds to an ion with a mass of 45, which is a carboxylic acid group
  - $[\text{COOH}]^+$
- The only molecule with this functional group is option A

**B, C and D** are incorrect because none of the molecules contain the correct structure

3

The correct answer is **A** because:

- The peak representing the **molecular ion ( $M^+$  or  $M^+$ )** is called the **molecular ion peak**. Excluding any peaks due to the presence of heavier isotopes, this is the peak with the highest  $m/e$  ratio
  - This is the whole molecule just that has lost an electron
- Chlorine has two isotopes, so there are 5 possible molecular ions depending on the combinations of the two isotopes:

	$^{35}\text{Cl}$	$^{37}\text{Cl}$
C <sub>4</sub> H <sub>6</sub> plus	4	0
	3	1
	2	2
	1	3
	0	4

4

The correct answer is **B** because:

- The peak representing the **molecular ion ( $M^+$  or  $M^+$ )** is called the **molecular ion peak**. Excluding any peaks due to the presence of heavier isotopes, this is the peak with the highest  $m/e$  ratio
  - This is the whole molecule just that has lost an electron
- Bromine has two isotopes, so there are 2 possible molecular ions:
  - $M - (^{79}\text{Br}) m/e = 122$
  - $M + 2 - (^{81}\text{Br}) m/e = 124$

**A** is incorrect because isotopes' reactivities are almost identical

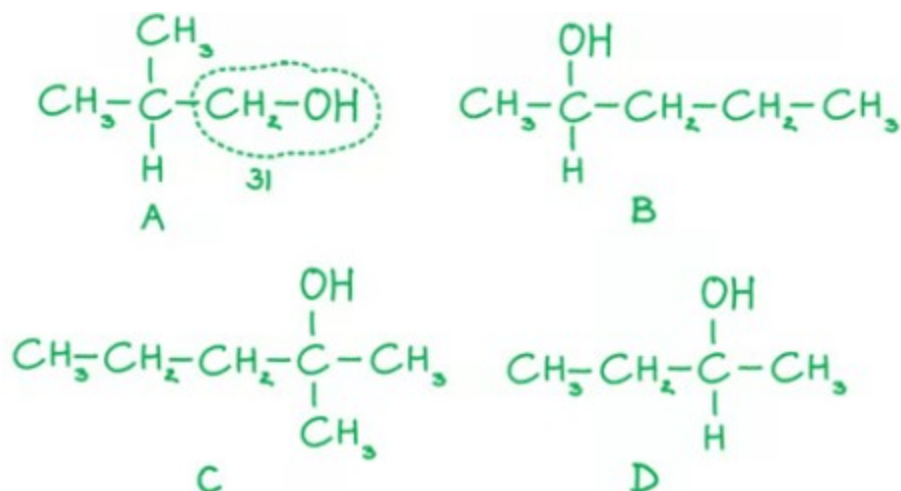
**C** is incorrect because the differences in the number of neutrons do not affect atomic radii

**D** is incorrect because the differences in the number of neutrons do not affect the ionisation energy

5

The correct answer is **A** because:

- A line at  $m/e = 31$  corresponds to an fragment with a mass of 31:
  - $[\text{CH}_2\text{OH}]^+$
- Molecule A is 2-methylpropan-1-ol will have a fragment at  $m/e = 31$  as it has a  $[\text{CH}_2\text{OH}]^+$  fragment

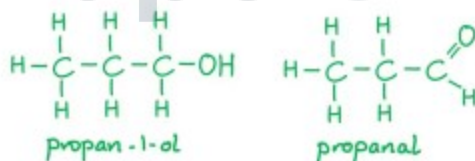


**Exam tip:** Always draw out the displayed structures to see more easily what fragments are possible

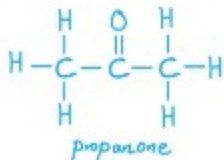
6

The correct answer is **A** because:

- A line at  $m/e = 29$  corresponds to a fragment with a mass of 29 which is an ethyl group:
  - $[C_2H_5]^+$
- The two compounds with this fragment are propan-1-ol and propanal

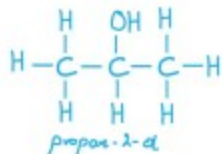


**B** is incorrect because propanone does not have the  $[C_2H_5]^+$  fragment





**C & D** are incorrect because propan-2-ol does not have the  $[C_2H_5]^+$  fragment



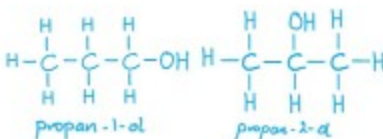
7

The correct answer is **D** because:

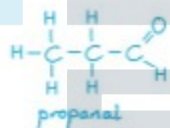
- The infrared spectrum shown in the question has a peak at 1680 – 1695 which means an aldehyde or ketone is present
- Propanone and propanal has a  $C=O$  in the structure giving this characteristic peak
- The absence of C-H peaks for aldehydes, means it can only be the ketone
- Comparing this to the data table in the question this matches the propanone structure



**A** and **B** are incorrect because propan-1-ol and propan-2-ol would not have a peak at 1680 – 1695 but have a broad peak at 3750 – 3200 corresponding to the alcohol group



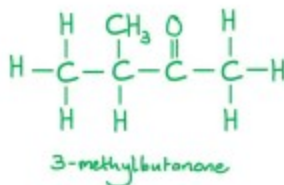
**C** is incorrect because propanal would have a peak at 1680 – 1695 but also a peak at 2900 – 2820 and 2775 – 2700 which is not present in this spectrum



8

The correct answer is **C** because:

- A line at  $m/e = 57$  corresponds to a fragment with a mass of 57 for example:
  - $[\text{C}_4\text{H}_9]^+$
  - $[\text{C}_2\text{H}_5\text{C}=\text{O}]^+$
- 3-methylbutanone will not have either of these fragments



**A** is incorrect because hexan-3-one has  $m/e$  at 57 due to the fragment ion  $[C_2H_5C=O]^+$

**B** is incorrect because pentan-3-one has  $m/e$  at 57 due to the fragment ion  $[C_2H_5C=O]^+$

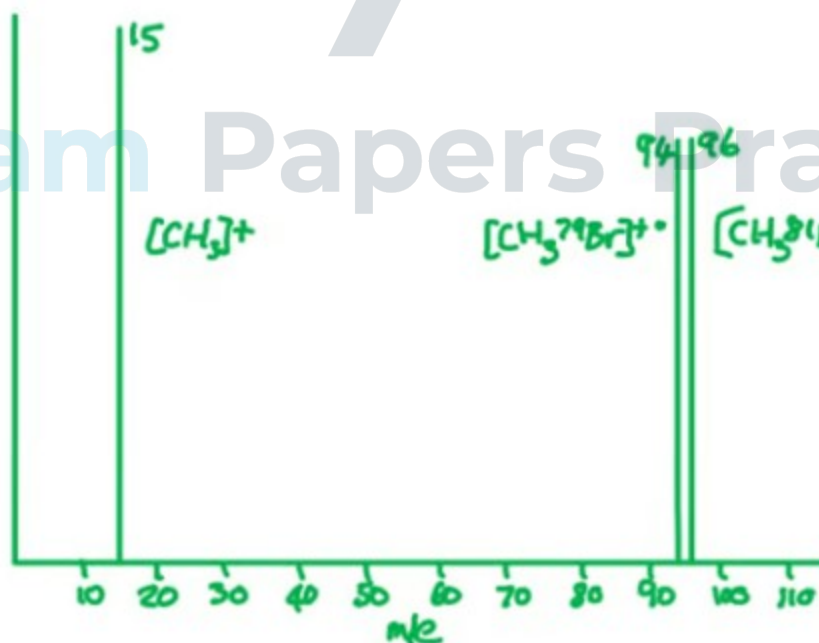
**D** is incorrect because butanone has  $m/e$  at 57 due to the fragment ion  $[C_2H_5C=O]^+$

9

### Model Answer 20 - CIE IAS 4.1 Analytical Techniques - MEDIUM

The correct answer is **D** because:

- Bromomethane will fragment to 3 peaks
  - $CH_3^{81}Br \rightarrow [CH_3^{81}Br]^+ + e^-$  at  $m/e$  96
  - $CH_3^{79}Br \rightarrow [CH_3^{79}Br]^+ + e^-$  at  $m/e$  94
  - $[CH_3Br]^+ \rightarrow [CH_3]^+ + Br$  at  $m/e$  15

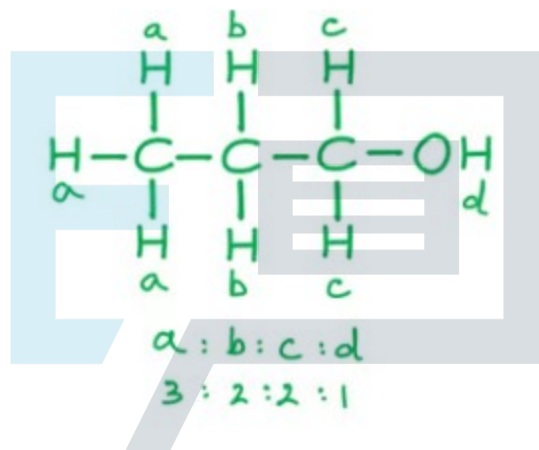




10

The correct answer is **A** because:

- The correct answer is **A** because: The NMR spectrum shows there are four different hydrogen environments
- The correct answer is **A** because: The ratio of the hydrogen nuclei in those environments is 2 : 1: 2 : 3
- The correct answer is **A** because: The only molecule this corresponds to is propan-1-ol



**B** is incorrect because propan-2-ol would show three peaks in the ratio 6:1:1

**C** is incorrect because methoxy ethane would show three peaks in the ratio 3:2:3

**D** is incorrect because pentan-2-one would should four peaks in the ratio 3:2:2:3