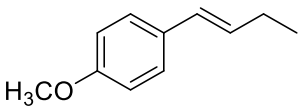
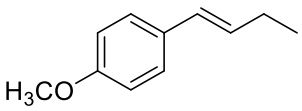
CHEM 8M, Lecture 4
- ^{1}H NMR Structural Analysis
- Spectral Analysis of Benzhydrol

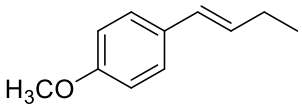
^{1}H NMR Chemical Equivalency, Integration, & Chemical Shifts

How many **^{1}H NMR absorptions** are expected below (how many **types of non-equivalent protons**)?

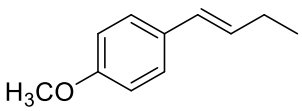




What is the ratio of peak areas expected upon **integration** of the spectrum?



Approximate the **chemical shift** for each type of proton.
- What is the *chemical environment* of each proton?
- **H**-C-("Group") used to assign most appropriate chemical shift range



Can you use the structure to explain the relative chemical shift ranges?

What's the resonance frequency, Kenneth?

Chemical shift (ppm) = $\frac{\text{frequency of proton relative to TMS}}{\text{Maximum operating frequency of instrument (MHz)}}$

Ex. *tert*-butyl acetate is dissolved in a solution of $CDCl_3$ (w/ 0.1 % TMS) and ^{1}H NMR spectra are run on two different instruments.

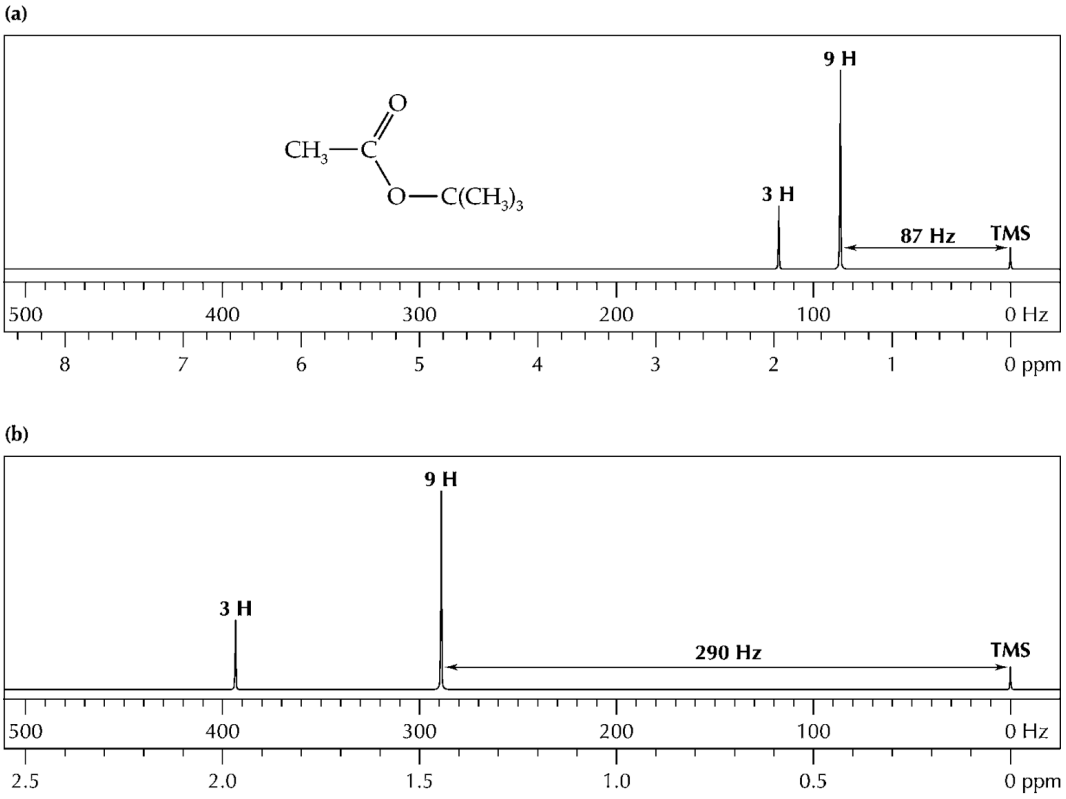


FIGURE 22.12 ^{1}H NMR spectra of *tert*-butyl acetate in the region from 0 to 500 Hz at (a) 60 MHz and (b) 200 MHz. The chemical shift of each signal is the same regardless of the spectrometer frequency.

How can ^{1}H NMR be used to determine or confirm chemical structures?

- Chemical shift, integration, & splitting (more on splitting in future lectures)

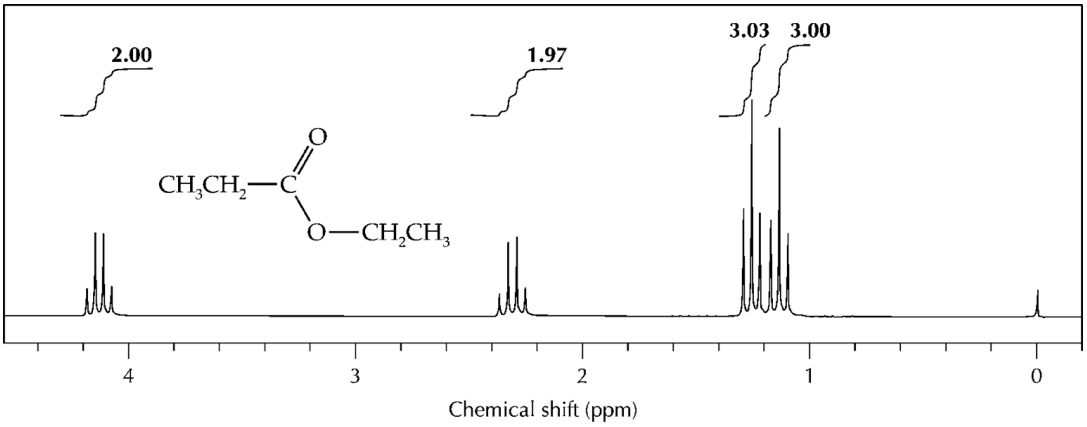


FIGURE 22.11 ^{1}H NMR spectrum of ethyl propanoate at 200 MHz.

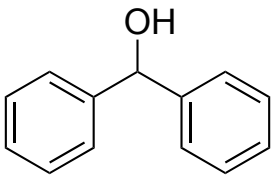
^{1}H NMR Analysis (on paper)

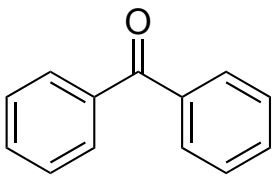
1. How many types of non-equivalent protons are in benzhydrol?

2. What is the relative ratio of H's for each signal?

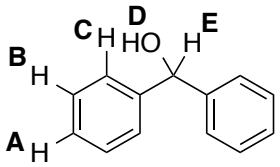
3. What is the chemical shift for each signal?

1. Look for symmetry – **equivalent protons** and for asymmetry – **non-equivalent protons**





2. How many of each type of proton?
3. Identifying **chemical shift** ranges in benzhydrol



Benzhydrol

Calculating expected chemical shifts using chemical shift correlation tables

Base value + Additive parameter (based on group and proximity)

Correlate / assign to signals on given spectrum

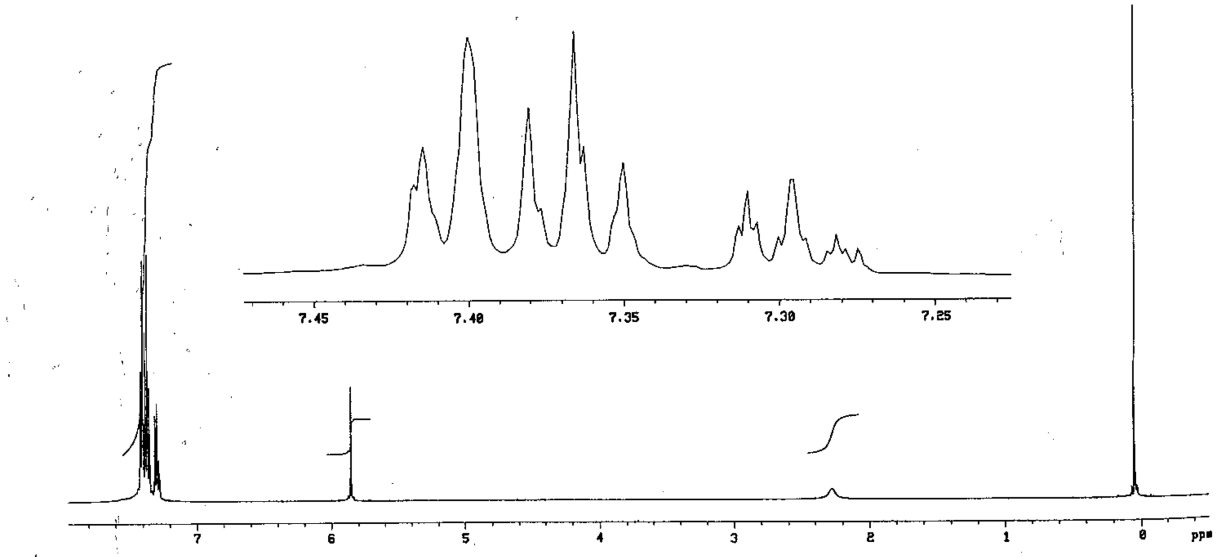
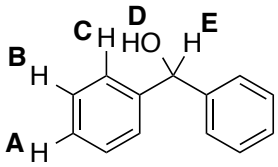


Figure 21.6 500-MHz ^{1}H-NMR spectrum of benzhydrol in $CDCl_3$.

Put it all together…

Table 3. ^{1}H NMR Analysis of Benzhydrol

	Signal	Integration (# of H's)	Expected Chemical Shift (ppm)	Observed Chemical Shift (ppm)
 **Benzhydrol**	**A**			
	B			
	C			
	D			
	E			

Next week in lab: ^{1}H NMR Activity & drawer check

Next week in lecture: Oxidation of Benzhydrol