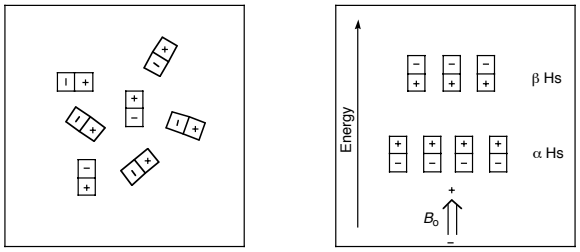
Techniques utilized by organic chemists:

NMR - Nuclear Magnetic Resonance Spectroscopy gives information about environment and overall structure.

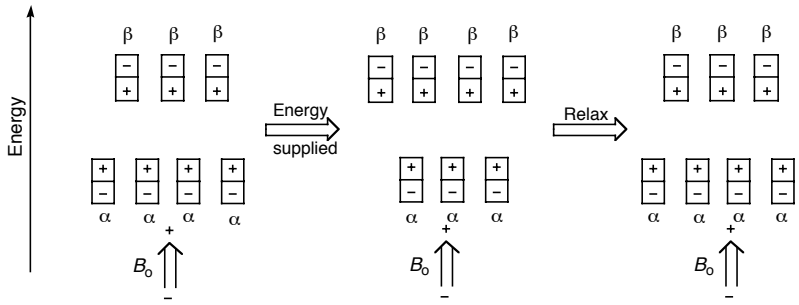


In the absence of a magnetic field

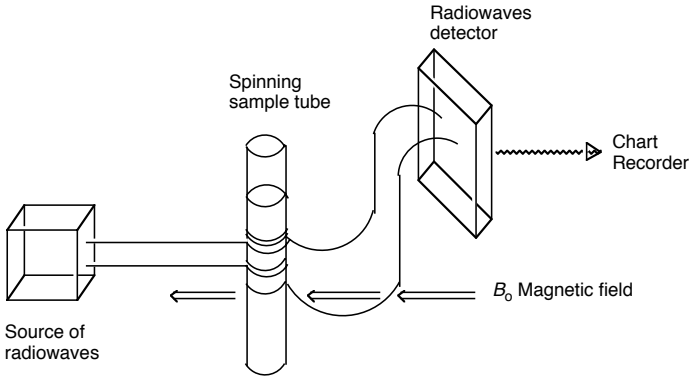
In the presence of an applied magnetic field, B_0

Nuclear spins in the absence and presence of a magnetic field.

Absorption of energy can "flip" a nuclear spin, converting the low energy orientation into the higher one.



A schematic of an NMR spectrometer.



Chemical Shifts (δ) – see table (measured in ppm)

Chemically equivalent – have the same signal

Identical

Enantiomeric – nuclei related by a mirror plane

Chemical shift is defined as the place on the chart at which a nucleus absorbs

Use TMS (tetramethylsilane) as our 0 point.

Upfield – towards 0 ppm

Downfield – towards 12 ppm

Integration

The area under each peak is proportional to the number of protons causing that peak.
Measured in a stair-step manner

Spin-spin splitting

The phenomenon of multiple absorptions caused by the interaction of the nuclear spins of neighboring atoms
Follows Pascal's triangle
The general rule is the $n + 1$ rule

1. *Chemically equivalent protons don't show spin-spin splitting.*
2. *The signal of a proton with equivalent neighboring protons is split into a multiplet of n + 1 peaks with a coupling constant J in Hz*
3. *Two groups of protons coupled to each other have the same coupling constant J.*

IR Spectroscopy

When a molecule is irradiated with electromagnetic radiation, energy is absorbed if the frequency of the radiation matches the vibrational frequency. (measured in cm^{-1})
It increases the amplitude for the vibration.
Need a dipole moment – cannot be symmetrical
From the vibration, we can tell what functional groups are present because functional groups have characteristic infrared absorptions that do not change from one compound to another.

Four Regions of IR

1. 4000 to 2500 cm^{-1} – N-H, C-H, and O-H bond stretches
   a) N-H and O-H absorb around 3600 – 3000 cm^{-1}
   b) C-H around 3000 cm^{-1} (above 3000 cm-1 aromatic below 3000 cm^{-1} aliphatic)
2. 2500 to 2000 cm^{-1} – triple bonds absorb nitriles and alkynes
3. 2000 to 1500 cm^{-1} – double bonds absorb C=O, C=N, and C=C
   a) carbonyl groups specifically – 1750 – 1680 cm^{-1}
   b) C=C 1680-1640 cm^{-1}
4. Region below 1500 cm^{-1} is the *fingerprint region.*

Taken from McMurry, J. *Fundamentals of Organic Chemistry*, 4th ed.; Brooks/Cole Publishing: Pacific Grove, 1998; Chapter 13 and Jones, Maitland *Organic Chemistry*, 2nd ed.; Norton Publishers, New York, 2001.