ORGANIC CHEMISTRY 2 LECTURE GUIDE 2019

BY RHETT C. SMITH, PH.D.

Marketed by Proton Guru

Find additional online resources and guides at protonguru.com.

There is a lot of online video content to accompany this book at the Proton Guru YouTube Channel! Just go to YouTube and search "Proton Guru Channel" to easily find our content.

Correlating these reactions with your course: The homepage at protonguru.com provides citations to popular text books for further reading on each reaction in this book, so that you can follow along using this book in any course using one of these texts.

Instructors: Free PowerPoint lecture slides to accompany this text can be obtained by emailing IQ@protonguru.com from your accredited institution email account. The homepage at protonguru.com provides a link to citations to popular text books for further reading on each Lesson topic in this primer.

Executive Editor: Rhett C. Smith, Ph.D. You can reach him through our office at:
IQ@protonguru.com

Cover photo courtesy of William C. Dennis, Jr.

Printed in the United States of America

10 9 8 7 6 5 4 3 2 1

ISBN 978-0578415017 (IQ-Proton Guru)

Lesson VII.5. Introduction to Nuclear Magnetic Resonance
NMR active nuclei

NMR stands for:

A

NMR spectroscopy is a technique that is used to identify compounds.
A NMR Spectrum is a plot of

B

vs.

C

Many common nuclei are NMR active, including:

D

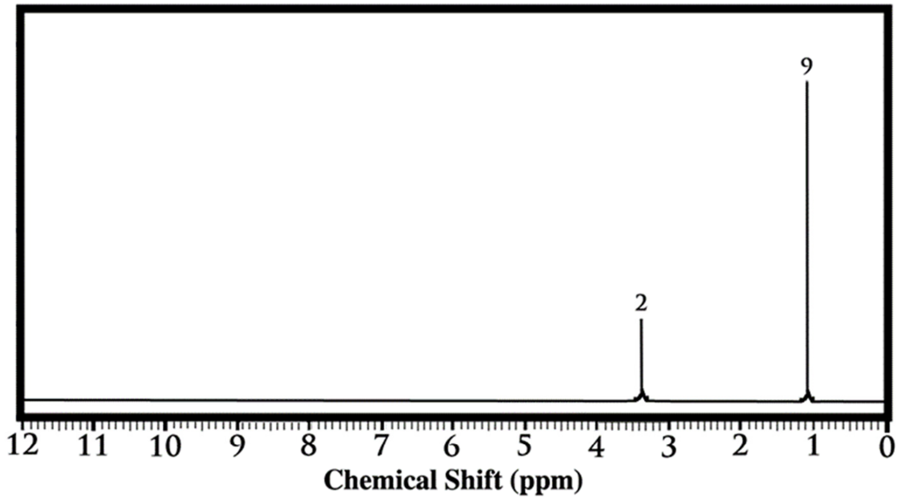
In this Lecture Guide, we will focus on ^{13}C and ^{1}H NMR spectrometry

Notes

Lesson VII.5. Introduction to Nuclear Magnetic Resonance

NMR spectrum

A representative spectrum is shown here:



The energy at which we observe a peak can tell us

D

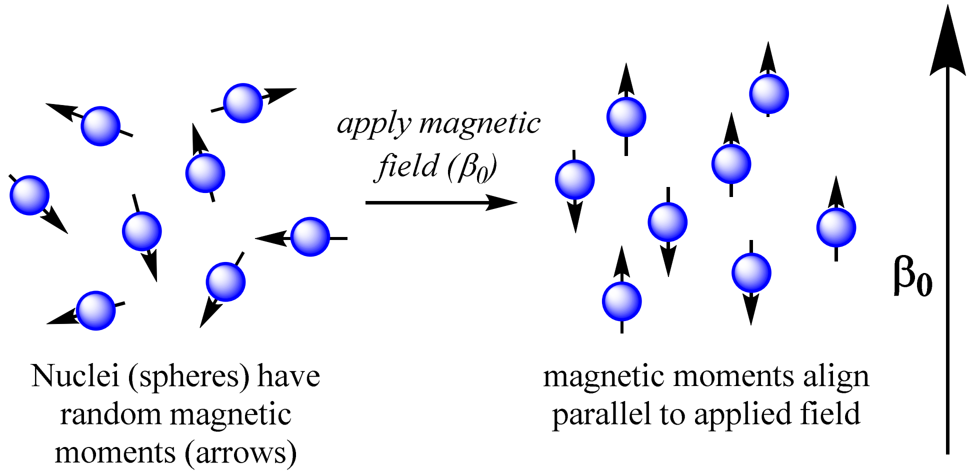
thus aiding in the compound's identification.

Notes

Lesson VII.5. Introduction to Nuclear Magnetic Resonance

NMR theory

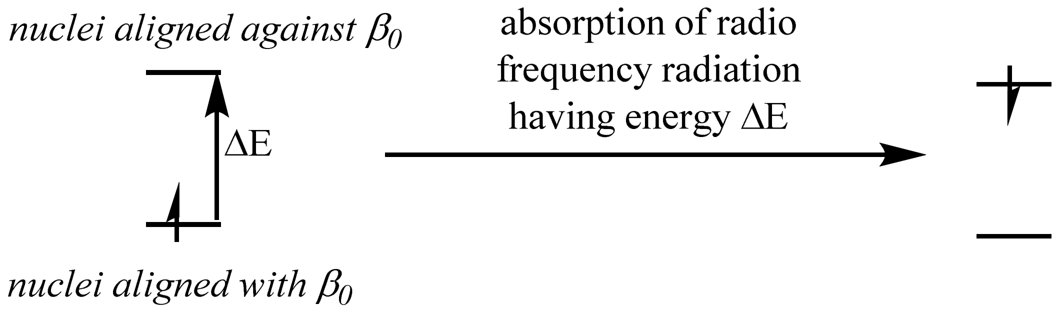
Nuclei are charged. Charged particles interact with magnetic fields. A 'resonating' nucleus generates a magnetic field of its own. This generated magnetic field may be aligned with or oppose the applied field. It takes more energy to oppose the applied field.



Notes

Lesson VII.5. Introduction to Nuclear Magnetic Resonance
NMR theory

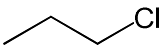
One can add energy to get the nucleus' magnetic field to 'flip' direction. By measuring the energy needed to accomplish this flip, we generate a NMR spectrum:

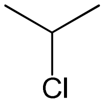


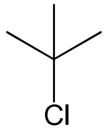
Notes

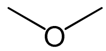
Lesson VII.5. Introduction to Nuclear Magnetic Resonance
Magnetically equivalent nuclei

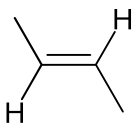
Each set of **magnetically equivalent** nuclei absorb a certain energy of photon. Free rotation about single bonds averages the signal, so that nuclei that can be interconverted by single bond rotation are equivalent. Consider how many types of H nuclei are in each of these molecules:

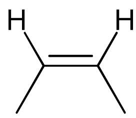

A)

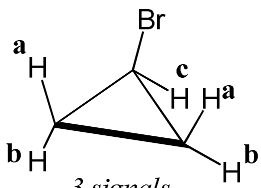

B)


C)


D)


E)


F)


3 signals
3 magnetically inequivalent proton sets

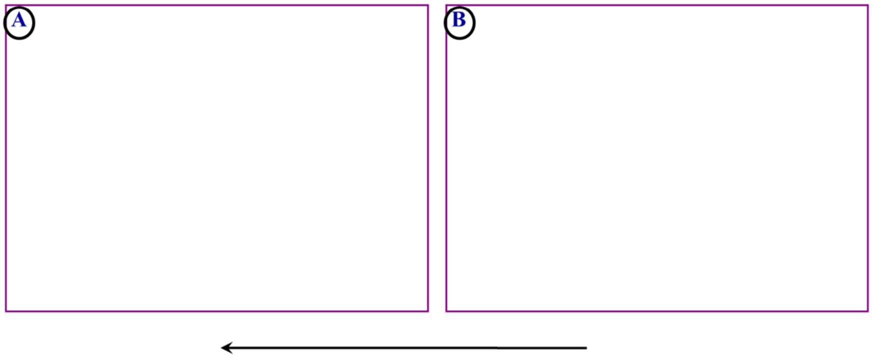
Notes

Lesson VII.5. Introduction to Nuclear Magnetic Resonance

Shielding by electrons in NMR spectra

Nuclei in molecules have electrons around them. Since electrons are oppositely charged compared to nuclei, they exert an opposing effect on the applied magnetic field. More electron density thus **shields** a nucleus and lowers the energy needed to flip it. In this way, NMR is an indirect way to measure electron density, which allows us to deduce the type of group containing the nucleus.

Protons in Electron Poor environment: **Protons in Electron Rich environment:**



Frequency increases

δ Increases

Higher number on x axis in spectrum

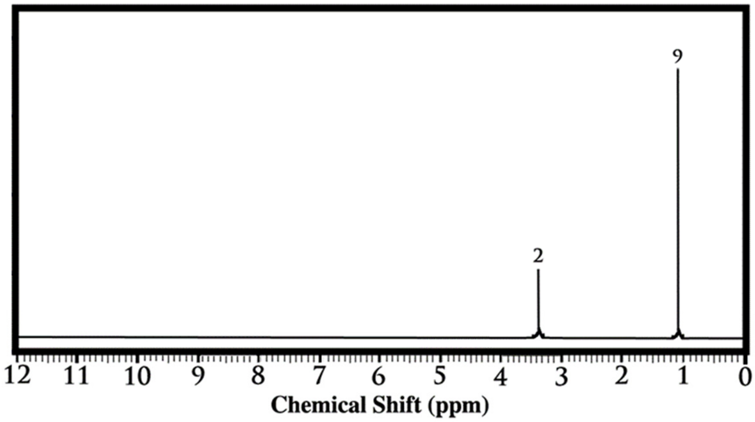
Notes

Lesson VII.5. Introduction to Nuclear Magnetic Resonance

NMR Integration

The area under each signal in an NMR spectrum is proportional to the number of nuclei giving the signal. The area under the peak is called the **integration.**

The integrations are printed above the peaks in this book. Consider this ^{1}H NMR spectrum:

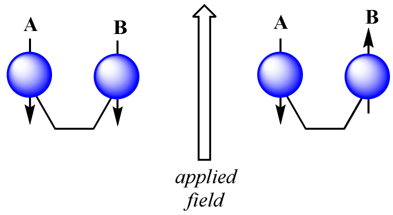


The ratio of peaks is 2:9. This could mean that one peak is attributable to 2 H nuclei and the other is attributable to 9, or one to 4 H and one to 9 H; we only know the ratio.

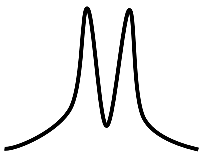
Notes

Lesson VII.5. Introduction to Nuclear Magnetic Resonance
Splitting and multiplicity in NMR

If there is an NMR active nucleus (i.e., one which resonates thus creating a magnetic field) near another NMR-active nucleus, the two will influence each other. Depending on the direction of nucleus **A**'s magnetic field, nucleus **A** may shield or reinforce the magnetic field experienced by its neighboring nucleus **B**:



This causes the signal for nucleus **A** to split slightly into two peaks. The shape of the peak will be:



This shape is called a:

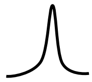
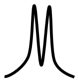
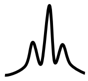
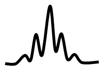
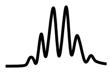
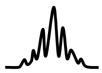
A

As there are more and more NMR-active nuclei adjacent to nucleus **A**, the splitting gets more elaborate …

Notes

Lesson VII.5. Introduction to Nuclear Magnetic Resonance
Multiplets in NMR

For 1H NMR, the **multiplicity** (*m*, the number of smaller peaks into which the signal is split) is equal to *n*+1, where *n* is the number of H on neighbor C:

#H on neighbor C:	Type of peak		Ratio of heights
	singlet		1
	doublet		1:1
	triplet		1:2:1
	quartet		1:3:3:1
	quintet		1:4:6:4:1
	sextet		1:5:10:10:5:1
	septet		1:6:15:20:15:6:1

Notes