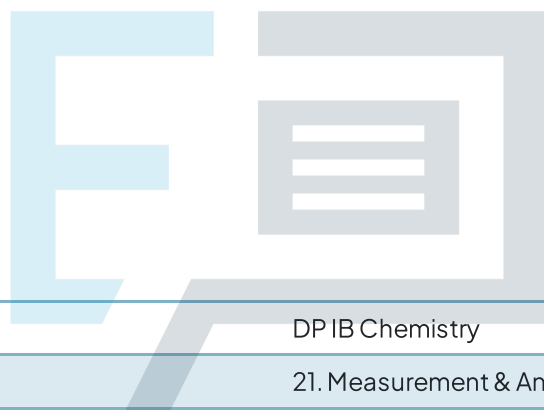




# 21.1 Spectroscopic Identification of Organic compounds

## Mark Schemes



Course	DP IB Chemistry
Section	21. Measurement & Analysis (HL only)
Topic	21.1 Spectroscopic Identification of Organic compounds
Difficulty	Medium

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 **C** because:

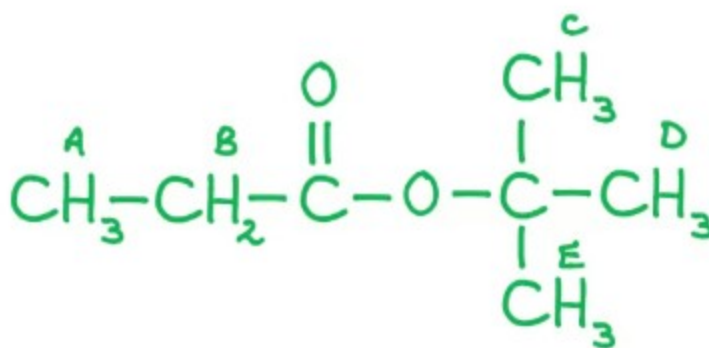
- X ray diffraction generates electron density maps of crystalline solids from which the location of atoms can be determined
- The separation between atoms is the bond length and their relative position to each other will give the bond angles

<b>A</b> is incorrect as	this technique is used to find relative molecular mass, molecular fragments and the existence of isotopes
<b>B</b> is incorrect as	this technique is used to find the types of bonds in a molecule
<b>D</b> is incorrect as	this technique is used to determine molecular structure

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# Exam Papers Practice

The correct answer is **B** because:



- The hydrogens labelled A have two neighbouring hydrogens
  - By the  $n + 1$  rule, this gives  $2 + 1 = 3$  and therefore a triplet
- The hydrogens labelled B have three neighbouring hydrogens
  - By the  $n + 1$  rule, this gives  $3 + 1 = 4$  and therefore a quartet
- The hydrogens labelled C, D and E all have no neighbouring hydrogens
  - By the  $n + 1$  rule, this gives  $0 + 1 = 1$  and therefore a singlet
- Option B is the only one that satisfies all of the splitting patterns

<b>A</b> is incorrect as	this answer has just used the groups that are labelled and not applied any NMR analysis techniques, e.g.  $\text{CH}_2 =$ doublet because of the number 2  $\text{CH}_3 =$ triplet because of the number 3
<b>C</b> is incorrect as	none of the hydrogens have a single neighbouring hydrogen to create a doublet splitting pattern
<b>D</b> is incorrect as	this answer has not recognised that the $\text{CH}_3$ groups containing hydrogens C, D and E are all equivalent / in the same chemical environment and therefore will all be part of the same singlet peak with a greater peak area ratio

3

The correct answer is **C** because:

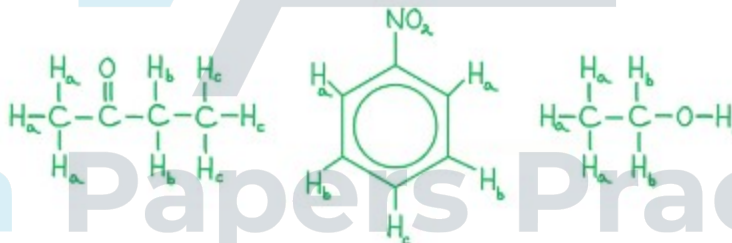
- The structure has 12 protons that are in the same chemical environment and produce one large signal that is far from proton signals typically found in organic molecules so it makes a suitable reference signal in a  $^1\text{H}$  NMR spectrum

<b>A</b> is incorrect as	TMS is very unreactive and its reactivity would not affect the NMR signal
<b>B</b> is incorrect as	TMS would have chain isomers, but this is not the reason it is used as a reference standard
<b>D</b> is incorrect as	TMS has a low boiling point, but this would not affect its use as a reference standard

4

The correct answer is **D** because:

- All three molecules have three unique proton environments (a, b, c)
- This is best seen from structural formulas:



<b>A, B &amp; C</b> are incorrect as	all three molecules have three peaks in NMR
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The correct answer is **C** because:

- There are three different proton environments which matches the three peaks on the spectrum
- You can also see the spectrum has a singlet, triplet and quartet which matches the splitting pattern for  $\text{CH}_3\text{COCH}_2\text{CH}_3$

<b>A</b> is incorrect as	this molecule has two proton environments as it is symmetrical about the central oxygen
<b>B</b> is incorrect as	this molecule has five unique proton environments
<b>D</b> is incorrect as	this molecule has four unique proton environments

# Exam Papers Practice