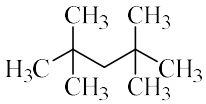
Structural Elucidation of 2,2,3,3-Tetramethylbutane NMR, IR and Mass spectral data

2,2,3,3-Tetramethylbutane (C_8H_{18}) is a highly branched alkane. To elucidate its structure, we can use a combination of IR, NMR, and MS



Infrared (IR) Spectroscopy

Since 2,2,3,3-tetramethylbutane is a saturated alkane, its IR spectrum will show characteristic peaks of C-H bonds in alkanes.

C-H Stretch (sp^3 hybridized): A series of peaks between 2850-2960 cm^{-1}, typical of the C-H stretching in methyl (CH_3) groups.

C-H Bending (Methyl group): Medium intensity bands around 1375-1475 cm^{-1} corresponding to the bending vibrations of the methyl (CH_3) groups.

Overall, the IR spectrum suggests a completely saturated hydrocarbon structure without any polar functional groups or unsaturation.

1H NMR (Proton NMR)

In the ^1H NMR spectrum, we would observe a single, sharp singlet around δ 0.85-1.0. This corresponds to the 18 equivalent protons of the six methyl groups. All the methyl groups are chemically equivalent due to the high symmetry of the molecule, resulting in just one signal.

Mass Spectrometry (MS)

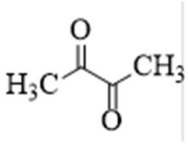
● Molecular Ion Peak (M^+): The molecular ion peak should be observed at m/z 114, which corresponds to the molecular weight of 2,2,3,3-tetramethylbutane (114 g/mol).

● Fragmentation Pattern:

m/z 57: This peak is due to the loss of a neutral methyl radical (CH_3), resulting in a tertiary butyl cation ($C_4H_9^+$), which is a common and stable fragment.

m/z 43: This peak corresponds to the propyl cation ($C_3H_7^+$), another common fragmentation product in branched alkanes.

Structural Elucidation of Butane-2,3-dione NMR, IR and Mass spectral data



Butane-2,3-dione is a diketone, with the structure consisting of two adjacent carbonyl groups (-C=O) on the 2nd and 3rd carbon atoms of the butane chain. This compound can be analyzed using various spectroscopic techniques like IR, NMR and MS to confirm its structure.

Infrared (IR) Spectroscopy

The IR spectrum of butane-2,3-dione will exhibit key absorption bands related to the carbonyl functional groups and C-H bonds.

Carbonyl Stretch (C=O): Strong absorption bands are expected around 1725-1750 cm^{-1} due to the symmetric and asymmetric stretching of the carbonyl (C=O) groups. Since this is a diketone, there will be two carbonyl peaks, but they might overlap or appear as a single broad peak depending on their symmetry.

C-H Stretch (Alkyl groups): Peaks around 2850-2960 cm^{-1} corresponding to the C-H stretching vibrations of the alkyl groups (CH_3) attached to the carbon backbone.

C-H Bending (Methyl group): Medium intensity bands around 1375-1450 cm^{-1}, characteristic of the bending vibrations of the methyl groups (CH_3).

These IR absorption patterns confirm the presence of two carbonyl groups and alkyl groups, indicating a diketone structure.

1H NMR (Proton NMR)

Methyl Protons (CH_3 groups): The two methyl groups attached to the carbonyl carbons (CH_3-C=O) will appear as a singlet around δ 2.1-2.4 ppm. Since these two methyl groups are adjacent to carbonyl groups, they are slightly downfield.

The spectrum is relatively simple due to the high symmetry of the molecule, resulting in just one signal for the two equivalent methyl groups.

Mass Spectrometry (MS)

Molecular Ion Peak (M^+): The molecular ion peak is expected at m/z 86, corresponding to the molecular weight of butane-2,3-dione (86 g/mol).

Fragmentation Pattern:

m/z 43: A common peak, resulting from the loss of one carbonyl group (-CO), leaving behind a methyl cation (CH_3^+) or acetyl fragment.

m/z 29: This corresponds to the loss of an ethyl group ($C_2H_5^+$), a common fragmentation in smaller alkyl chains. The molecular ion peak and the fragmentation pattern support the structure of butane-2,3-dione as a small alkyl chain with two adjacent carbonyl groups.

Structural Elucidation of Propanoic acid NMR, IR and Mass spectral data

Propanoic acid **(CH_3-CH_2-COOH)** is a simple carboxylic acid, and its structure can be elucidated using multiple spectroscopic techniques such as IR, NMR and MS. Here is an integrated description of its spectral data.

Infrared (IR) Spectroscopy

O-H Stretch (Hydroxy group): A broad, strong band around 2500-3300 cm^{-1} indicates the presence of the carboxylic acid (O-H stretch) group, characteristic of hydrogen-bonded carboxylic acids.

C=O Stretch (Carbonyl group): A strong, sharp peak around 1700-1725 cm^{-1} confirms the presence of a carbonyl (C=O) group, typical for carboxylic acids.

C-O Stretch: A band around 1200-1300 cm^{-1} represents the C-O stretch of the carboxyl group.

C-H Stretch (Aliphatic chain): Peaks between 2850-2960 cm^{-1} indicate the C-H stretching from the methyl (CH_3) and methylene (CH_2) groups.

1H NMR (Proton NMR):

Methyl Protons (CH_3 group): A triplet at δ 1.0-1.2 ppm due to the three protons of the CH_3 group, which are adjacent to a CH_2 group.

Methylene Protons (CH_2 group): A quartet around δ 2.2-2.4 ppm arises from the two protons of the CH_2 group adjacent to the CH_3 group and the carbonyl carbon (COOH).

Carboxylic Proton (COOH group): A broad singlet around δ 10-12 ppm corresponds to the acidic proton of the carboxylic acid group.

Mass Spectrometry (MS)

Molecular Ion Peak (M^+): The molecular ion peak at m/z 74 confirms the molecular weight of propanoic acid (74 g/mol).

Fragmentation Patterns:

m/z 45: This peak is attributed to the loss of a carboxyl group (COOH, 29 mass units), yielding the ethyl fragment ($CH_3CH_2^+$).

m/z 29: This peak is due to the ethyl cation ($CH_3CH_2^+$), confirming the presence of the aliphatic chain.

Structural Elucidation of Methyl propionate NMR, IR and Mass spectral data

Methyl propionate **(CH_3-CH_2-$COOCH_3$)** is an ester with the molecular formula $C_4H_8O_2$. It consists of a propionate group ($CH_3CH_2COO–$) attached to a methyl group (-CH_3). The structure will be elucidated using techniques such as IR, NMR and MS spectroscopy.

Infrared (IR) Spectroscopy

The IR spectrum of methyl propionate will show characteristic absorption bands for the ester functional group as well as alkyl groups:

C=O Stretch (Ester Carbonyl): A strong, sharp absorption band around 1735-1750 cm^{-1}, typical of the carbonyl stretch in esters.

C-O Stretch (Ester Bond): A medium-intensity peak between 1050-1300 cm^{-1}, corresponding to the C-O single bond in the ester.

C-H Stretch (Alkyl Groups): Absorption bands between 2850-3000 cm^{-1}, corresponding to the C-H stretching vibrations of the methyl (CH_3) and methylene (CH_2) groups.

C-H Bending (Methyl Group): Medium peaks around 1370-1450 cm^{-1}, typical for C-H bending in the CH_3 group.

1H NMR (Proton NMR)

Methoxy Protons (-OCH_3 group): The methyl group attached to the oxygen atom (-OCH_3) will appear as a singlet around δ 3.6-3.7 ppm. The singlet nature is due to the absence of neighbouring protons to couple with.

Methylene Protons (CH_2 adjacent to C=O): The methylene protons (CH_2) adjacent to the carbonyl group (C=O) will appear as a triplet around δ 2.2-2.4 ppm. The triplet arises due to coupling with the neighbouring CH_3 group.

Methyl Protons (CH_3 group): The terminal methyl group (CH_3) of the propionate chain will show up as a quartet around δ 1.0-1.2 ppm, caused by coupling with the neighbouring methylene group (CH_2).

Mass Spectrometry (MS)

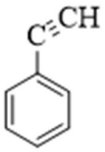
Molecular Ion Peak (M^+): The molecular ion peak should be observed at m/z 88, corresponding to the molecular weight of methyl propionate (88 g/mol).

Fragmentation Pattern:

m/z 59: A peak corresponding to the loss of the methoxy group (-OCH_3), leaving behind a propionyl fragment ($CH_3CH_2CO^+$).

m/z 43: This peak is due to the formation of the acylium ion ($CH_3CH_2C^+$), a common fragment in esters. The molecular ion peak at m/z 88 and the characteristic fragment ions provide strong evidence for the structure of methyl propionate.

Structural Elucidation of Phenylacetylene NMR, IR and Mass spectral data



Phenylacetylene is an aromatic alkyne, consisting of a benzene ring attached to an acetylene group. The combination of aromatic and alkyne functional groups can be elucidated using various spectroscopic techniques such as IR, NMR and MS spectroscopy.

Infrared (IR) Spectroscopy

Phenylacetylene contains both an aromatic ring and an alkyne group, each of which contributes characteristic absorption bands in the IR spectrum:

Alkyne (C≡C) Stretch: A strong, sharp peak around 2100-2200 cm^{-1} due to the stretching of the carbon-carbon triple bond (C≡C).

Terminal Alkyne (C-H) Stretch: A sharp peak around 3300 cm^{-1} characteristic of the stretching vibration of the terminal alkyne C-H bond. This peak is usually sharper and more intense than typical alkane C-H stretches.

Aromatic C-H Stretch: Peaks between 3000-3100 cm^{-1}, characteristic of the C-H stretching in the aromatic ring.

Aromatic C=C Stretch: Weak to medium-intensity peaks between 1500-1600 cm^{-1}, which correspond to the C=C stretching vibrations in the benzene ring.

These peaks indicate the presence of both an aromatic system and a terminal alkyne group.

1H NMR (Proton NMR)

Alkyne Proton (C≡C-H): The proton attached to the terminal alkyne group (C≡CH) will appear as a sharp singlet around δ 3.0-3.2 ppm. This signal is downfield due to the electronegative nature of the sp-hybridized carbon in the alkyne.

Aromatic Protons: The five protons on the phenyl ring (benzene) will show up between δ 7.2-7.5 ppm as a multiplet. These protons are in different electronic environments due to the influence of the alkyne group, leading to complex splitting patterns that may appear as overlapping signals.

Mass Spectrometry (MS)

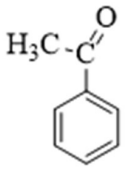
Molecular Ion Peak (M^+): The molecular ion peak would be observed at m/z 102, corresponding to the molecular weight of phenylacetylene (102 g/mol).

Fragmentation Pattern:

m/z 77: A common peak resulting from the loss of the acetylene group (-C≡CH), which corresponds to the phenyl cation ($C_6H_5^+$).

m/z 51 and m/z 39: Additional peaks can be seen due to further fragmentation of the phenyl group or the loss of small fragments such as acetylene or benzene. This fragmentation pattern supports the presence of both an aromatic ring and an alkyne group in the molecule.

Structural Elucidation of Acetophenone NMR, IR and Mass spectral data



Acetophenone ($C_6H_5COCH_3$) is a simple aromatic ketone and its structure can be elucidated using several spectroscopic techniques, including IR, NMR, and MS spectroscopy.

Infrared (IR) Spectroscopy

C=O Stretch (Carbonyl group): A strong absorption band around 1680-1700 cm^{-1} indicates the presence of a carbonyl (C=O) group, typical for ketones.

C-H Stretch (Aromatic ring): Peaks in the region of 3000-3100 cm^{-1} suggest aromatic C-H stretching, characteristic of the phenyl group.

C-H Stretch (Methyl group): Peaks near 2850-2960 cm^{-1} correspond to the C-H stretching of the methyl group (CH_3).

C=C Stretch (Aromatic ring): Weak to medium-intensity bands around 1600 cm^{-1} and 1500 cm^{-1} indicate the presence of an aromatic ring.

1H NMR (Proton NMR):

Methyl Protons (CH_3 group): A singlet around δ 2.6-2.7 ppm is attributed to the three equivalent protons of the methyl group (CH_3) attached to the carbonyl carbon.

Aromatic Protons (C_6H_5 group): A set of multiplets between δ 7.2-7.8 ppm arises from the five aromatic protons of the phenyl ring (C_6H_5), showing characteristic splitting patterns based on their positions (ortho, meta, para) relative to the carbonyl group.

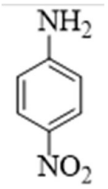
Mass Spectrometry (MS)

Molecular Ion Peak (M^+): The molecular ion peak at m/z 120 confirms the molecular weight of acetophenone (120 g/mol).

Base Peak: A base peak at m/z 105 is due to the loss of a methyl group (CH_3, 15 mass units), yielding the phenyl ketone fragment ($C_6H_5CO^+$).

Other Fragmentation Patterns: Additional peaks such as m/z 77 (benzyl cation, $C_6H_5^+$) and m/z 43 (acetyl cation, CH_3CO^+) support the presence of the phenyl group and the carbonyl methyl fragment.

Structural Elucidation of p-Nitroaniline NMR, IR and Mass spectral data



p-Nitroaniline is an aromatic compound with a nitro group (-NO_2) at the para position relative to an amino group (-NH_2) on a benzene ring. The structure of p-nitroaniline can be elucidated using IR, NMR and MS spectroscopy.

Infrared (IR) Spectroscopy

The IR spectrum of p-nitroaniline provides clear evidence for the presence of both the nitro group and the amino group, as well as the aromatic ring:

N-H Stretch (Amino Group, -NH_2): A pair of broad absorption bands in the range 3300-3500 cm^{-1} due to asymmetric and symmetric stretching of the N-H bonds in the amino group.

NO_2 Stretch (Nitro Group): The nitro group (-NO_2) exhibits two characteristic strong bands:

Asymmetric Stretch: A strong band around 1510-1550 cm^{-1}.

Symmetric Stretch: Another strong band between 1330-1370 cm^{-1}.

Aromatic C=C Stretch: Peaks in the range of 1450-1600 cm^{-1} correspond to the stretching vibrations of the C=C bonds in the aromatic ring.

C-H Stretch (Aromatic Ring): Peaks around 3050-3100 cm^{-1} due to the C-H stretching vibrations of the aromatic system.

These features confirm the presence of both nitro and amino groups on the benzene ring.

1H NMR (Proton NMR)

Aromatic Protons: The protons on the benzene ring (C_6H_6) will appear as two doublets in the range of δ 6.5-8.0 ppm. These doublets arise due to the splitting from the neighbouring protons, with the typical coupling constant for an aromatic system. The splitting is indicative of the para-substitution pattern of the nitro and amino groups on the ring, with two sets of equivalent protons.

Amino Protons (NH_2 group): The protons of the -NH_2 group appear as a singlet around δ 4.5-5.5 ppm. This signal may be broad due to the ex-changeable nature of the amino protons.

Mass Spectrometry (MS)

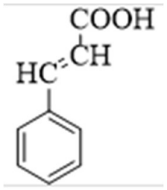
Molecular Ion Peak (M^+): The molecular ion peak is observed at m/z 138, which corresponds to the molecular weight of p-nitroaniline (138 g/mol).

Fragmentation Pattern:

m/z 121: This peak corresponds to the loss of a hydroxyl group (-OH) from the nitro group.

m/z 65: A significant fragment due to the presence of the nitro group or a resonance-stabilized fragment of the benzene ring.

Structural Elucidation of Cinnamic acid NMR, IR and Mass spectral data



Cinnamic acid is an α, β unsaturated aromatic Carboxylic acid. The structure of Cinnamic acid can be elucidated using IR, NMR and MS spectroscopy.

Infrared (IR) Spectroscopy

$C{=}O$ stretch: A strong absorption around 1693 cm^{-1} indicates the presence of a carbonyl group in the carboxylic acid.

$O{-}H$ stretch: A broad absorption band in the range of 3200−2500cm^{-1} is characteristic of the hydrogen-bonded $O{-}H$ group in a carboxylic acid.

$C{=}C$ stretch: An absorption around 1622cm^{-1} corresponds to the stretching of the C=C in the alkene portion of the molecule.

Aromatic C-H stretch: Absorption bands above 3000 cm^{-1} confirm the presence of aromatic C-H bonds.

1H NMR (Proton NMR)

Olefinic protons: Two doublets appear at δ 6.47 and δ7.81 ppm.

Aromatic protons: Signals at δ 7.4-7.6 ppm region represent the protons on the mono substituted benzene ring.

Carboxylic acid proton: A very broad singlet appears at a low field δ 12.20 ppm representing the acidic proton, which is highly deshielded and has a variable chemical shift depending on the solvent and concentration.

Mass Spectrometry (MS):

Molecular ion M+: The molecular ion peak at (m/z=148) corresponds to the molecular weight of cinnamic acid ($C_9H_8O_2$).

Fragmentation: The molecular ion can fragment into characteristic ions, such as a fragment corresponding to the loss of the carboxyl group $[M\text{-}45]^+$, loss of (COOH) or other fragments resulting from the cleavage of the molecule.