

NMR I

An Inquiry based lab

In this lab we will be looking at various proton NMR spectra and attempting to see patterns that correlate the spectra with the chemical structures. In class we will hopefully try to get a handle on the theory behind these patterns.

Lets begin by taking a look at the NMR spectrum of ethane.

☺ What are the units on the x-axis?

The peak at zero is the calibration standard and should be ignored.

Lets now look at the NMR spectrum for chloroethane. This spectrum introduces the concepts of integration, chemical shift and splitting.

☺ What is deuterium (D)?

☺ Does it show up on NMR?

Integration is a measurement of the area of the peak. It is related to the number of protons that peak represents.

Chemical shift. Heteroatoms change the chemical environment and tend to push the peaks to the left.

Splitting. The sub peaks a full peak is split into is related to the number of proton neighbors it has. In this spectrum, you see a triplet and a quartet.

Please look through the following spectra and describe the correlation between integration and the number of protons.

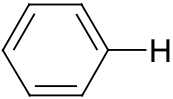
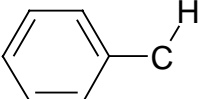
☺ **Integration:**

Please look through the following spectra and describe the correlation between splitting and the number of protons next to the atom.

☺ **Splitting:**

Please look through the following spectra and describe the correlation between chemical shift and the various functional groups.

© **Chemical Shift:**

	chemical shift	deshielding effect
standard	~1	none
$\begin{array}{c} \text{H} \quad \text{O} \\ \quad \\ \text{C}-\text{C} \end{array}$		
$\begin{array}{c} \text{H} \\ \\ \text{C}-\text{O} \end{array}$		
$\begin{array}{c} \text{H} \\ \\ \text{C}-\text{X} \end{array} \text{ (halogen)}$	<i>varies</i>	
$\begin{array}{c} \text{H} \\ \\ \text{C}=\text{C} \end{array}$		
$\begin{array}{c} \text{H} \quad \text{C} \\ \quad \\ \text{C}-\text{C} \end{array}$		
$\begin{array}{c} \text{O} \\ \\ \text{H}-\text{C} \end{array}$		
$\begin{array}{c} \text{O} \\ \\ \text{HO}-\text{C} \end{array}$		
$\text{HO}-\text{C}$		
	7	+6
	2	+1

Lab Report

What are equivalent hydrogens? Answer in complete sentences.

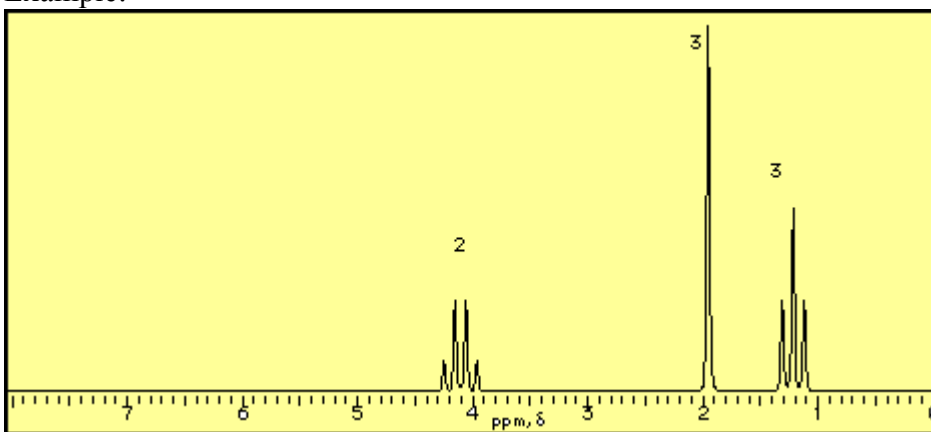
Spectrum number 1

The following structure is ethyl acetate. On the spectrum write the structure and label nonequivalent protons a, b, c..... Identify those peaks on the spectra.

Create a table with the following headings.

Proton, chemical shift, deshielded by, split by

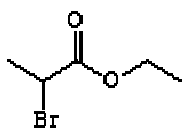
Example:



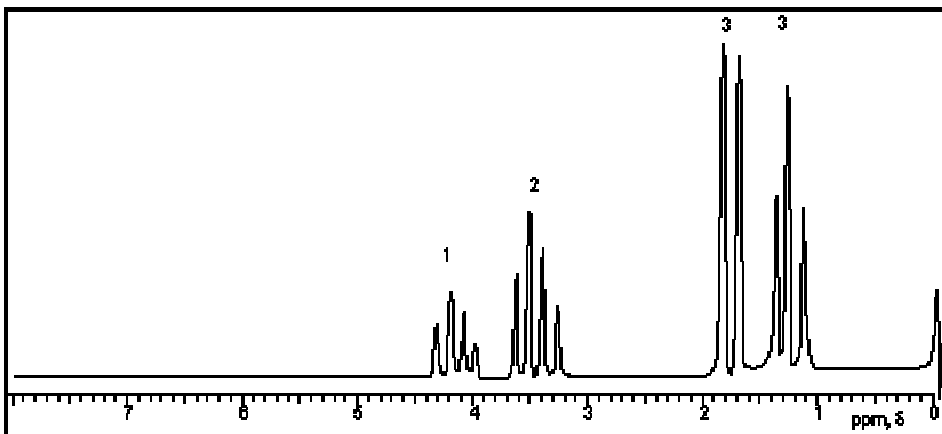
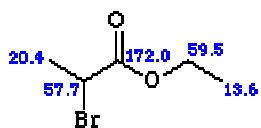
Proton	Chemical shift	Deshielded by	Split by

Spectrum number 2

Structure:



^{13}C NMR Assignments:



Proton	Chemical shift	Deshielded by	Split by

Are chemical shifts additive? Answer in complete sentences using examples from the lab.