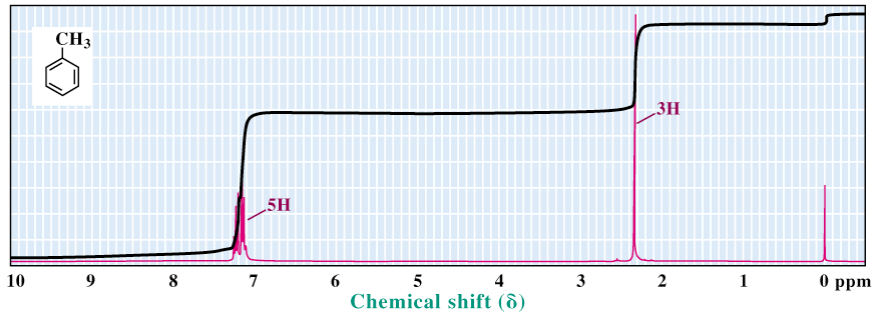
Integration of ^{1}H NMR

Information about the total number of hydrogen atoms

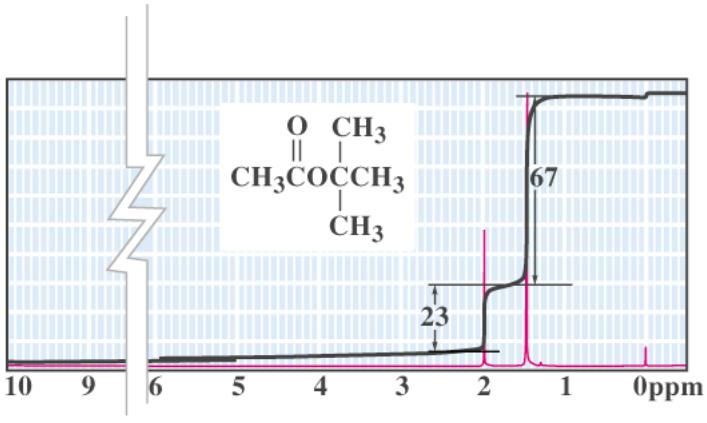
Signal Areas

- **Relative areas of signals are proportional to the number of hydrogens giving rise to each signal.**
- **All modern NMR spectrometers electronically integrate and record the area of each signal.**

^{1}H-NMR spectrum of toluene



^{1}H-NMR spectrum of *tert*-butyl acetate

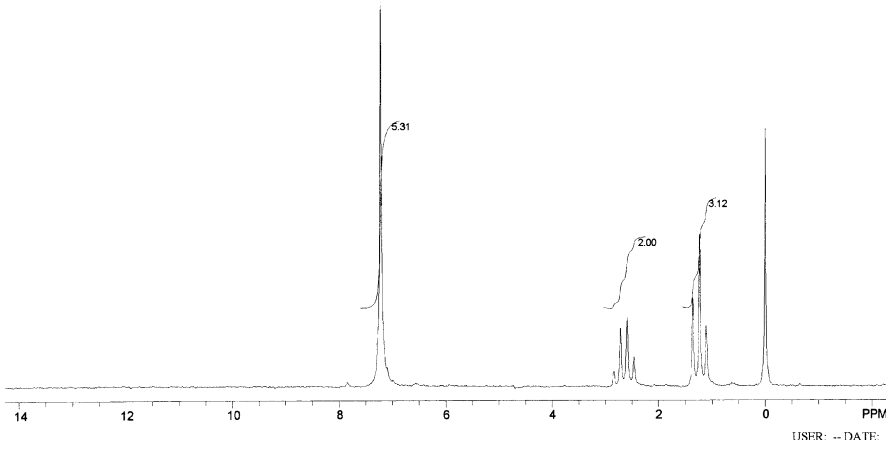


Peak splitting in ^{1}H NMR

Information about the number of nearby hydrogen atoms

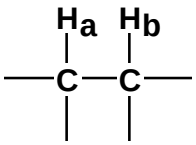
Typical ^{1}H splitting

ethylbenzene

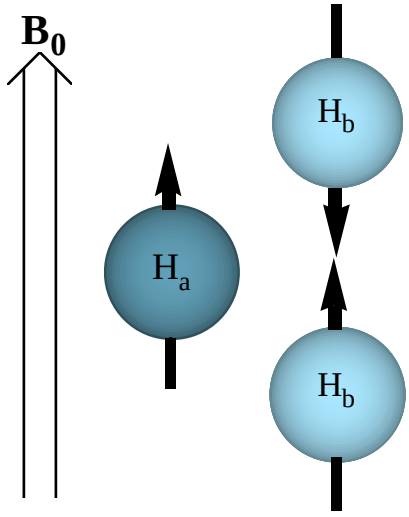


Origins of Signal Splitting

- Spin-½ nucleii are influenced by neighboring spin-½ nucleii. This is a magnetic effect.
- When the chemical shift of one nucleus is influenced by the spin of another, the two are said to be coupled.
- Consider nonequivalent hydrogens H_a and H_b on adjacent carbons:



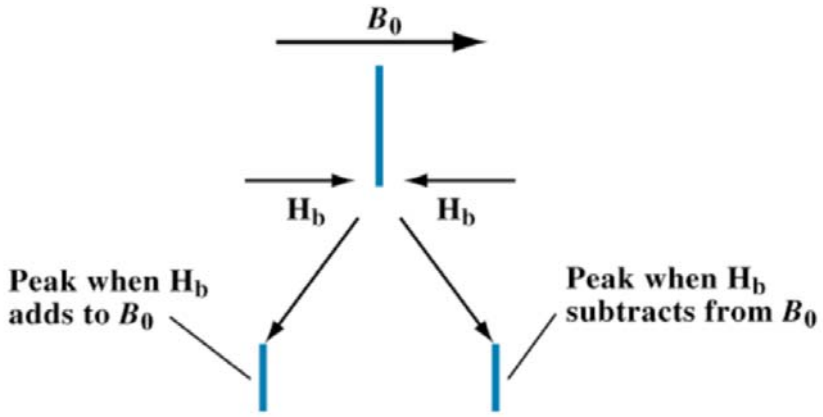
Origins of Signal Splitting



H_b reduces the field felt by H_a; H_a signal is shifted upfield.

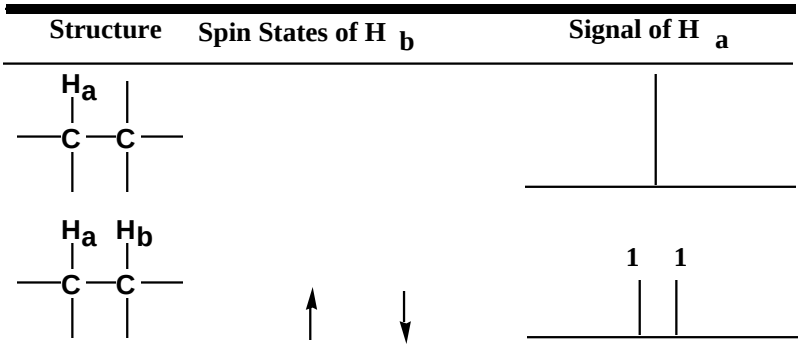
H_b increases the field felt by H_a; H_a signal is shifted downfield.

Origins of Signal Splitting

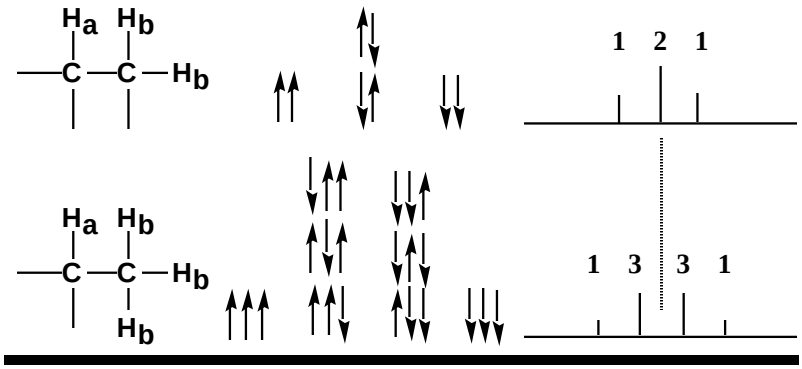


Origins of Signal Splitting

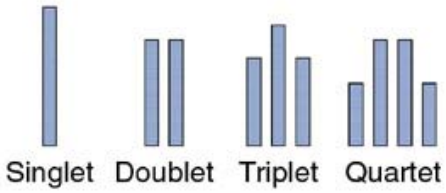
- **Observed signal splitting patterns for an H with 0, 1, 2, and 3 equivalent neighboring hydrogens**



Origins of Signal Splitting



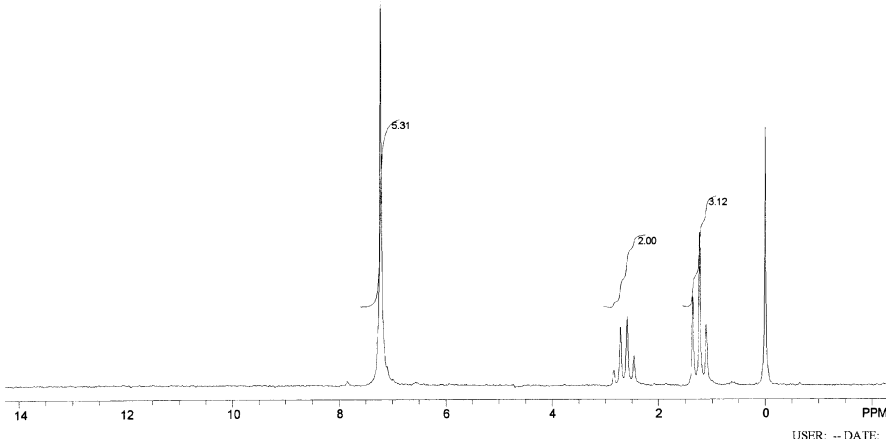
The (n+1) rule



- **Peak:** **the units into which an NMR signal is split; doublet, triplet, quartet, etc.**
- **(n + 1) rule:** **the NMR signal of a set of equivalent spin-½ nucleii is split into (n + 1) peaks by a nonequivalent set of n equivalent neighboring spin-½ nucleii**

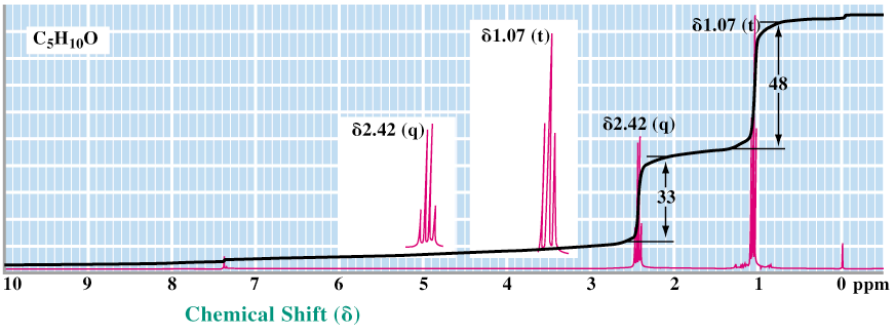
The (n+1) rule

ethylbenzene



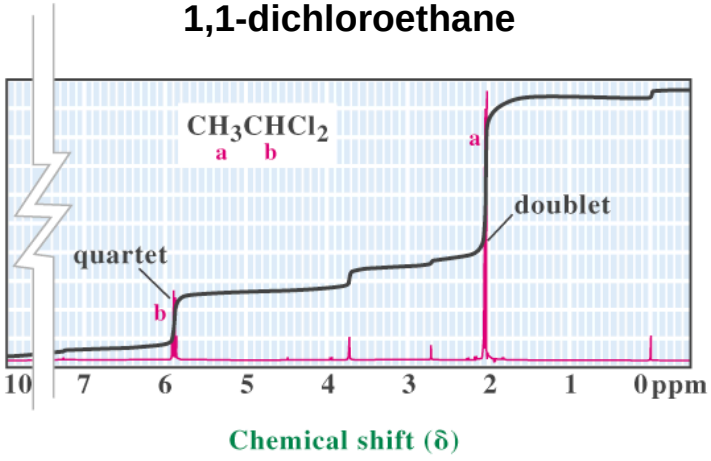
The (n+1) rule

3-pentanone



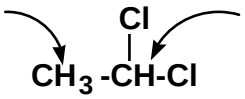
The (n+1) rule

1,1-dichloroethane



Signal Splitting (n + 1)

n = 1. Their signal is split into (1 + 1) or 2 peaks ; a doublet

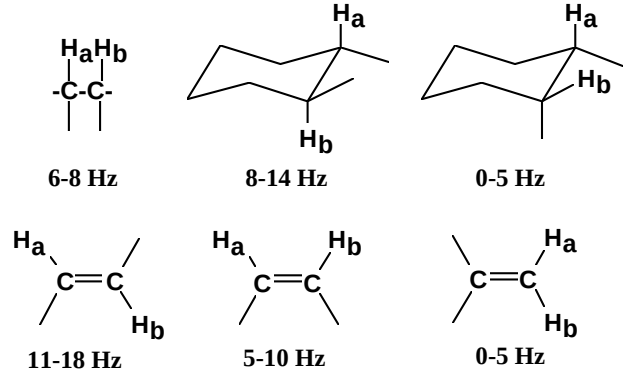


n = 3. Its signal is split into (3 + 1) or 4 peaks; a quartet

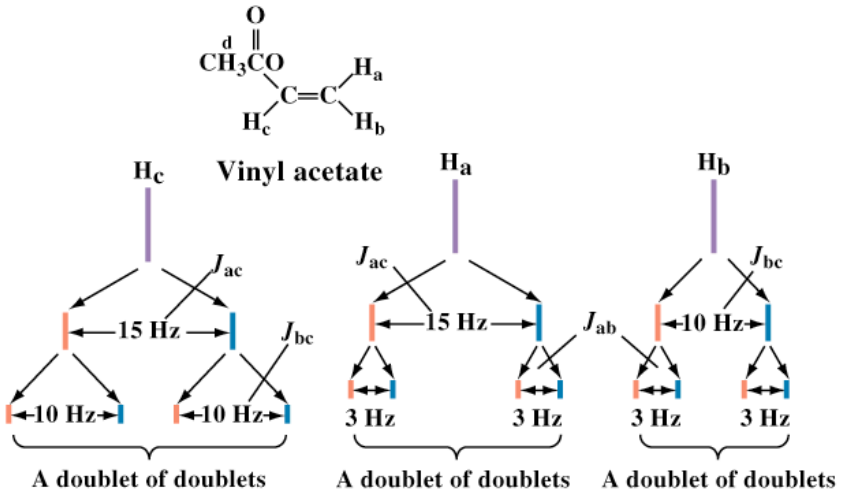
- **Problem:** **predict the number of ^{1}H-NMR signals and the splitting pattern of each**

Coupling Constants

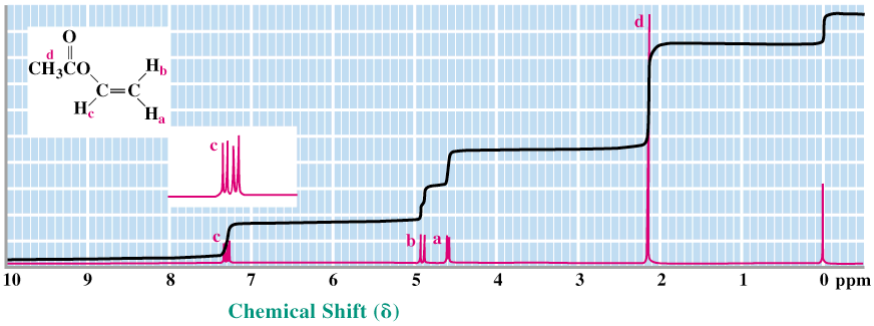
- **Coupling constant (J):** the distance between peaks in an NMR multiplet, expressed in hertz
  - J is a quantitative measure of the magnetic interaction of nuclei whose spins are coupled



Splitting in vinyl acetate



300-MHz ^{1}H-NMR spectrum of vinyl acetate



60-MHz ^{1}H-NMR spectrum of vinyl acetate