Chem 342

Lecture Summary 01
January 14, 2004

Introduction

Tips for Learning Organic Chemistry

Learning organic chemistry is very much like learning a foreign language. You need the vocabluary (terms, structures, etc) and the grammar (reactivity, functional group properties) to put it together. Here are some suggestions for success: Read before coming to class. Come to class. Rewrite your notes using all your senses. Do problems. Use flash cards. Form a study group. Get a set of molecular models. And most important - DON’T FALL BEHIND.

Structure Determination

To figure out the structures of molecules, we use techniques to probe the physical features.

Elemental Analysis - atomic composition

Mass Spectrometry - molecular formula, elemental identification, connectivity

Vibrational (IR) Spectroscopy - functional groups

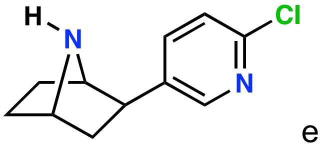
Electronic (UV-VIS) Spectroscopy - conjugated pi-systems

X-Ray Crystallography - 3D position of atoms.

NMR Spectroscopy - most useful for organic chemists - atom connectivity, functional group identification, stereochemistry, higher order structure.

Real-Life Example - Epibatidine

The molecule, epibatidine, was isolated from the skins of an Ecuadorean tree frog. It possesses analgesic activity. The structure was elucidated using many of the techniques described above. High resolution Mass Spectrometry provided the elemental identity and indicated that chlorines were present. UV Spectroscopy and IR Spectroscopy indicated the presence of the nitrogen containing ring (a pyridine ring). Key to solving the structure was the proton and carbon NMR data. This showed conclusively the connectivity and different types of hydrogens and carbons.

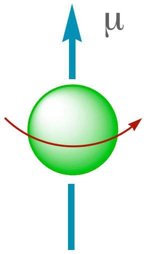


epibatidine - *J. Am. Chem. Soc.* **1992**, *112*, 3475.

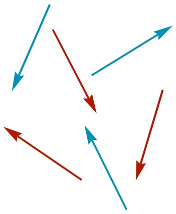
Chapter 13 - Nuclear Magnetic Resonance Spectroscopy

Provides detailed information about the structure of molecules

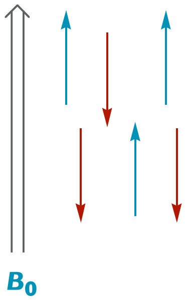
The NMR phenomenon occurs due to the spins of nuclei. A charged particle (like a proton) has a spin. This generates a magnetic field with a vector component. If a molecule is placed in an applied magnetic field (B_o), the nuclear spins can align with the field or against the field.



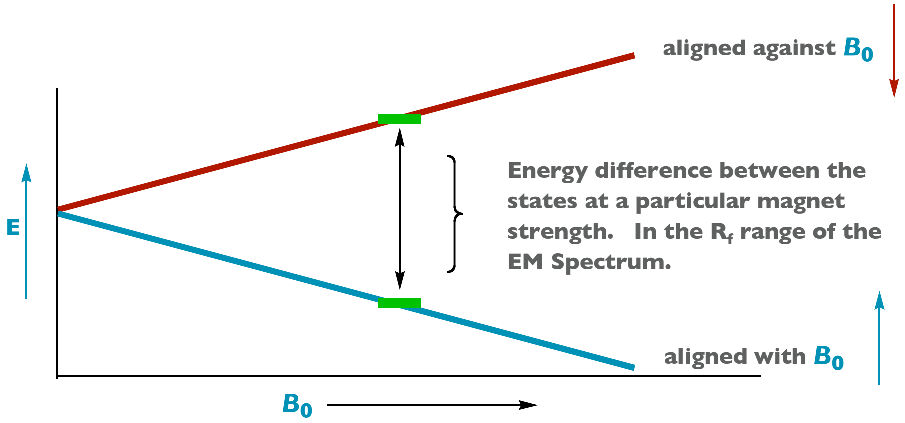
A spinning charged particle generates a magnetic field.
A nucleus with a spin angular momentum will generate a magnetic moment (m).



When placed in a magnetic field (**Bo**), they will adopt two different states - one aligned with the field and one aligned against the field.



Those nuclei that are aligned with the external field are lower in energy than those opposed to the applied magnetic field. This energy is in the range of radio frequencies. Thus, when radio waves are passed through the sample, the frequency corresponding to this energy difference will be absorbed and cause the spins to flip - this is termed resonance.



Many nuclei are “NMR Active”. They are observable if the atom’s Spin Quantum Number (I) does note equal zero. ^{1}H and ^{13}C are the most common nmr active nuclei used for organic structures. Others include ^{1}H (D), ^{14}N, ^{19}F, and ^{31}P. Atoms like ^{12}C and ^{16}O cannot be observed.

The NMR phenomenon is the same utilized for medical Magnetic Resonance Imaging.