

## Nuclear Magnetic Resonance (NMR)

A structure determination tool

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## Spectroscopy (General)

- Spectroscopy is the study of the interaction between energy and matter
- Different energy types are used in different types of spectroscopy

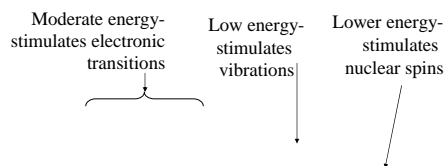


Figure 9.2 from text

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## NMR Background I

- Nuclei of some isotopes ( $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$ ...) possess nuclear spins
- All nuclei are positively charged, therefore those that spin generate a magnetic field

Figure 9.7 from text

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## NMR Background II

- These magnetic fields will align in one of two orientations when an external magnetic field is applied

Figure 9.8 from text

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## NMR Background III

- The alignments do not have the same energy, and radio frequency energy can be used to probe the energy difference
- Different magnet strengths, however, change the energy difference
- Therefore a normalized scale (ppm) is used

Figure 9.9 from text

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## NMR Spectral Interpretation

- 4 features of an NMR spectrum provide information about structure
  - Number of peaks
  - Position of peaks (chemical shift)
  - Relative peak areas
  - Peak splitting

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## NMR Spectra (Example)

$^1\text{H}$  peaks occur in range from 0-12ppm  
 $^{13}\text{C}$  peaks occur in range from 0-200ppm

This spectra is a  $^1\text{H}$  spectra with:

3 peaks @

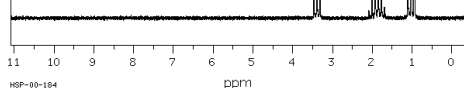
1.0 ppm: split into triplet

1.9 ppm: split into multiplet

3.4 ppm: split into triplet

Relative areas not provided

although 1.0 ppm peak > 3.4 ppm peak



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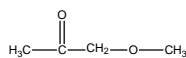
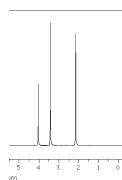
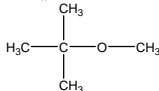
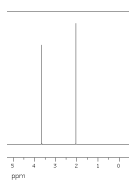
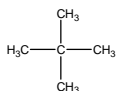
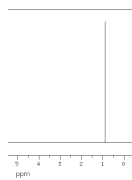
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## Number of Peaks

- What structural reasons can you suggest for the different numbers of peaks in the following spectra?  
 (none had peaks at > 5 ppm)




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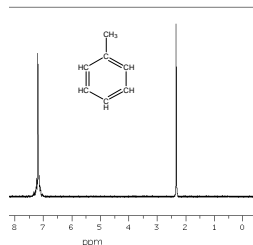
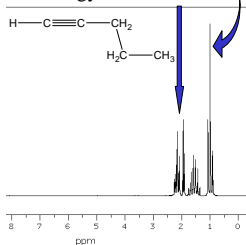
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## Position of Peaks (Chemical Shift)

- Electrons (as moving charged particles) generate magnetic fields and influence the energy a nucleus absorbs
- >energy = shielded
- <energy = deshielded




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## Chemical Shifts to Know

- Terminal alkane: ~1ppm
- Mid-alkane: slightly > 1ppm
- Near electronegative atom: depends on atom but ~ 3.5ppm
- Alkene (vinyl) protons: ~5ppm
- Aromatic protons: ~7ppm

Relate protons in other environments to the most relevant of these!

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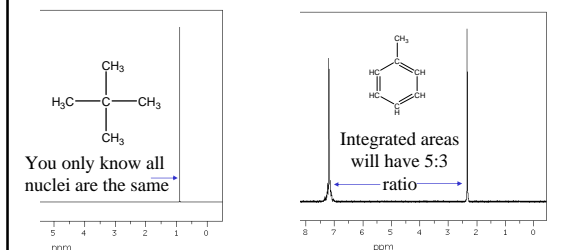
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## Relative Peak Areas

- Relative (but not absolute) peak areas relate to the number of nuclei contributing to the signal




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## Peak Splitting

- Since spinning nuclei generate magnetic fields, neighboring nuclei of different spins result in different energy absorbances



• Splitting<sub>a</sub> = (n<sub>b</sub>+1)(n<sub>c</sub>+1)(n<sub>d</sub>+1)...

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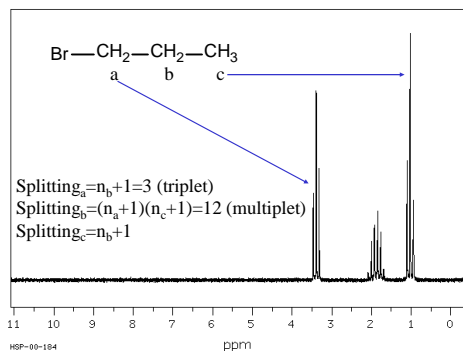
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## Splitting Example



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## Splitting Notes

- Splittings > 4 are generally called multiplets
- Most instruments do not provide sufficient resolution to show all signals in a multiplet
- Splitting is generally only observed between nuclei within 3 bonds of each other

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## Problem 1

- What features do you expect to see in the  $^1\text{H}$  NMR spectrum for 2-bromobutane?

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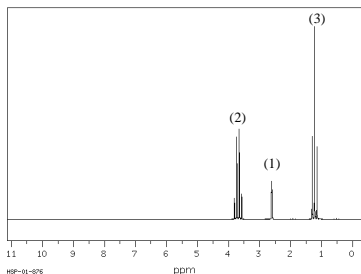
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## Problem 2

- What structure do you think gave the following spectra? (The compound gives a broad absorbance @  $3245\text{ cm}^{-1}$  in its IR spectra) Relative peak areas are shown above each peak.



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## Problem 3

- Two structures with formulas  $\text{C}_3\text{H}_8\text{O}$  gave the spectra on the following slides (IR,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR)
- Determine their structures, their IUPAC names, and their structural relationship

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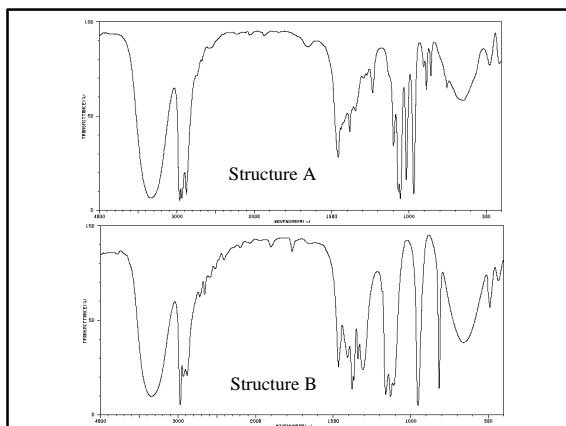
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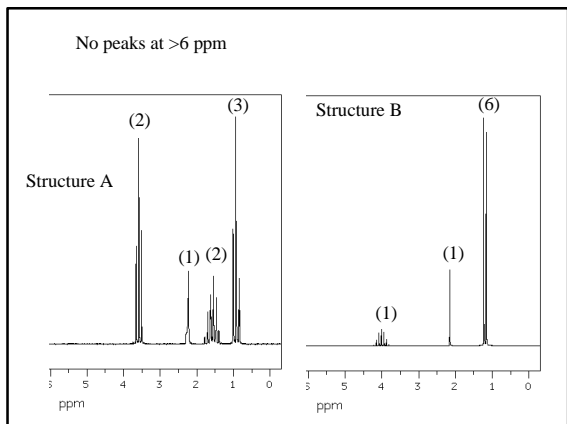
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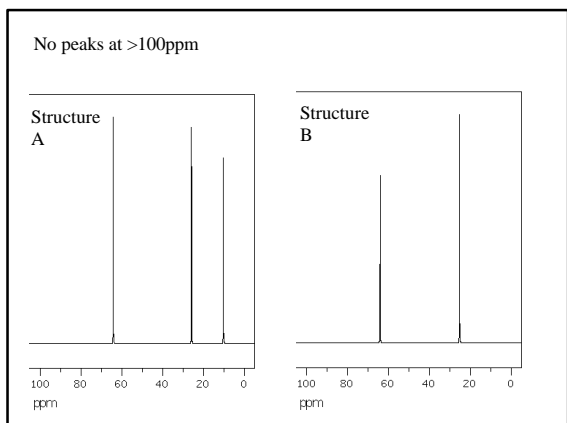
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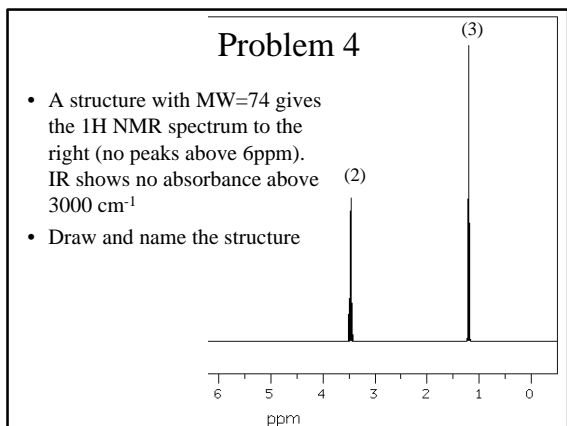
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