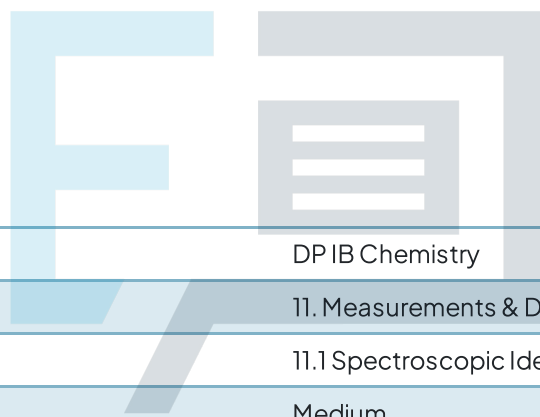




11.1 Spectroscopic Identification

Mark Schemes



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

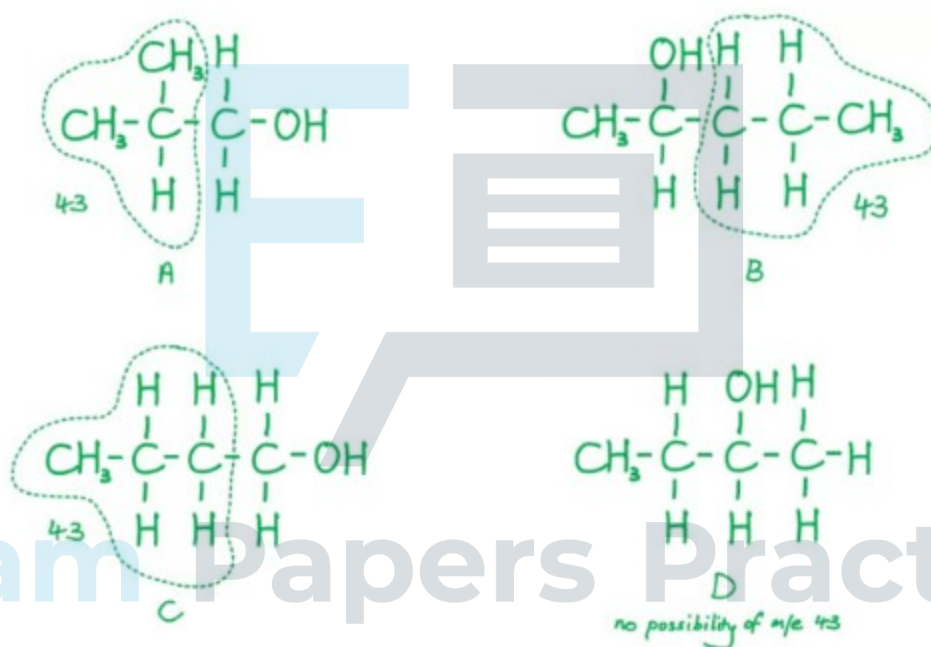
Exam Papers Practice

To be used by all students preparing for DP IB Chemistry SL
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}Cl	^{37}Cl
C ₄ H ₆ 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

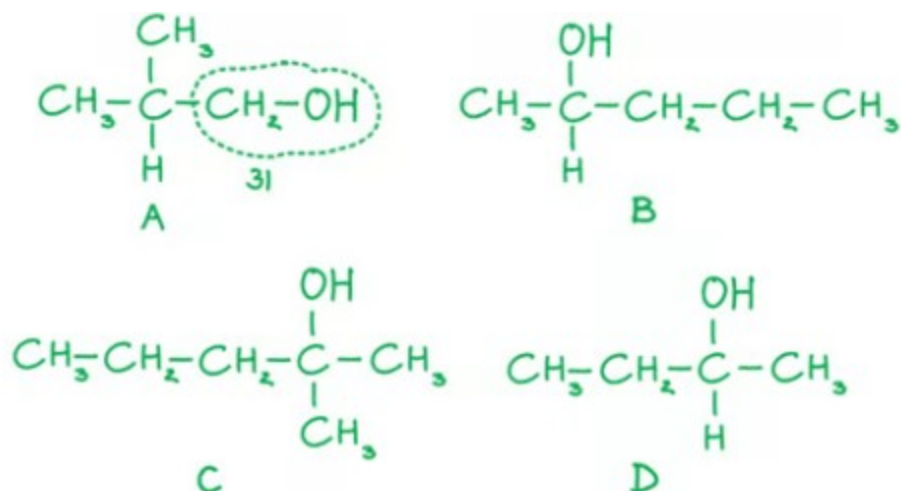
C is incorrect because the differences in the number of neutrons do not affect atomic radii

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

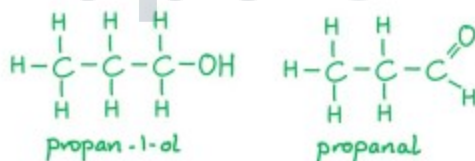


Exam tip: Always draw out the displayed structures to see more easily what fragments are possible

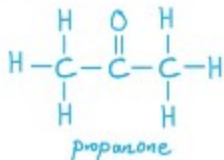
6

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

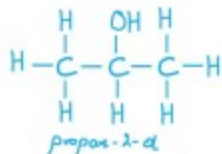


B is incorrect because propanone does not have the $[C_2H_5]^+$ fragment





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



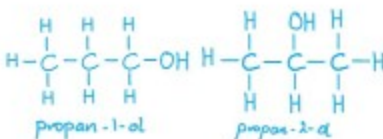
7

The correct answer is **D** because:

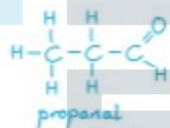
- The infrared spectrum shown in the question has a peak at 1680 – 1695 which means an aldehyde or ketone is present
- Propanone and propanal has a $C=O$ in the structure giving this characteristic peak
- The absence of $C-H$ peaks for aldehydes, means it can only be the ketone
- Comparing this to the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



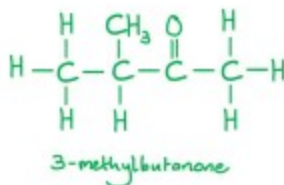
C is incorrect because propanal would have a peak at 1680 – 1695 but also a peak at 2900 – 2820 and 2775 – 2700 which is not present in this spectrum



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 $[C_2H_5C=O]^+$

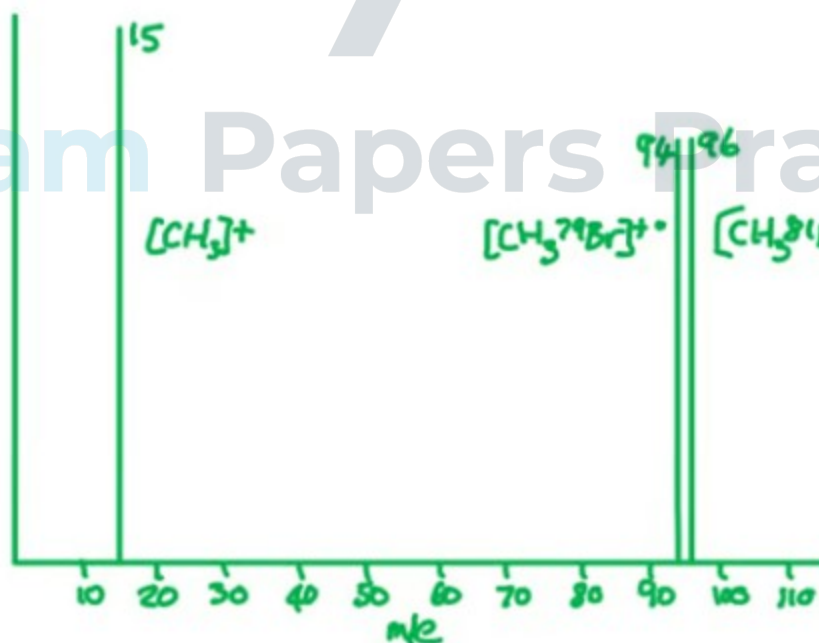
D is incorrect because butanone has m/e at 57 due to the fragment ion $[C_2H_5C=O]^+$

9

Model Answer 20 - CIE IAS 4.1 Analytical Techniques - MEDIUM

The correct answer is **D** because:

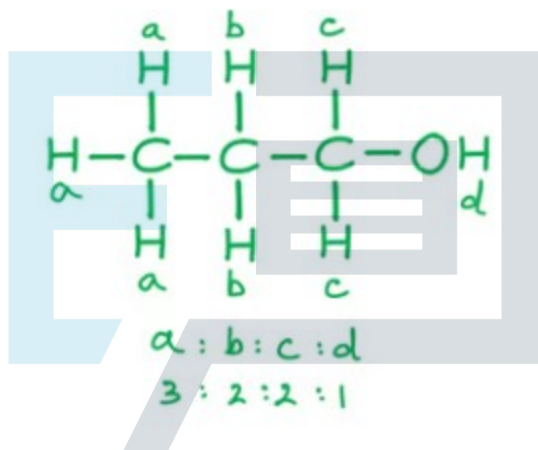
- Bromomethane will fragment to 3 peaks
 - $CH_3^{81}Br \rightarrow [CH_3^{81}Br]^+ + e^-$ at m/e 96
 - $CH_3^{79}Br \rightarrow [CH_3^{79}Br]^+ + e^-$ at m/e 94
 - $[CH_3Br]^+ \rightarrow [CH_3]^+ + Br$ at m/e 15



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