CHEM 222 section 01

LECTURE #11

Tues., Oct.09, 2007

Lecture topics & readings

# Today's class

- NMR spectroscopy (Ch.13)

## Before next class

- read sections 13.1-7

## Next class

- continue NMR

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# CHARACTERIZATION METHODS - PART II Ch.13: Nuclear Magnetic Resonance (NMR) Spectroscopy

<u>Chapter Goals & hints</u>

Learn the basic principles of NMR & how to interpret <sup>1</sup>H & <sup>13</sup>C spectra.

- Learn the basic theory behind how an NMR spectrometer works.
- Learn to extract structural information from <sup>1</sup>H & <sup>13</sup>C NMR spectra.

Topics Outline:

13.1-2	What NMR involves
13.3-10	Basic information from <sup>1</sup> H NMR spectra
13.11	Examples of <sup>1</sup> H NMR spectra
13.12-18	More advanced information from <sup>1</sup> H NMR spectra
13.19-20	<sup>13</sup> C NMR
13.21	2D NMR
13.22	MRI

## 13.1 Nuclear magnetic resonance (NMR) spectroscopy basic principles



- **Result:** with appropriate photons  $\Rightarrow$  excite nuclei  $\Rightarrow$  flip spins  $\alpha \rightarrow \beta$ (3) then measure resulting small changes in overall field
  - 13.2 An NMR spectrometer the basic set-up



An NMR experiment: flip spins, then monitor small field changes...





A 300 MHz NMR spectrometer (like our research instrument)

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http://www.curie.u-psud.fr/U350/1999/photosequipements/bruk306big.jpg

### NMR spectroscopy = another absorption spectroscopy





#### Larger magnet $\Rightarrow$ more sensitive & better resolution



## 13.4 Shielding: why not all <sup>1</sup>Hs absorb exactly the same frequency

#### Local field differences due to nearby electron clouds...

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• e-s spin  $\Rightarrow$  small mag. fields line up against  $B_0 \Rightarrow$  cancel some of  $B_0$ 



If experience SAME field strength ⇒ absorb SAME frequency

### 13.4 How many peaks should be in the spectrum? Chemically equivalent <sup>1</sup>Hs appear as the same peak

Each DIFFERENT type of <sup>1</sup>H yields one peak...



...with intensity matching how many H's of that type

#### Things to remember:

single bonds rotate quickly - faster than NMR data is acquired

π-bonds do NOT rotate



If experience SAME field strength ⇒ absorb SAME frequency

#### 13.5 Chemical shift: frequency relative to reference

**Chemical shift**  $\delta$  = how far downfield peak is from TMS...

- **ppm** = parts-per-million shift in frequency
- H<sub>3</sub>C CH<sub>3</sub> CH<sub>3</sub>C CH<sub>3</sub>

#### = <u>how far downfield from TMS (in Hz)</u> operating freq. of spectrometer (in MHz)

 $\Rightarrow$  peak positions ( $\delta$ ) same on any strength of spectrometer





13.6-7 Characteristic chemical shift values

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#### 13.8 Diamagnetic anisotropy (different in different directions) = why some functional groups look like extreme EWGs



