NMR Assignment

Purpose: The purpose of this assignment is to get you accustomed to another type of organic chemistry analyzing technique called NMR or Nuclear Magnetic Resonance. There are several different types of NMR (e.g. ^{1}H-NMR, ^{9}F-NMR, ^{13}C-NMR, ^{31}P-NMR). We will be focusing on the ^{1}H-NMR, or nuclear magnetic Resonance that focuses on analyzing the hydrogen atoms of a molecule (a.k.a. proton NMR).

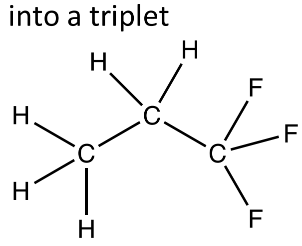
Background

Remember that the average hydrogen atom only has 1 proton (so it weighs 1 a.m.u.) hence the ^{1}H prefix of this type of NMR. Another name you might here would be proton-NMR for the indicating ^{1}H as well. Other types of NMR are ^{13}C- or ^{9}F-NMR (to look at the carbons or fluorines in a molecule), but those are used in graduate school or research labs. NMR is a useful tool for organic chemists because it allows the user to map a molecule's structure. The readout of the NMR shows peaks on a graph similar to an infrared spectrometer, except in the case of ^{1}H-NMR, these peaks indicate the different types of hydrogens in the molecule.

When interpreting a proton-NMR there are generally 4 things to keep in mind:

1. **Number of peaks**- the number of peaks represent types of hydrogens in a compound considering the hydrogens that are equivalent to each other. For example, if you look at a methyl group (CH_3-R), there are 3 hydrogens attached to a single Carbon. Even though there are three hydrogens, they will show up as one peak on a proton-NMR because they are 'equivalent' by being attached to the same carbon. Another way that hydrogens can be equivalent are if they are attached to a different carbon, but the compound is symmetrical, and the hydrogens are on the 'mirrored' carbon.

2. **Peak splitting**- the number of peaks represents the types of carbons, but each peak can be 'split'. The splitting indicated how many hydrogens are on the carbon(s) adjacent to the carbon to which the examined hydrogen is attached, and the peaks are split into the [peak split = n +1] format where "n" is the number of neighbors on the adjacent carbon(s). For example- if I had 1,1,1-trifluoropropane (shown below), there are 2 carbons with hydrogen on them, so there would be two peaks. The middle carbon is attached to two carbons. There are 3 hydrogens attached to those two carbons to which it is attached, so the peak that would represent the middle carbon would be split into 4 tinier peaks. The carbon with hydrogens on the end is attached to 1 carbon that has 2 hydrogens, so the peak representing that carbon would be split into a triplet



1,1,1-trifluoropropane

3. **Peak Height**- the height of the peak is representative of the number of hydrogens that the peak is representing. In the case of 1,1,1-trifluoropropane, the peak that represents the middle carbon is representing 2 hydrogens, and the peak that represents the carbon on the end is representing 3 hydrogens. In this case the peak that represents the carbon on the end (with 3H) would be 50% taller than the peak representing the middle carbon (with 2H).

4. **Peak Location on NMR spectrum**- As mentioned earlier the peaks in an NMR spectrum are located along similar style graph as an IR except this time, the peaks come up from the bottom of the graph. The bottom axis, instead of being read in wavenumbers (cm^{-}) as in IR, are read in 'parts per million' (ppm) that generally go from 12 on the left side to 0 on the right side (12ppm – 0ppm). Hydrogens that are attached to non-electronegative atoms are generally closer to 0ppm. When the hydrogens are attached to more and more polar carbons, or directly to more electronegative atoms, they will move toward 12ppm.

The videos below will provide more details on NMR, the first video goes over the above information a more detail with more examples. Then there is a more complicated example by the same person in the second video. The third video is longer, and by the same person who did the IR video (but not quite as long), but has many more examples.

Assignment

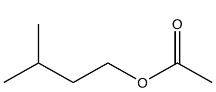
Watch the videos and write a short paragraph (4-5 sentences) about what you learned and how NMR spectroscopy is important. Then match the following compounds to their ^{1}H-NMR spectrum. Along with matching them, tell me which peaks go with which hydrogen types.

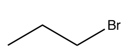
YouTube videos to watch

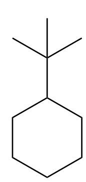
The first two videos do a better job of explaining the terminology of examining an NMR, and the last video is by the same person in the IR assignment video. I would recommend watching the first two before you watch the third one. All together they are about 55 minutes long.

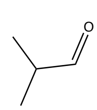
https://www.youtube.com/watch?v=k0eR8YqcA8c
https://www.youtube.com/watch?v=OrvAUDgVoT8
https://www.youtube.com/watch?v=MhiiIKpm5Xw

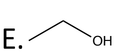
Compounds

A. 

B. 

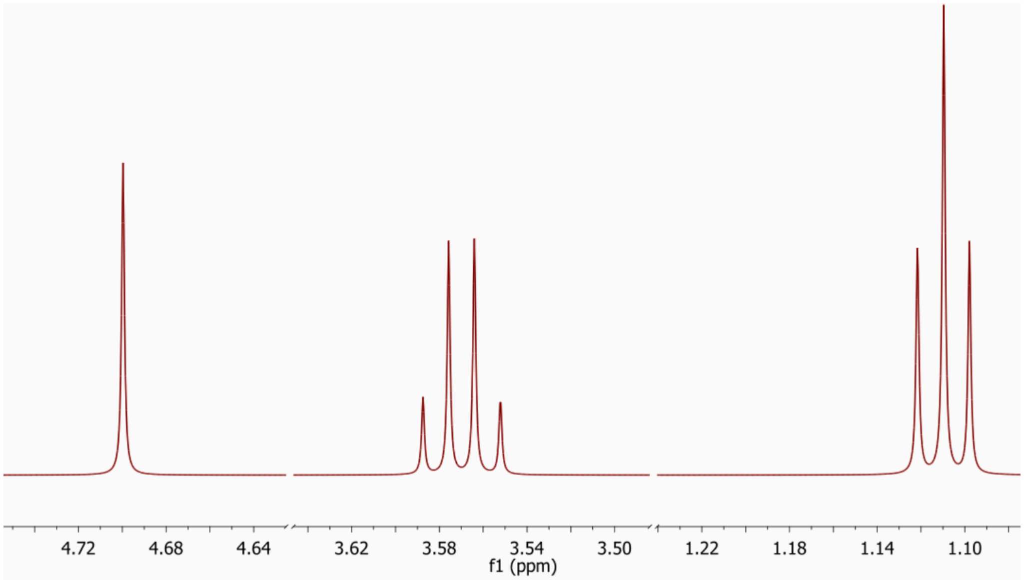
C. 

D. 

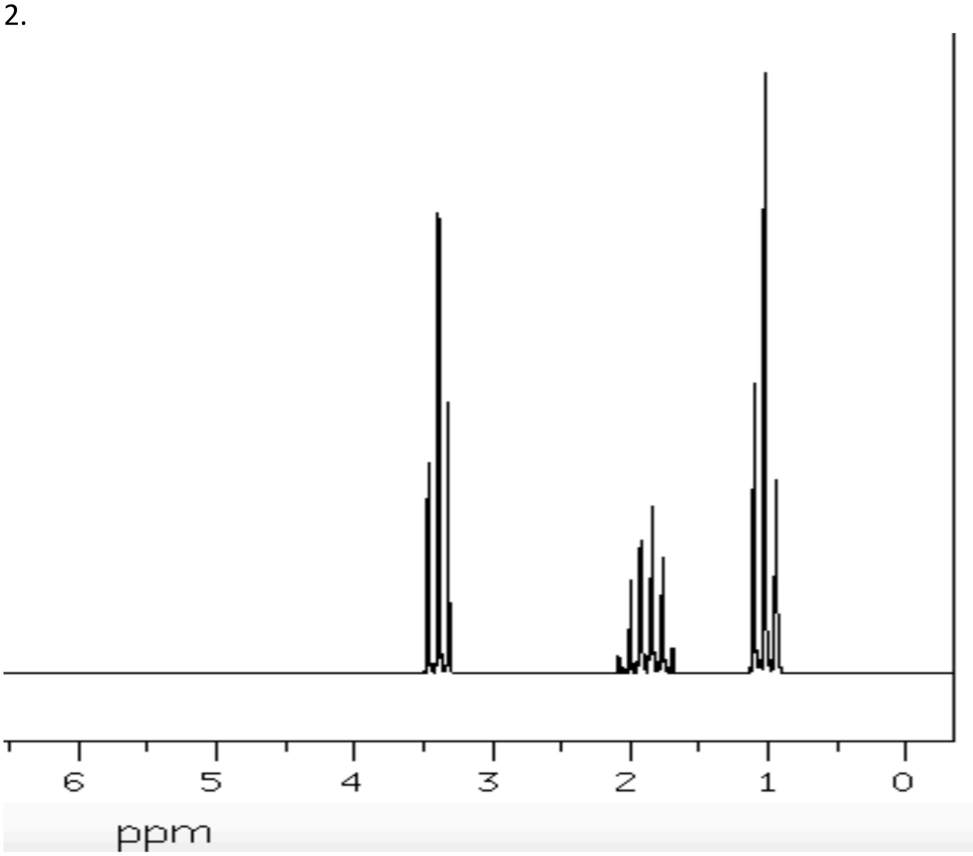
E. 

Spectra to match to compounds.

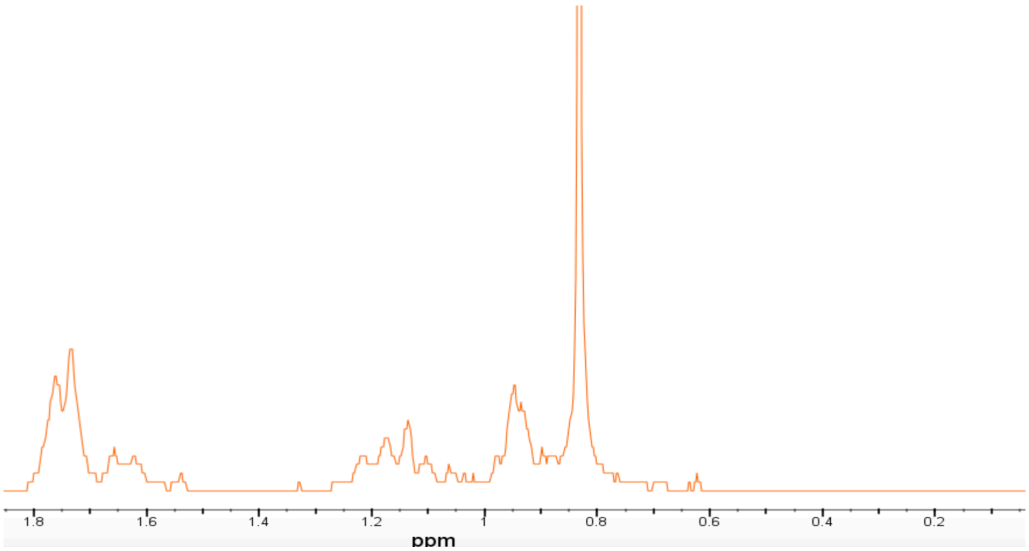
1.



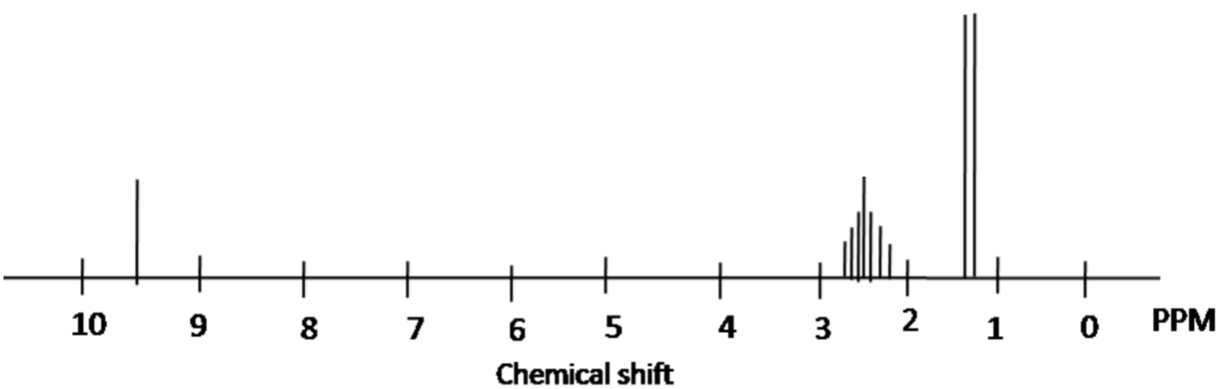
2.



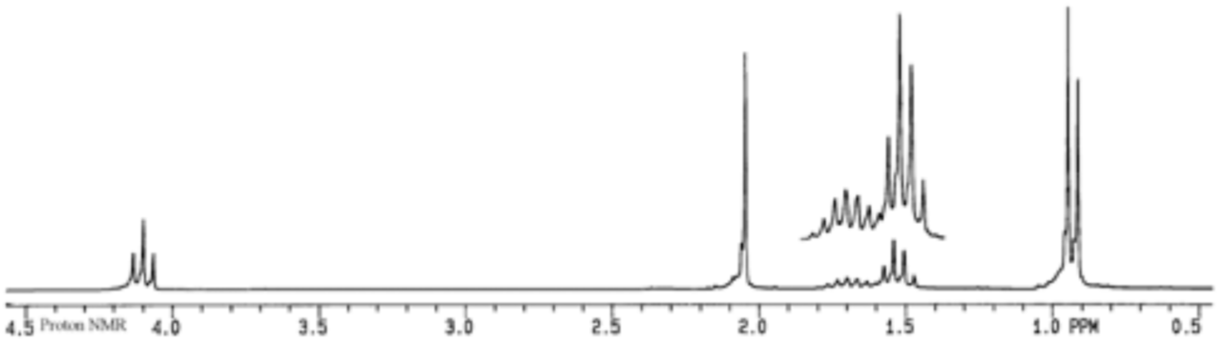
3.



4.



5.



(In addition to the spectrum from 4.5 to 0.5, this picture shows a zoomed in area from 1.8 to 1.4 to show more clearly that there are two different peak types, each with their own number of splits)