Citrus College

O. Chem. 220 ***Prof. Badieh Farahani***

^{13}C-NMR

NMR spectroscopy is not limited to the study of protons. Any element with a nuclear spin (^{2}D, ^{13}C, ^{17}O, ^{19}F, ^{31}P) will give rise to an NMR signal.

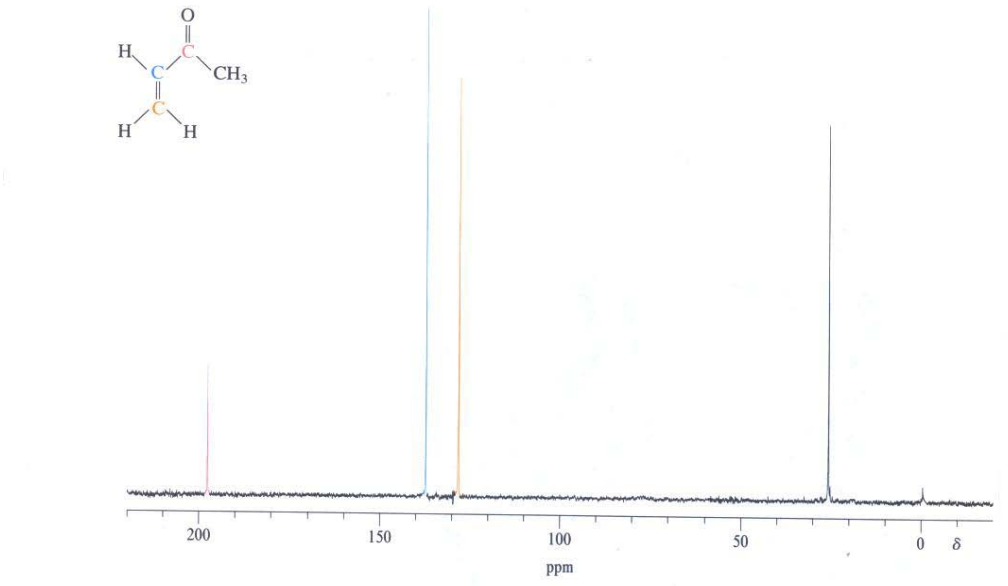
The idea & theory behind ^{13}C-NMR is the same as with ^{1}H-NMR just a different nucleus.

Electronegativity, hybridization, and anisotropy all affect ^{13}C chemical shift nearly the same fashion as ^{1}H shift.

B_o = 7.05 T & υ = 75 MHz (for ^{1}H υ = 300 MHz)

C-13 has a nuclear spin (I = +1/2 & -1/2) and make up 1.1% of naturally occurring carbon (C-12 is NMR inactive).

The range of chemical shift for C-13 (0-220 ppm) is much larger than H-1 (0-12 ppm) due to direct attachment of C to other elements (C=O, C-X,…). This wide range makes the overlaps of the peaks less likely.



Each C appears as a sharp singlet – by using a technique called **broadband decoupling**.

No ^{13}C-^{13}C coupling is observed due to low natural abundance of this isotope. However coupling between C-H (even several bonds away) is strong and result is complex spectrum.

Off-resonance decoupling allows spin coupling between C & H that are directly attached.

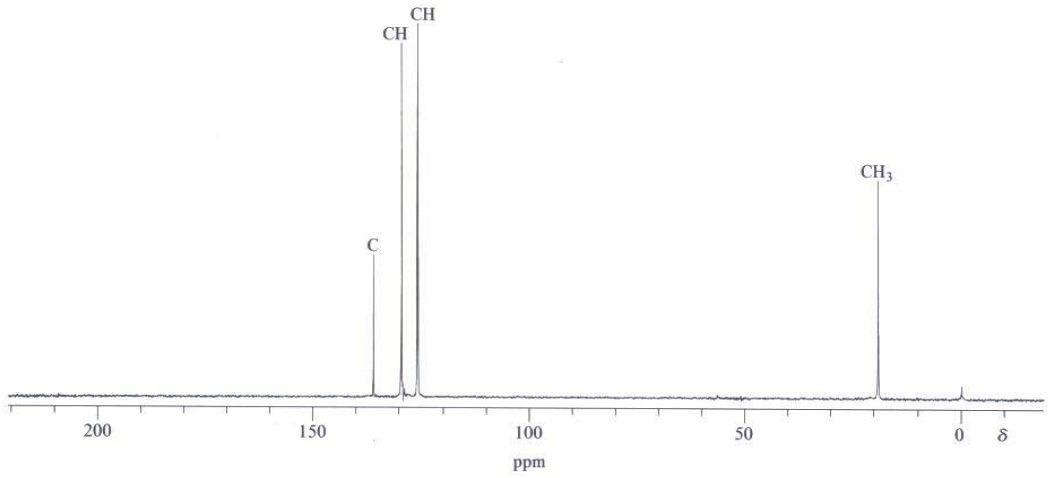
CH_3 → quartet
CH_2 → triplet
CH → doublet
C → singlet

A newer technique called **DEPT-NMR** (**D**istortionless **E**nhancement by **P**olarization **T**ransfer) is used to determine the # of H attached to each carbon.

Typical Chemical Shifts in ^{13}C-NMR Spectra

Structure	Chemical Shift (ppm)
Carbonyl (ketone)	205-220
Carbonyl (aldehyde)	190-200
Carbonyl (ester, acid)	160-185
Carbonyl (amide)	150-180
Aromatic	110-170
Alkene	100-150
Alkyne	60-90
Alcohol, Ether	50-90
Alkyl Halide (Cl, Br)	25-65
Amine	35-60
R_4C, R_3CH	20-60
R_2CH_2	15-55
RCH_3	8-30

^{13}C-NMR of C_8H_{10} is given below. Propose a structure.



^{13}C-NMR of $C_6H_{12}O$ is given below. Propose a structure.