^{13}C-NMR Spectroscopy

- Each nonequivalent ^{13}C gives a different signal.
  - The number of signals equals the number of different carbons in the molecule.
  - Less than one ^{13}C per molecule; **there is no carbon-carbon coupling.**
- A ^{13}C is split by the ^{1}H bonded to it according to the (n + 1) rule.
  - Coupling constants of 100-250 Hz are common, which means that there is often significant overlap between signals, and splitting patterns can be very difficult to determine.

^{13}C-NMR Spectroscopy

- In a **hydrogen-decoupled mode**, a sample is irradiated with two different radio frequencies
  - one to excite all ^{13}C nuclei
  - a second is a broad spectrum of frequencies that causes all hydrogens in the molecule to undergo rapid transitions between their nuclear spin states
- On the time scale of a ^{13}C-NMR spectrum, each hydrogen is in an average or effectively constant nuclear spin state, with the result that ^{1}H-^{13}C spin-spin interactions are not observed; they are **decoupled**

^{13}C-NMR and the Nuclear Overhauser Effect

- NOE is an interaction between a target nucleus and its radiatively-saturated neighbors.
- Spin is transferred from the target nucleus to its saturated neighbors, increasing the population of low-spin target nuclei. This **increases the signal** of the target nucleus.
- **As a result, during a standard H-decoupled experiment, ^{13}C atoms attached to hydrogens show enhanced signals compared to quaternary ^{13}C atoms.**

Interpreting ^{13}C NMR

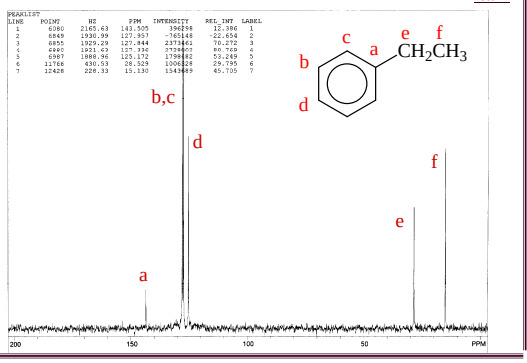
- **Number of peaks shows the number of types of carbon in the sample.**
- **Chemical shifts show what types of carbon are in the sample.**
- **Peak size shows up quaternary carbons in the sample.**

^{13}C NMR chemical shifts

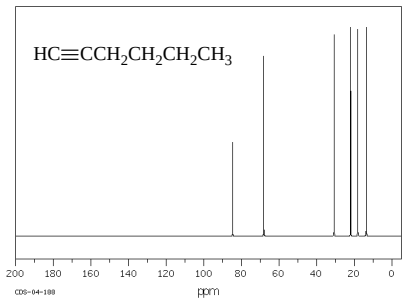
Type of Carbon	Chemical Shift (δ)	Type of Carbon	Chemical Shift (δ)
RCH_3	0–40		110–160
RCH_2R	15–55		
R_3CH	20–60		160–180
RCH_2I	0–40		
RCH_2Br	25–65		165–180
RCH_2Cl	35–80		
R_3COH	40–80		175–185
R_3COR	40–80		
$RC{\equiv}CR$	65–85		180–210
$R_2C{=}CR_2$	100–150		

^{13}C-NMR spectrum of ethylbenzene

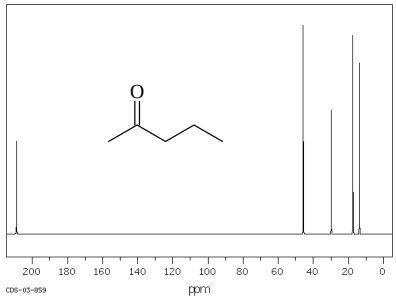
return



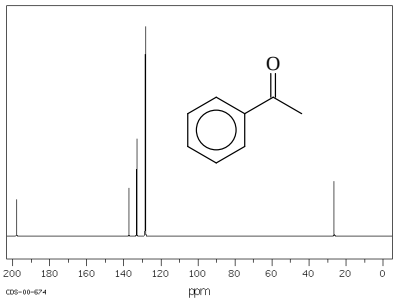
^{13}C-NMR spectrum of 1-hexyne



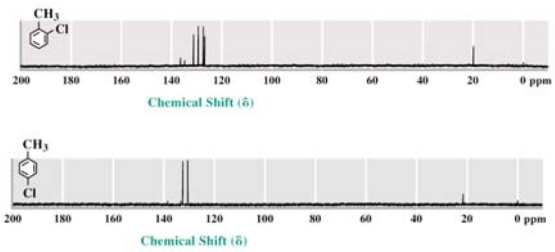
^{13}C-NMR spectrum of 2-pentanone



^{13}C-NMR spectrum of acetophenone



^{13}C-NMR spectra of 2- and 4-chlorotoluene



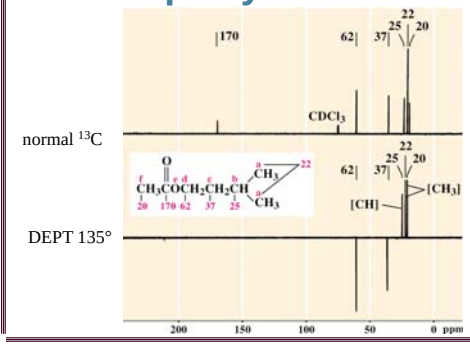
The DEPT method

- In the hydrogen-decoupled mode, information on spin-spin coupling between ^{13}C and attached hydrogens is lost
- The Distortionless Enhancement by Polarization Transfer (DEPT) method is an instrumental mode that provides a way to acquire this information
  - DEPT is an NMR technique for distinguishing among ^{13}C signals for CH_3, CH_2, CH, and quaternary carbons

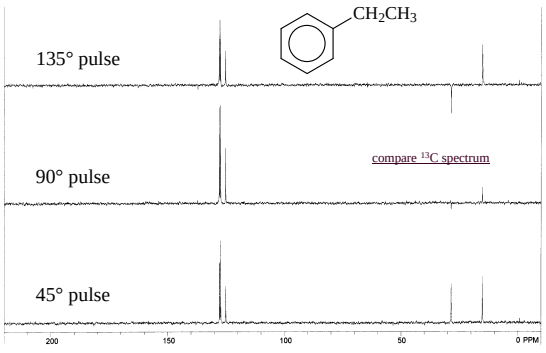
The DEPT method

- The DEPT methods uses a complex series of pulses in both the ^{1}H and ^{13}C ranges: a 45° pulse, a 90° pulse and a 135° pulse
  - quaternary carbons give no signal
- 45° pulse: all H-bearing peaks are positive
- 90° pulse: only CH carbons are seen
- 135° pulse: carbon signals show different phases
  - signals for CH_3 and CH carbons give positive signals
  - signals for CH_2 carbons give negative signals

^{13}C and DEPT-135° spectra of isopentyl acetate



DEPT spectrum of ethylbenzene



Interpreting ^{13}C NMR

- Number of peaks shows the **number of types** of carbon in the sample.
- Chemical shifts show **what types** of carbon are in the sample.
- Peak size shows up **quaternary carbons** in the sample.
- DEPT detects **primary**, **secondary**, and **tertiary** carbons