CHAPTER OUTLINES/WORKSHEETS

CHAPTER 13

STRUCTURE DETERMINATION: NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

NMR spectroscopy offers a map of the carbon-hydrogen framework of a molecule. You don't need to know all of the theory behind NMR spectroscopy. The numerical calculations are shown just so you can get an idea of how this type of spectroscopy compares to IR and UV spectroscopy.

I. PRINCIPLES OF NMR SPECTROSCOPY

1. Nuclear spins in a magnetic field

2. Energy required to change spin states \((5.7 \times 10^{-7} \text{ kcals/mole @ 14,100 gauss})\)

3. Cause of chemical shift \(B_{\text{eff}} = B_{\text{applied}} - B_{\text{local}}\) \((B = \text{magnetic field})\)
   a. shielding and deshielding (chemical shift, delta scale)

4. Operation of a simple spectrometer

II. \(^{13}\text{C}\) NMR

1. Normal mode (proton noise – decoupled)
   a. Chemical shift correlation with environment

2. DEPT spectra (not too important)

III. \(^{1}\text{H}\) NMR

1. Number of absorptions (equivalent protons)

2. Chemical shifts (proton environment, table of chemical shifts)

3. Integration (proton counting)

4. Spin-spin splitting (proton coupling, coupling constant)
   a. no splitting occurs for chemically equivalent protons
   b. \(n+1\) rule (splitting due to equivalent protons, multiplicities)
c. Two groups which are coupled must have same coupling constant

5. Tree-diagrams

Chapter 13 Worksheet

What does NMR spectroscopy allow us to determine concerning an organic molecule?

What two nuclei are organic chemists most interested in studying?

In what two ways can a spinning nucleus (¹H, ¹³C) orient its magnetic field with an applied external field?

Which of these two orientations is lower in energy? How much is this energy difference at a field of 14,100 gauss? How does this energy compare with the typical energy required for an IR absorption?

What does it mean when we say that nuclei is "shielded"? Why is this shielding important in structural determination by NMR spectroscopy?

What is "chemical shift"? What is the delta scale? What is the typical standard for both proton and carbon NMR spectroscopy? What is the δ of the standard? What is a ppm?

How is the chemical shift of a carbon nucleus correlated with its chemical environment? How does the electronegativity of the atoms bonded to a carbon effect its chemical environment? How does the hybridization of carbon effect its chemical shift?

What is spin-spin splitting? What is coupling? What is a singlet? doublet? triplet?

How does spin-spin splitting arise? How does the multiplicity translate into the number of protons attached to a given carbon atom?

What are the four general features of NMR spectra?

What determines the number of resonances observed in an NMR spectrum?

How does the chemical shift range of proton resonances compare to that of carbon resonances?

What are the five general regions for absorptions in ¹H NMR spectra and protons attached to what functional group types absorb in these regions?

What is a coupling constant?

What are the three rules of spin-spin splitting in ¹H NMR?
What is a tree-diagram? How does it help analyze the coupling due to immediately adjacent non-equivalent protons?