ORGANIC CHEMISTRY 1 LECTURE GUIDE 2019

BY RHETT C. SMITH

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Organic Chemistry 1
Lecture Guide 2019

By Rhett C. Smith, Ph.D.

Companion Books from the Proton Guru:

Organic Chemistry 1 Reactions and Practice Problems 2019

by Rhett C. Smith

Organic Chemistry 1 Primer 2019,

by Rhett C. Smith, Andrew G. Tennyson, and Tania Houjeiry

Lecture Topic 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)

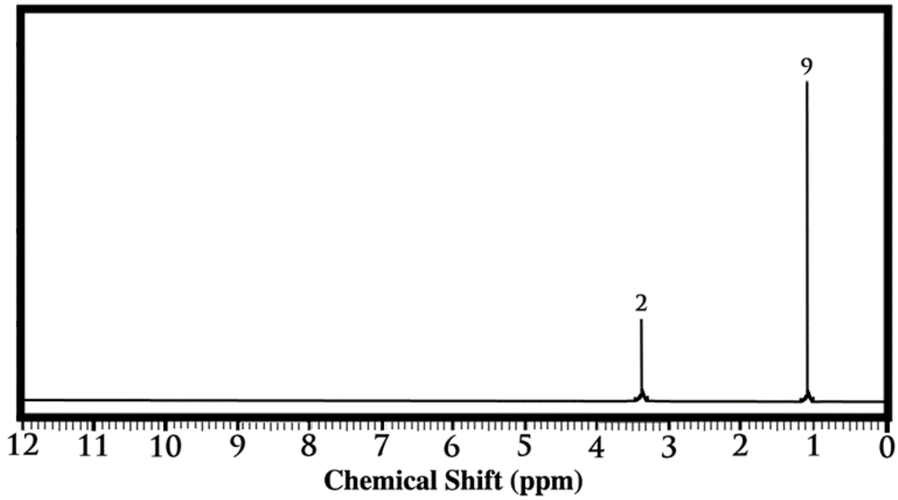
Many common nuclei are NMR active, including:

(D)

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

Notes

A representative spectrum is shown here:



The energy at which we observe a peak can tell us

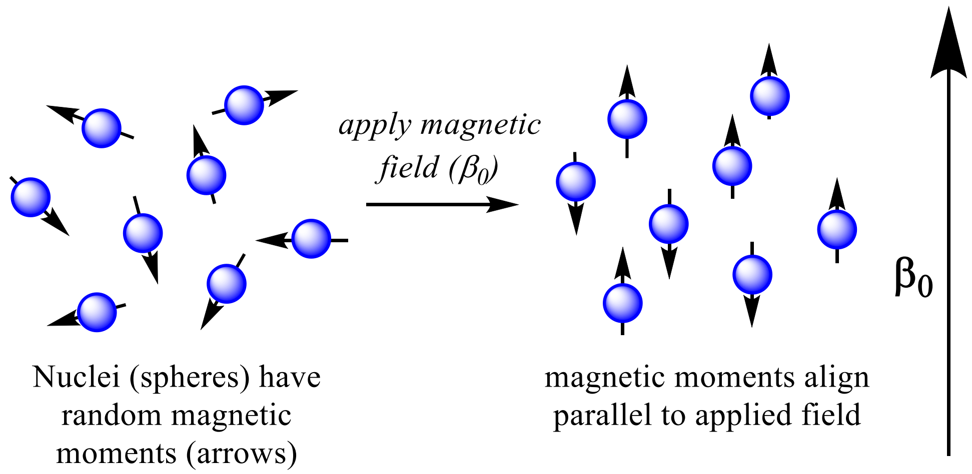
D

thus aiding in the compound's identification.

Notes

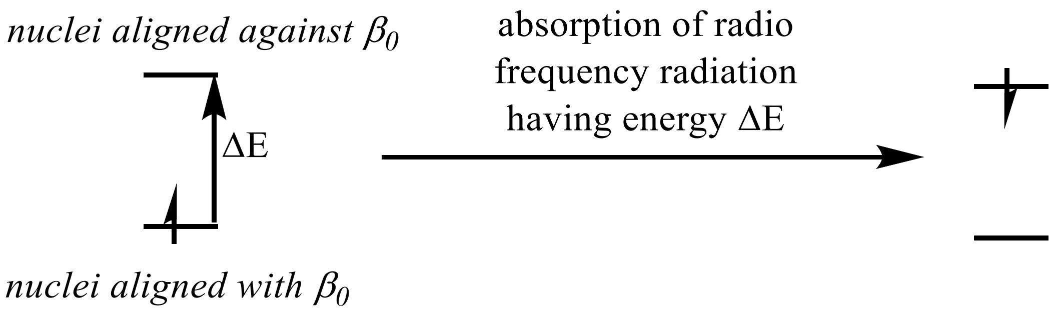
NMR theory

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

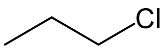
One can add energy to get the nucleus' magnetic field to 'flip' direction. By measuring the energy needed to accomplish this flip, we generate a NMR spectrum:



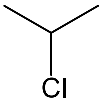
Notes

Lecture Topic VII.5. Introduction to Nuclear Magnetic Resonance
Magnetically equivalent nuclei

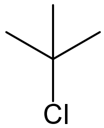
Each set of **magnetically equivalent** nuclei absorb a certain energy of photon. Free rotation about single bonds averages the signal, so that nuclei that can be interconverted by single bond rotation are equivalent. Consider how many types of H nuclei are in each of these molecules:



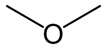
A)



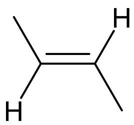
B)



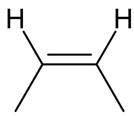
C)



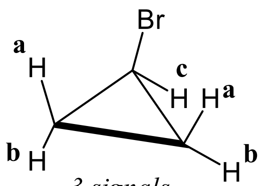
D)



E)



F)

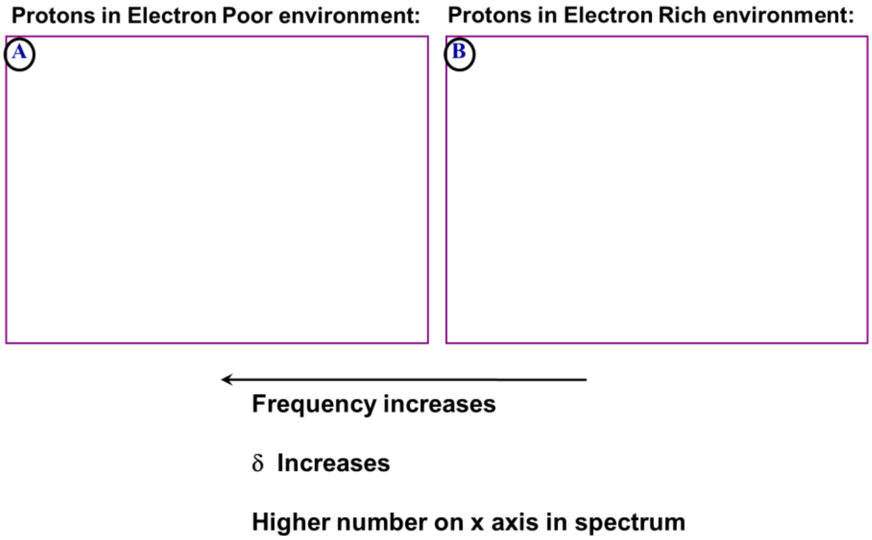


3 signals
3 magnetically inequivalent proton sets

Notes

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.

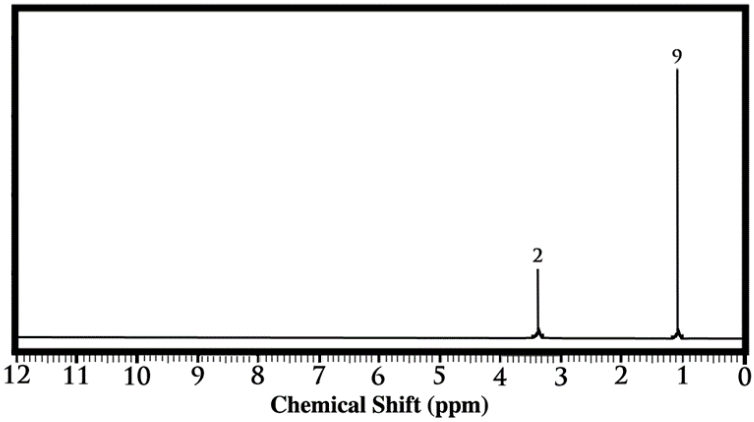


Notes

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 ^1H NMR spectrum:



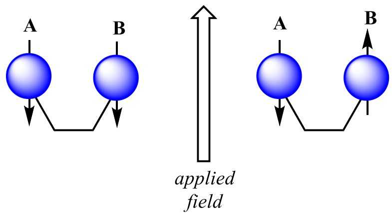
The ratio of peaks is 2:9. This could mean that one peak is attributable to 2 H nuclei and the other is attributable to 9, or one to 4 H and one to 9 H; we only know the ratio.

Notes

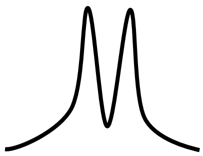
Lecture Topic VII.5. Introduction to Nuclear Magnetic Resonance

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:

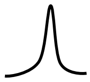
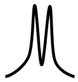
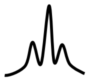
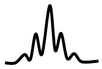
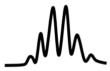
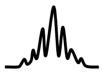
Ⓐ

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

Notes

Lecture Topic 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