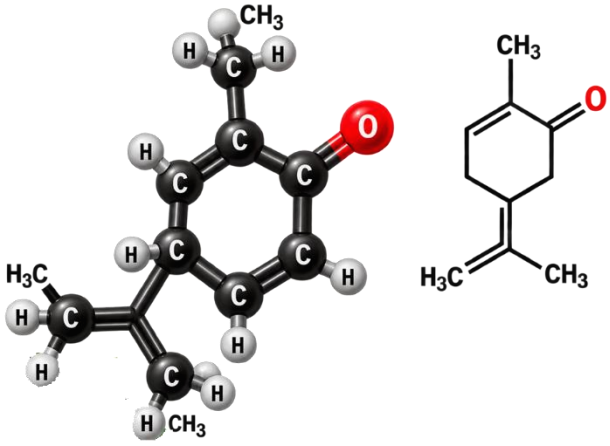
Structure Elucidation by Spectroscopic Techniques

Carvone

Introduction



- Carvone is a monocyclic monoterpene ketone.
- It is commonly found in caraway oil and spearmint oil.
- Molecular formula of carvone is $C_{10}H_{14}O$.

Structure Elucidation by UV Spectroscopy

Important Observation

- Carvone contains a conjugated carbonyl group.
- Conjugation causes absorption in the ultraviolet region.

UV Spectrum

- Absorption maximum appears around 230–250 nm.

Interpretation

- The absorption indicates the presence of an α,β-unsaturated ketone system.
- The UV spectrum confirms the conjugated double bond attached to the carbonyl group.

Structure Elucidation by IR Spectroscopy

Important Absorption Bands

Functional Group	IR Absorption
Carbonyl (C=O)	1670–1715 cm^{-1}
Alkene (C=C)	1600–1650 cm^{-1}
C-H Stretch	2850–3000 cm^{-1}

Interpretation

- A strong peak near 1670 cm^{-1} indicates a conjugated ketone.
- Peaks near 1600 cm^{-1} indicate carbon-carbon double bonds.

Structure Elucidation by Mass Spectrometry (MS)

Molecular Ion Peak

- Molecular ion peak appears at m/z 150.

Interpretation

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- The peak confirms molecular weight of 150.
- Fragmentation pattern supports the presence of a monoterpene ketone structure.

Structure Elucidation by ^{1}H NMR

Important Signals

- Olefinic protons appear between δ 5.5–7.0 ppm.
- Methyl protons appear around δ 1.0–2.0 ppm.
- Ring protons appear between δ 2.0–3.0 ppm.

Interpretation

- Signals confirm alkene and methyl groups in the molecule.

Structure Elucidation by ^{13}C NMR

Important Signals

- Carbonyl carbon appears around δ 190–210 ppm.
- Alkene carbons appear around δ 120–160 ppm.
- Methyl carbons appear around δ 15–30 ppm.

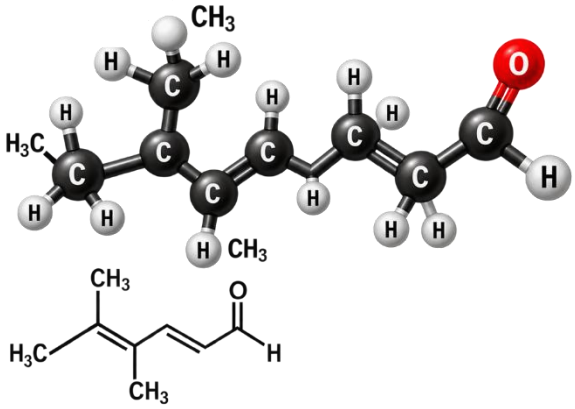
Interpretation

- Presence of ketone carbon and double bond carbons confirms carvone structure.

First Hope

Citral

Introduction



- Citral is an acyclic monoterpene aldehyde.
- It occurs mainly in lemongrass oil and citrus oils.
- Molecular formula of citral is $C_{10}H_{16}O$.

Structure Elucidation by UV Spectroscopy

Important Observation

- Citral contains conjugated double bonds and an aldehyde group.

UV Spectrum

- Absorption maximum occurs around 230–240 nm.

Interpretation

- The absorption indicates a conjugated aldehyde system.

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Structure Elucidation by IR Spectroscopy

Important Absorption Bands

Functional Group	IR Absorption
Aldehyde C=O	1680–1740 cm^{-1}
Aldehyde C-H	2720–2820 cm^{-1}
Alkene C=C	1600–1650 cm^{-1}

Interpretation

- Strong carbonyl peak confirms aldehyde group.
- Aldehyde hydrogen peak is characteristic of citral.

Structure Elucidation by Mass Spectrometry (MS)

Molecular Ion Peak

- Molecular ion peak appears at m/z 152.

Interpretation

- The peak confirms molecular weight of citral.
- Fragmentation pattern indicates presence of aldehyde and unsaturated chain.

Structure Elucidation by ^{1}H NMR

Important Signals

- Aldehyde proton appears around δ 9–10 ppm.
- Olefinic protons appear between δ 5–7 ppm.
- Methyl protons appear around δ 1–2 ppm.

Interpretation

- Presence of aldehyde proton clearly confirms aldehyde functionality.

Structure Elucidation by ^{13}C NMR

Important Signals

- Aldehyde carbon appears around δ 190–200 ppm.
- Alkene carbons appear around δ 120–160 ppm.
- Methyl carbons appear around δ 15–30 ppm.

Interpretation

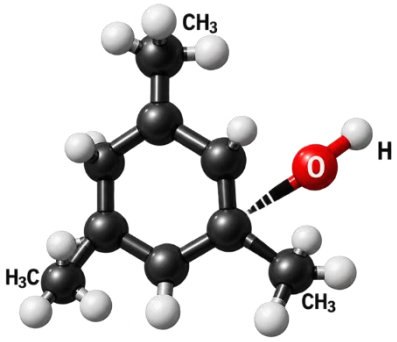
- Signals confirm aldehyde carbon and conjugated double bonds.

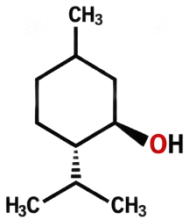
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Menthol

Introduction





- Menthol is a cyclic monoterpene alcohol.
- It is the major constituent of peppermint oil.
- Molecular formula of menthol is $C_{10}H_{20}O$.

Structure Elucidation by UV Spectroscopy

Important Observation

- Menthol does not contain conjugated double bonds.
- Therefore, very weak ultraviolet absorption is observed.

Interpretation

- Lack of strong UV absorption indicates absence of conjugated systems.

Structure Elucidation by IR Spectroscopy

Important Absorption Bands

Functional Group	IR Absorption
O-H Stretch	3200–3600 cm^{-1}
C-O Stretch	1050–1260 cm^{-1}
C-H Stretch	2850–3000 cm^{-1}

Interpretation

- Broad O-H peak confirms alcohol group.
- C-O stretching confirms alcoholic functionality.

Structure Elucidation by Mass Spectrometry (MS)

Molecular Ion Peak

- Molecular ion peak appears at m/z 156.

Interpretation

- Molecular weight confirms menthol structure.
- Characteristic fragmentation pattern supports cyclic alcohol nature.

Structure Elucidation by ^1H NMR

Important Signals

- Hydroxyl proton appears around δ 1–5 ppm.
- Methyl protons appear around δ 0.8–1.2 ppm.

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- Ring protons appear between δ 1–3 ppm.

Interpretation

- Signals confirm cyclohexane ring and alcohol group.

Structure Elucidation by ^{13}C NMR

Important Signals

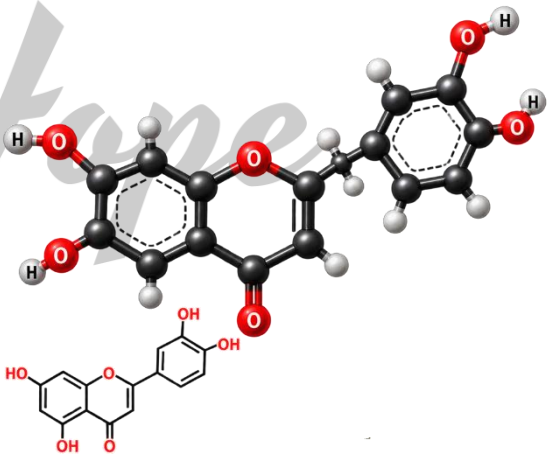
- Carbon attached to hydroxyl group appears around δ 60–80 ppm.
- Methyl carbons appear around δ 15–30 ppm.
- Ring carbons appear around δ 20–50 ppm.

Interpretation

- Carbon bearing hydroxyl group confirms menthol structure.
- Remaining signals support saturated cyclic monoterpene skeleton.

Luteolin

Introduction



- Luteolin is a naturally occurring flavonoid.
- It is commonly found in parsley, celery, thyme, and many medicinal plants.
- The molecular formula of luteolin is $C_{15}H_{10}O_6$.

Structure Elucidation by UV Spectroscopy

Important Observation

- Luteolin contains an aromatic flavone nucleus.
- It has conjugated double bonds and phenolic hydroxyl groups.

UV Spectrum

- Band I appears around 330–350 nm.
- Band II appears around 250–270 nm.

Interpretation

- Band I indicates the cinnamoyl system of ring B.
- Band II indicates the benzoyl system of ring A.
- These bands confirm the flavone structure.

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