Spectroscopy Review: The Basics of the Basics

Infrared Spectroscopy - allows us to determine functional groups present in a molecule

Characteristic arrangements of atoms (functional groups) have about the same frequencies of vibration in any molecule

Stronger the bond - higher the vibrational frequency, higher the wavenumber

Heavier the atoms - lower the vibrational frequency, lower the wavenumber

Nuclear Magnetic Resonance Spectroscopy - allows us to determine the carbon/hydrogen skeleton

chemical shift - (where the signal occurs) compared to standard - TMS

depends on the magnetic field strength "felt" by the nucleus (effective field strength - H_{eff})

H_{eff} depends on the electron density around the nucleus because the circulation of electrons generates a magnetic field (H_i)that shields the nucleus from the field applied by instrument (H_0)

greater the electron density, the more "shielded" the nucleus, the higher the necessary field strength (H_0)to produce a signal, therefore the more upfield the signal

smaller the electron density, the less "shielded" the nucleus, the lower the necessary field strength to produce a signal, therefore the more downfield the signal

factors that affect electron density affect chemical shift:

electronegative atoms -

pi electrons of a double bond -

pi electrons of a triple bond -

signal multiplicity - (appearance of signal - how many peaks?)

adjacent, nonequivalent nuclei generate magnetic fields that affect the appearance of a signal in the NMR spectrum

N + 1 Rule: The signal for a given nucleus is split into N + 1 peaks by N adjacent nuclei

remember: The N nuclei must be nonequivalent to the nucleus of interest and must be equivalent to each other. If the nucleus of interest is adjacent to more than one kind of nucleus, the N + 1 rule is used for each kind.

Examples: