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CHEMISTRY

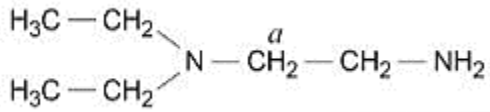
ORGANIC CHEMISTRY II

Level & Board	AQA (A-LEVEL)
TOPIC:	NMR SPECTROSCOPY
PAPER TYPE:	SOLUTION - 4
TOTAL QUESTIONS	10
TOTAL MARKS	/39

NMR Spectroscopy – 4

1.

(a)



- The ^{13}C NMR spectrum of this isomer will have **4 peaks**.
- The splitting pattern of the peak for the hydrogens labelled 'a' in the ^{1}H NMR spectrum is a **triplet**, because of the two hydrogen atoms on the adjacent carbon (CH_2CH_2 group).

(3)

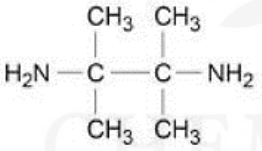
(b)

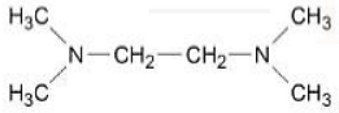
Structure of the isomer of $C_6H_{16}N_2$

(1)

(c)

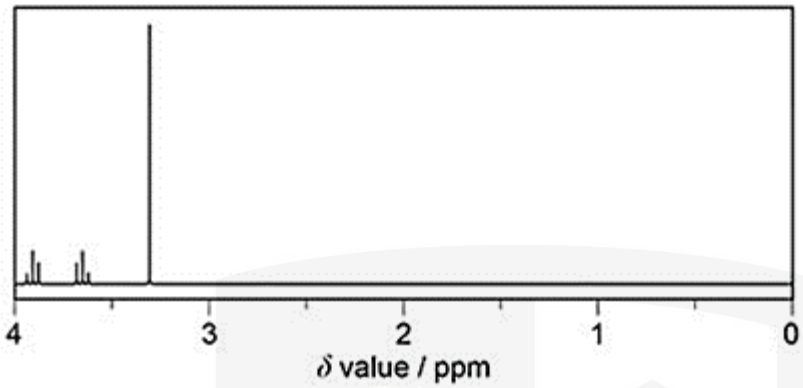
Following are the structure of the isomer of $C_6H_{16}N_2$ that contains two tertiary amine groups and has only two peaks in its ^{13}C NMR spectrum.





(1)

2.



The structure of Q is **CH_3-O-CH_2-CH_2-Cl**.

Integration Ratio:

- *The integration values correspond to a ratio of 2:2:3 when simplified.*

Analysis of Peaks:

Peak at 3.95 ppm:

- *Integration: 2 (suggesting 2 hydrogens)*
- ***Splitting pattern: Triplet***
  Explanation:
  This indicates that these two hydrogens are adjacent to a CH_2 group. So, this peak likely corresponds to Cl-CH_2, as chlorine is electronegative and can cause a downfield shift.

Peak at 3.65 ppm:

- *Integration: 2 (suggesting 2 hydrogens)*
- ***Splitting pattern: Triplet***
  Explanation:
  This indicates that these two hydrogens are adjacent to a CH_2 group. So, this peak likely corresponds to O-CH_2, as oxygen is electronegative and can cause a downfield shift.

Peak at 3.35 ppm:

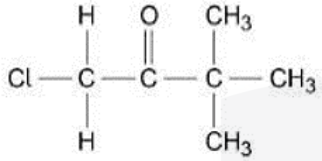
- *Integration: 3 (suggesting 3 hydrogens)*
- ***Splitting pattern: Singlet***
  Explanation:
  This indicates that these three hydrogens have no adjacent hydrogens. So, this peak likely corresponds to O-CH_3, as it has no neighboring hydrogens to split its signal.

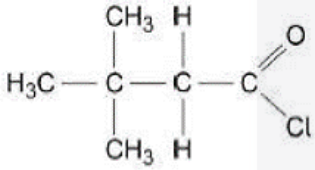
The structure of Q is **CH_3-O-CH_2-CH_2-Cl**.

(5)

3.

Structures of these two isomers are as:





(2)

4.

The splitting patterns for the labelled hydrogens are:

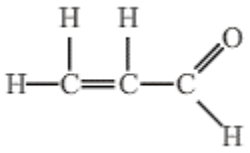
Hydrogens x on CH₃ :
Doublet

Hydrogen y on CH :
Quartet

Hydrogens z on CH₂ :
Doublet

(3)

5.



Hydrogen:

- *Propenal has three different types of hydrogen nuclei (hydrogen atoms or protons) each in a unique chemical environment:*
  The two hydrogens on the CH_2 group (vinyl group).
  The single hydrogen on the CH group (vinyl group).
  The single hydrogen on the CHO group (aldehyde group).

Three Peaks in the NMR Spectrum:

- *These different environments result in three distinct peaks in the ^1H NMR spectrum.*

Relative Areas Under the Peaks:

- *The relative areas of these peaks correspond to the number of hydrogen atoms in each environment:*
  - ***CH_2**: 2 hydrogens.*
  - ***CH**: 1 hydrogen.*
  - ***CHO**: 1 hydrogen.*

So

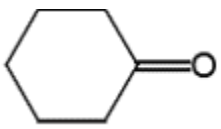
***Hydrogen nuclei** in three different environments.*
Relative areas** under the peaks: **2:1:1

(3)

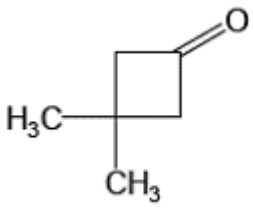
6.

(a)

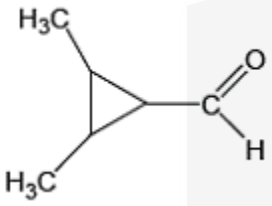
Structure for K



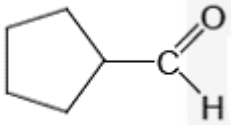
Or



Structure for L



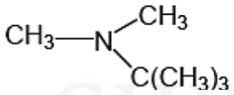
Or



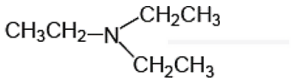
(2)

(b)

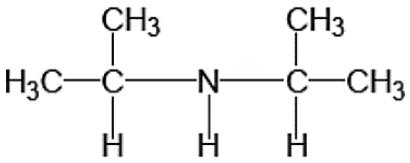
Structure for M



Or



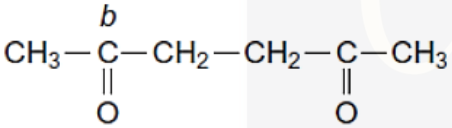
Structure for N



(2)

7. *N.m.r. spectroscopy can be used to study the structures of organic compounds.*

Compound K was studied using ^{13}C n.m.r. spectroscopy.



K

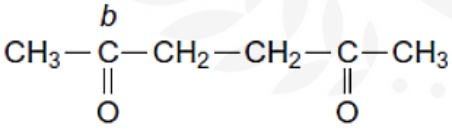
(a)

There are three number of peaks in the ^{13}C n.m.r. spectrum of K.

(1)

(b)

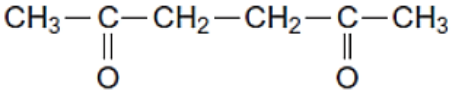
δ value of the peak is 190-220 (cm^{-1}) for the carbon labelled b. i.e. carbonyl group.



K

(1)

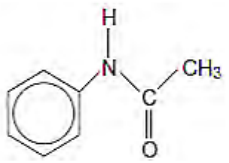
(c)



IUPAC name of K is **hexane-2,5-dione.**

(1)

8.



There are six number of peaks in the ^{13}C n.m.r. spectrum of N–phenylethanamide.

(1)

9.

High-resolution nuclear magnetic resonance (NMR) spectroscopy provides valuable information about a molecule through various means:

Chemical Shift (δ):

- *The chemical shift (δ) provides information about the type of proton or chemical environment.*
- *For example, a shift at 1.0 ppm might indicate aliphatic protons, while a shift at 7.0 ppm might indicate aromatic protons.*

Number of Peaks:

- *The number of peaks corresponds to the number of different types of protons or chemical environments in the molecule.*
- *For instance, if there are three peaks, it suggests the presence of three distinct proton environments.*

Relative Peak Areas:

- *The relative areas of the peaks give the relative number of protons contributing to each type.*
- *For instance, a peak with twice the area of another peak indicates twice as many protons in that environment.*

Splitting Patterns:

- *Splitting patterns arise due to spin-spin coupling between neighboring protons.*
- *The number of neighboring protons is revealed by the n+1 rule. For example, a doublet (2 peaks) suggests one neighboring proton, a triplet (3 peaks) suggests two neighboring protons, and so on.*

Deuterium Oxide (D_2O):

- *Deuterium oxide (D_2O) can be used to identify hydroxyl (OH) groups in the molecule.*
- *The exchange of hydrogen in OH groups with deuterium in D_2O leads to disappearance of the OH peak in the spectrum.*

(7)

10.

Purpose of $CDCl_3$ or CCl_4 Solvent:

$CDCl_3$ or CCl_4 Solvent:

- **Purpose:** Used as a solvent in ^1H NMR spectroscopy.
- **Explanation:**
  - **$CDCl_3$:** Polar covalent molecule, suitable for dissolving polar organic compounds.
  - **CCl_4:** Nonpolar, making it a good solvent for nonpolar organic molecules.
- **Inert:** Both solvents are inert, so they are unlikely to react with the sample, ensuring the integrity of the chemical analysis.

Purpose of TMS as Reference:

Tetramethylsilane (TMS) as Reference:

- **Purpose:** Used as a reference or calibration standard in ^1H NMR spectroscopy.

- **Explanation:**
  - **Reference/Peak at 0 ppm:**
    TMS provides a sharp single peak at 0 ppm, serving as a reference for chemical shift measurements.
  - **Equivalent Hydrogens:**
    TMS has 12 equivalent hydrogens, resulting in one signal, simplifying the spectrum interpretation.
  - **Signal Away from Others:**
    TMS signal is far from other typical hydrogen signals, ensuring it doesn't interfere with the signals of interest.
  - **Easy to Remove:**
    TMS is volatile with a low boiling point, making it easy to remove from the sample after the NMR experiment.

(6)

I am Sorry !!!!!

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