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Solving a Structure

Based on IR and NMR

Spectra Solving an

Unknown Organic

Structure using NMR,

IR, and MS Structure

Elucidation from

Spectroscopic Data in

Organic Chemistry

~~Organic Spectroscopy~~

~~Problem Series (Part 1) ||~~

~~Structure Determination~~

~~by Using NMR IR~~

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~~Mass|| Tricks NMR~~

~~Spectroscopy Structure~~

~~Determination of~~

~~Organic Compound~~

~~using NMR data~~

~~Organic Chemistry~~

~~Structure Elucidation~~

~~Monash Organic~~

~~Spectroscopy~~

~~Symposium: Part 1~~

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in Organic Chemistry -

Ethyl Acetate Structure

Elucidation Of Organic

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Compounds structure

elucidation 4 |

Interactive session |

Spectral interpretation

B.Sc. III Year |

Problems pertaining to
the structure elucidation

of compounds using

UV, IR and NMR

Structure Elucidation

with the support of

EIMS, IR, UV, ^1H

^{13}C NMR

Spectroscopy How to

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~~Structure Solve Based~~

~~On NMR, IR\&u0026~~

~~Mass spectroscopy~~

~~Practice Problem Part 3~~

Making Sense of

Chemical Structures

Hard NMR Made E-Z! -

Problem 1 | Part 1 |

(NMRs Made Easy Part

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Spectroscopy Total

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Proton NMR Skills
(Benzene Derivatives) -
Part 1 How to Structure
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IR & Mass
spectroscopy Practice
Problem Part 2 Mnova
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YOHIMBINE example
Determining the
structure of organic
compounds *Determine
Organic Structure from
IR/NMR/C NMR/ Mass*

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Spectroscopy Part 4

Practice Problem:

Assigning Molecular

Structure From an NMR

Spectrum

Proton NMR

Spectroscopy - How To

Draw The Structure

Given The Spectrum

Spectroscopy Problems

"Structure Elucidation

by Using Spectral

Data" by Mr. D. M.

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Solved example- ^1H -

NMR spectroscopy-

Structure elucidation-

How to predict structure

from spectral data

**Structure elucidation
problems using ^1H and
 ^{13}C NMR**

spectroscopic data

~~Special Class - GATE~~

~~Chemistry - Structural~~

~~Elucidation with NMR~~

~~through PYQs - A Sethi~~

Structural Elucidation

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Part 2 20200923

Wednesday CHE 255

CHAT - Structure

Elucidation Using NMR

Organic Structure

Elucidation Work

Answers

3 Problem 3 Formula

Mass Spectrum (m/z) IR

(cm⁻¹) ¹H NMR (ppm)

¹³C NMR (ppm) C 9 H

12 UN=4 120 (M⁺) 105

(M-15) 91 (M-29) 3027,

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3062 2865, 2900 7.35

(m) 2.64 (t) 1.71 (sextet)

1.02 (t)

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Unknowns

UN7 144 M 117 M 27

90 M 54 77 M 67 3392

broad 3115 1514 1308

105 exchanges 776;

University of Illinois,

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technique for organic
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Answers 3 Problem 3

Formula Mass Spectrum

(m/z) IR (cm⁻¹) ¹H

NMR (ppm) ¹³C NMR

(ppm) C 9 H 12 UN=4

120 (M⁺) 105 (M-15)

91 (M-29) 3027, 3062

2865, 2900 7.35 (m)

2.64 (t) 1.71 (sextet)

1.02 (t) Organic

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C2 C5 C3, C4 Organic

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answers; Organic

Structure Elucidation

$C_7H_{11}O_4Br$. MW 238;

Question: Organic

Structure Elucidation

$C_7H_{11}O_4Br$. MW 238.

This problem has been
solved! See the answer.

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Structure Elucidation
C7H11O4Br. MW 238

...

NMR Spectroscopy is a useful technique for organic structure elucidation. We will devote three classes to learning the basics and how to use NMR for

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Structure determination.

However, it should be noted that there is an entire research field devoted to the subject and it can easily be (and has been) developed into a full semester course.

Solved: NMR

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Work Answers 4 ^1H

NMR (ppm) ^{13}C NMR

(ppm) 1644 1070, 1238

6.35 (dt) 4.66 (m) 3.97

(t) 1.98 (q) 1.84 144.0

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101.7 65.7 22.7, 19.4

C=C stretch C-O
stretches H1 H2 H5 H3
H4 C1 C2 C5 C3, C4

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