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**Chemistry 320M/328M
Dr. Brent Iverson
Practice NMR Problems
December 2, 2024**

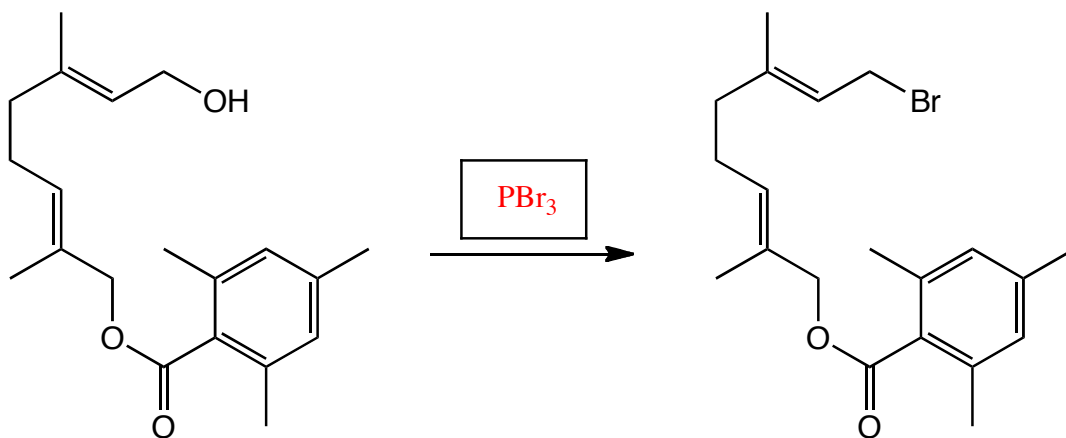
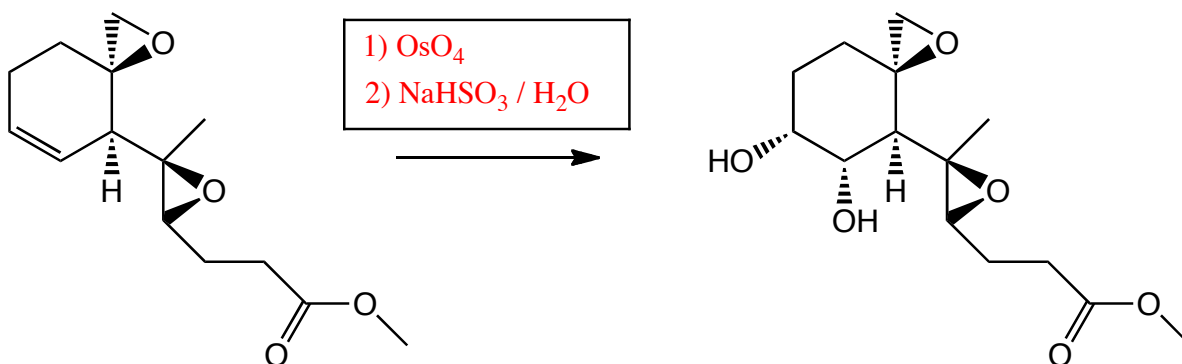
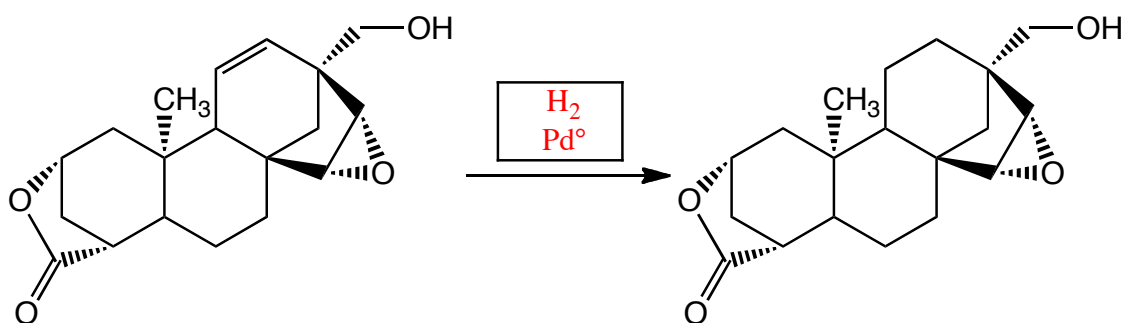
**Please print the
first three letters
of your last name
in the three boxes**

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Score: _____

1. One of the major concepts of organic chemistry is that functional groups such as alkene pi bonds, alcohol groups, or alkyl halides generally react the same whether they are in simple molecules or extraordinarily complex molecules. Below are three examples of very complex molecules that were part of famous organic syntheses by EJ Corey, who was awarded the Nobel prize for his contributions to organic synthesis. **Study the molecules and determine which functional groups were changed. Then, in the box over the arrows, indicate what reagents were used to carry out the transformation. DO NOT BE INTIMIDATED!!! YOU KNOW THIS CHEMISTRY even if you do not understand all there is to know about the structures of these complicated molecules.**

3 pts each



(1 pt. each) **Circle all the statements relating to the theory of NMR that are true.**

A magnetic field will cause charges to move.

A magnetic field will not cause charges to move.

Moving charge creates a magnetic field.

Moving charge does not create a magnetic field.

Electrons, neutrons, and protons are all charged.

Neutrons and protons are both charged.

Only electrons are charged.

Both electrons and protons are charged.

Atomic nuclei with an odd atomic mass or an odd atomic number have a quantum mechanical property called spin.

The best way to think about nuclear spin is as if nuclear positive charge (from the protons) were circulating within the nucleus, thereby creating a small magnetic field that can interact with a strong laboratory magnetic field.

^1H and ^{13}C nuclei have a spin quantum number of 2.

^1H and ^{13}C nuclei have a spin quantum number of 1.

^1H and ^{13}C nuclei have a spin quantum number of $1/2$.

The two spin states of a ^1H nucleus in a strong magnetic field are $+1/2$ and $-1/2$.

The two spin states of a ^1H nucleus in a strong magnetic field are $+1$ and -1 .

The two spin states of a ^1H nucleus in a strong magnetic field are $+2$ and -2 .

(1 pt. each) **Suppose you place a sample of a molecule in a very strong laboratory magnetic field. Circle the following statements that are true:**

A magnetic field will cause the electron density to circulate in the molecule.

The circulating electron density will create its own magnetic field that is in the same direction as the laboratory magnetic field.

The circulating electron density will create its own magnetic field that opposes the laboratory magnetic field.

A ^1H nucleus with spin $+1/2$ will be lower in energy than an equivalent nucleus with a spin of $-1/2$

The difference in energy between $+1/2$ and $-1/2$ spin states for a given ^1H nucleus is directly proportional to the strength of the external magnetic field.

If electromagnetic energy of the precise energy difference between the $+1/2$ and $-1/2$ spins states is used to irradiate the sample, the energy is absorbed as the spin "flips" from the $+1/2$ state to the $-1/2$ state.

"Resonance" in NMR refers to the phenomenon of absorption of energy when a nuclear spin "flips".

The magnetic field "felt" by any given nucleus in a molecule is actually the sum of (i) the external magnetic field plus (ii) the magnetic field of the electrons around the nucleus plus (iii) the magnetic fields caused by the different spin states of adjacent nuclei.

A ^1H nucleus surrounded by greater electron density feels a weaker net magnetic field (external magnetic field plus the induced magnetic field from the circulating electron density) compared to a ^1H nucleus surrounded by less electron density.

A ^1H nucleus surrounded by greater electron density feels a stronger net magnetic field (external magnetic field plus the induced magnetic field from the circulating electron density) compared to a ^1H nucleus surrounded by less electron density.

A ^1H nucleus surrounded by greater electron density is considered to be more shielded and comes into resonance (absorbs electromagnetic radiation) at a lower frequency (smaller ppm).

A ^1H nucleus surrounded by greater electron density is considered to be more shielded and comes into resonance (absorbs electromagnetic radiation) at a higher frequency (larger ppm).

(not graded) These two questions will not be graded, but turn them in anyway. They will help you organize your thoughts regarding NMR and MRI. Something like this might show up on the exam, and that will be graded!

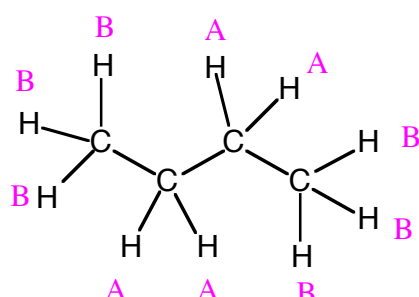
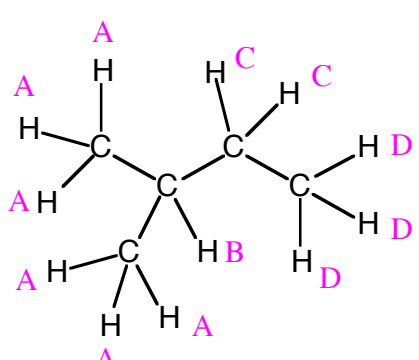
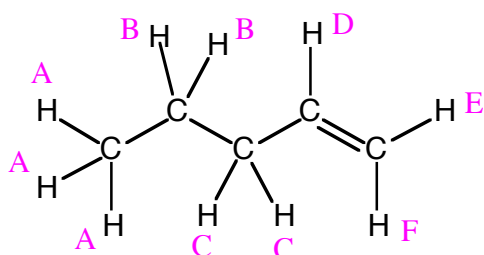
In no more than four sentences, explain what happens in a ^1H NMR experiment.

The ^1H NMR experiment is carried out by placing a sample in a strong magnetic field, then the sample is irradiated with electromagnetic radiation. When the energy of the electromagnetic radiation corresponds exactly to the difference in energy between the $+1/2$ and $-1/2$ nuclear spin states, the nuclei absorb the energy as the nuclear spins are excited (i.e. "flip" when they come into "resonance" with the electromagnetic radiation) from the lower energy spin state ($+1/2$) to the higher energy spin state ($-1/2$). The NMR spectrum is a plot of absorbance vs. frequency scaled for magnetic field strength, wherein chemical shift (distance from the TMS signal at 0 ppm) is correlated with the functional groups present, the connectivity of atoms in molecules can be determined by splitting, and the relative ratio of different equivalent H atoms in the molecule is proportional to the relative integrations of the different signals.

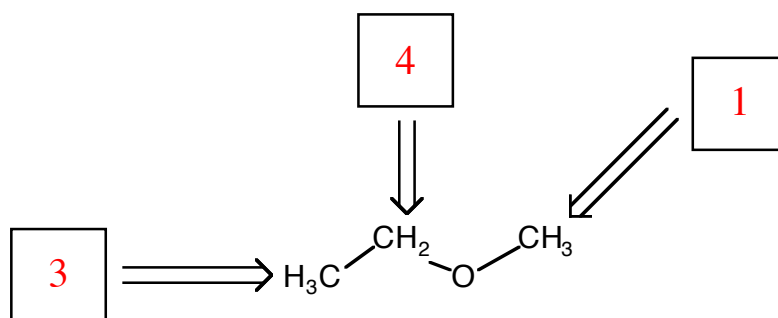
Suppose a relative of yours is having an MRI. In no more than four sentences, explain to them what is happening when they have the MRI scan. *****This will be on the first page of the final!!!*****
Please memorize this passage, the same one given to you in class.

The popular medical diagnostic technique of **magnetic resonance imaging (MRI)** is based on the **same principles as NMR**, namely the **flipping (i.e. resonance) of nuclear spins of protons by radio frequency irradiation** when a patient is placed in a **strong magnetic field**. **Magnetic field gradients** are used to gain imaging information, and **rotation of the gradient around the center of the object** gives imaging in an entire plane (i.e. **slice inside patient**). In an MRI image, you are looking at **individual slices that when stacked make up the three-dimensional image of relative amounts of protons, especially the protons from water and fat, in the different tissues**.

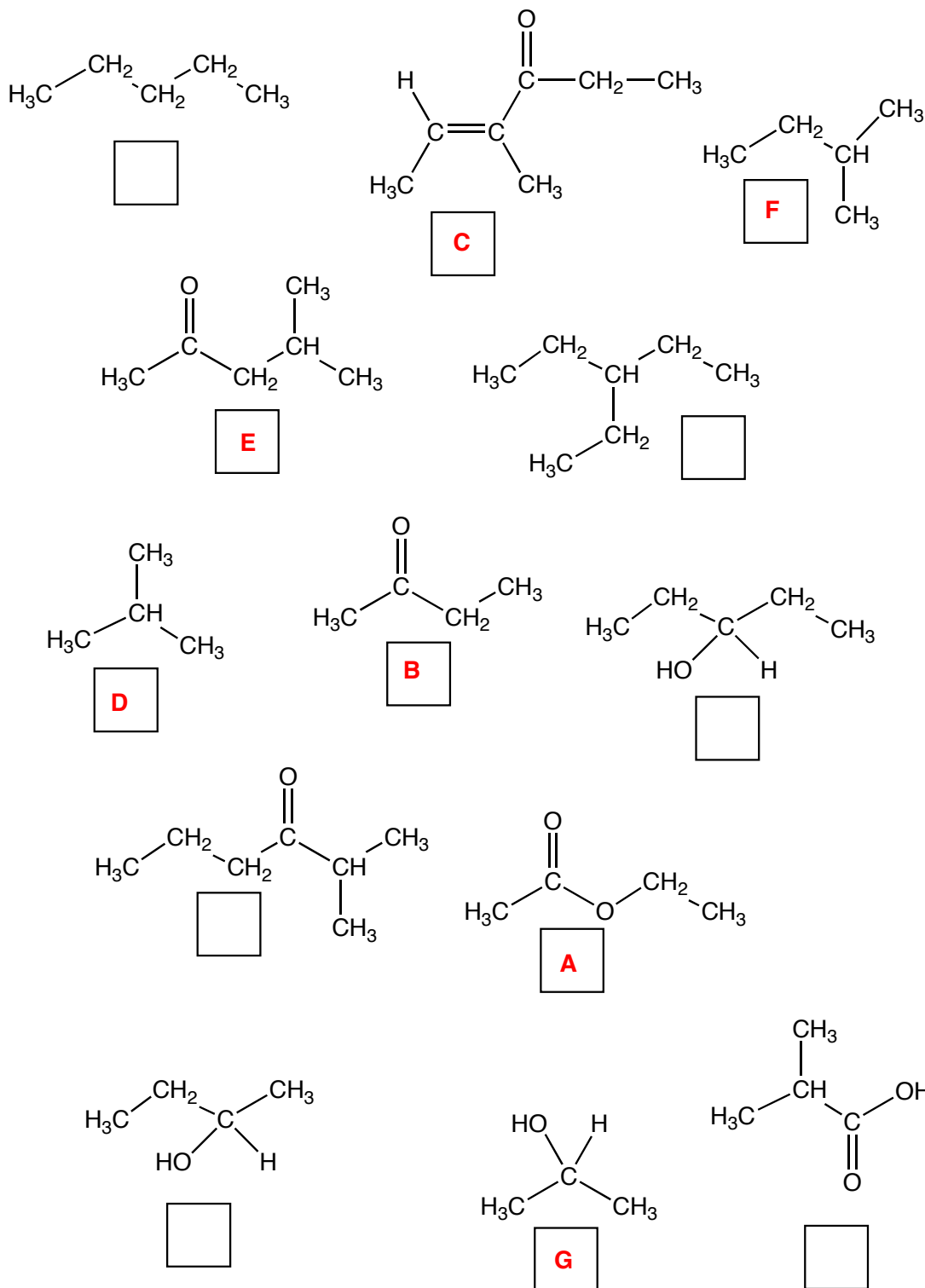
(1 pt. each) For this problem you need to ignore spin-spin splitting, in that we consider one signal to be derived from one set of equivalent H atoms, regardless of splitting pattern. For each of the next three molecules, on the lines provided state how many sets of equivalent sets of H atoms are present, next state how many different signals will appear in the ^1H NMR spectrum of each, and finally, the relative ratios of the integrations of the different signals (i.e. 1:2 or 1:2:6, etc.).

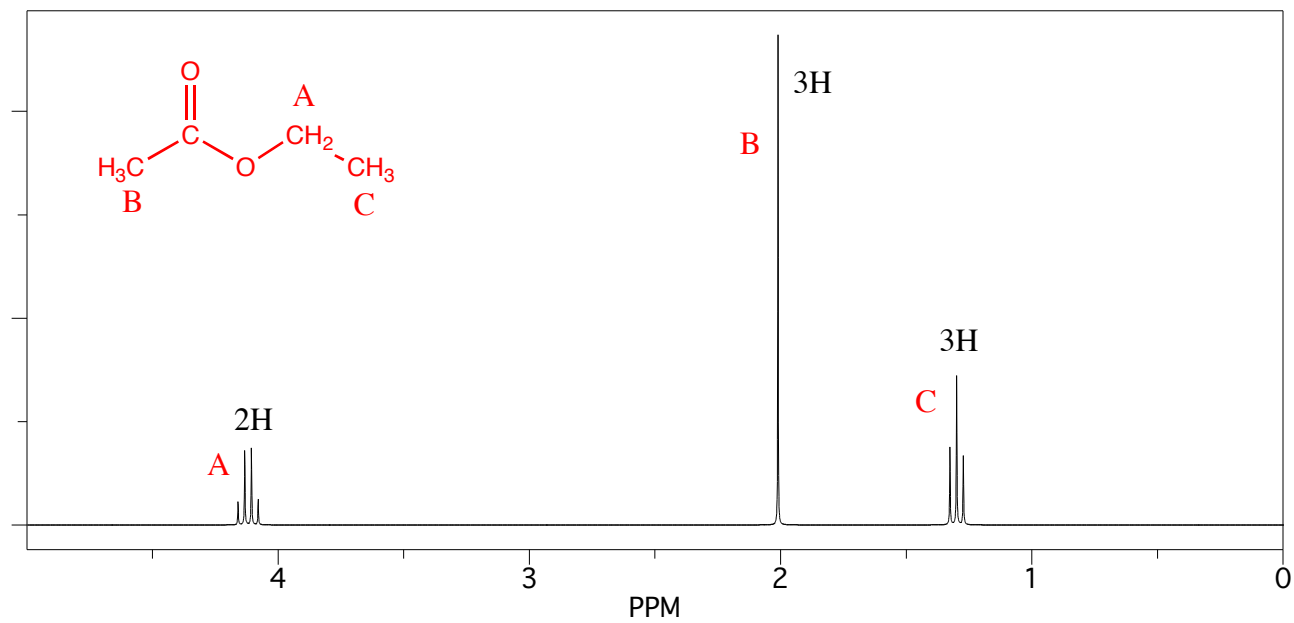
	Number of sets of equivalent H atoms	Number of different signals in the NMR spectrum	Ratio of signal integrations
	<u>2</u>	<u>2</u>	B:A <u>4:6 (or 2:3)</u>
	<u>4</u>	<u>4</u>	B:C:D:A <u>1:2:3:6</u>
	<u>6</u>	<u>6</u>	D:E:F:B:C:A <u>1:1:1:2:2:3</u>

(1 pt. each) For the following molecule, in the boxes provided, state the number of peaks you expect in each ^1H NMR signal due to spin-spin splitting.

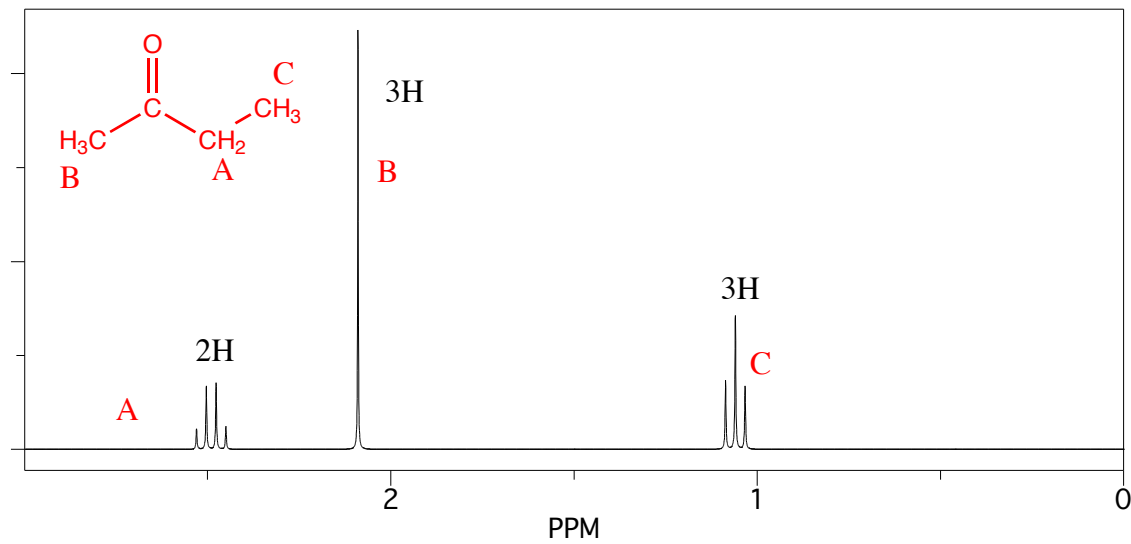


On the following pages there are NMR spectra. The relative integrations are given above each signal. Assign each spectra to the appropriate structure out of the following possibilities. **Each NMR spectrum has a letter on it. Write the appropriate letter underneath the molecules in the space provided.** Notice that not all of the molecules below will have letters underneath them, as there are only seven spectra but thirteen molecules. You didn't want us to make it too easy, did you? We recommend you print the problems as the spectra are easier to read when printed.

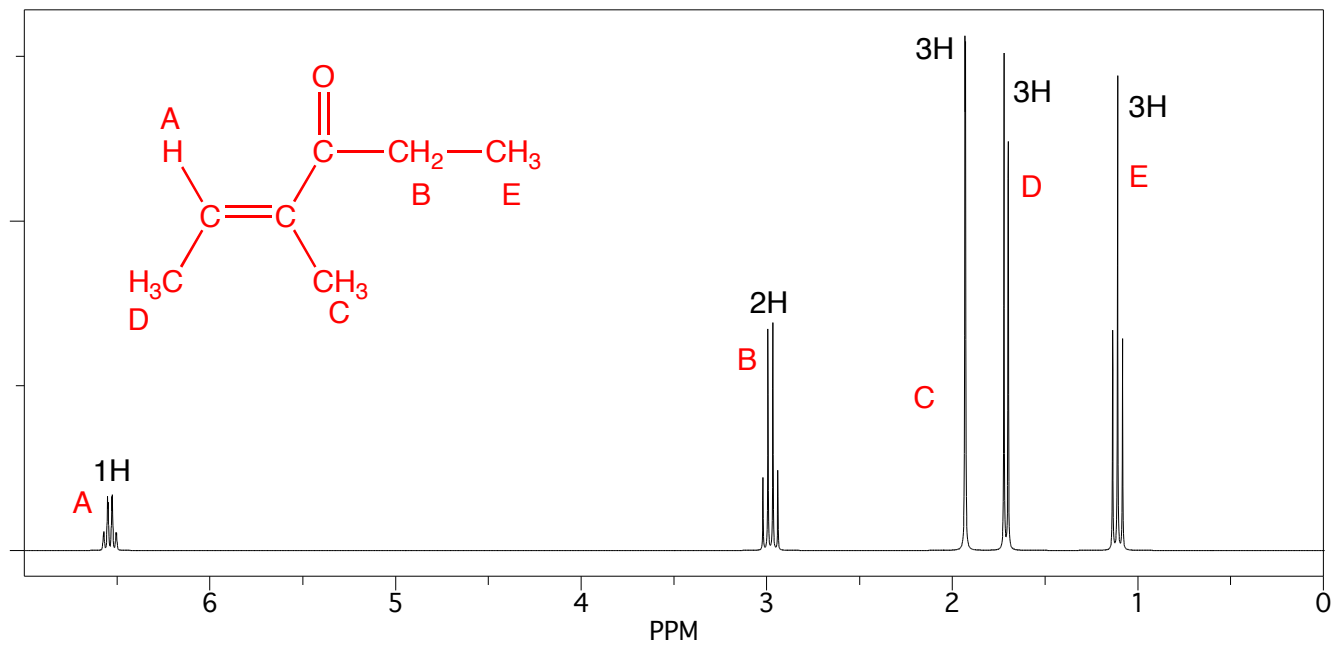


A

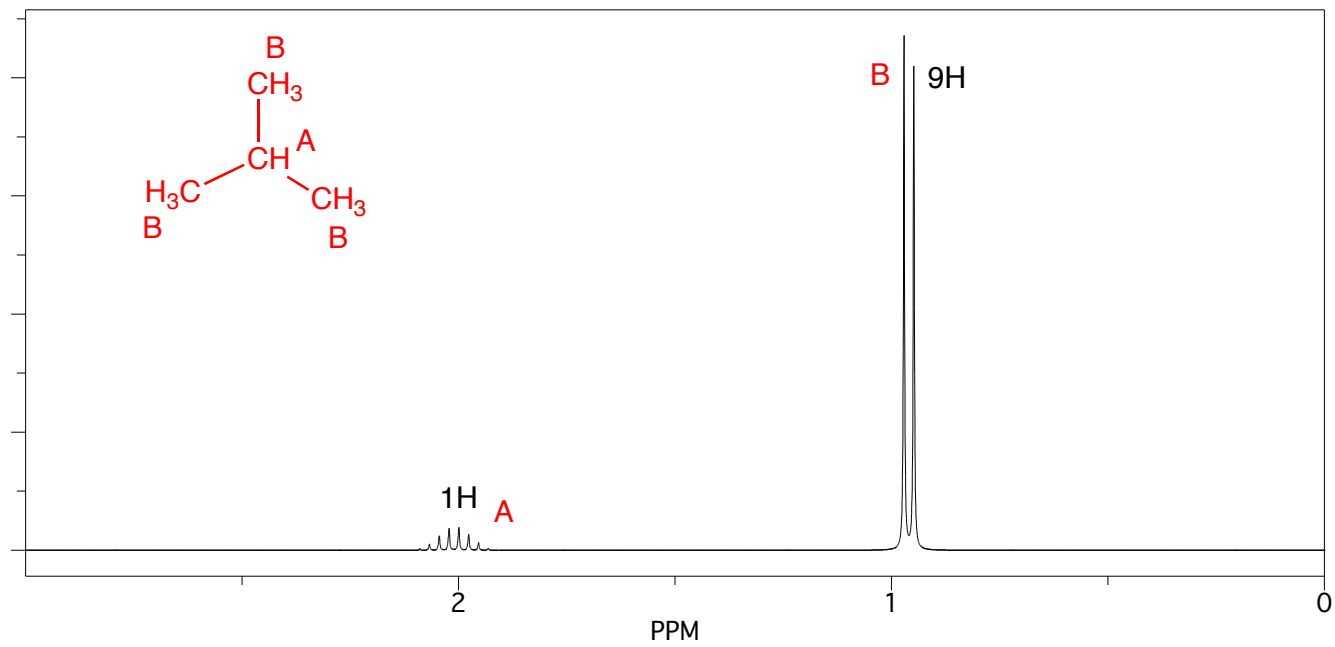
B



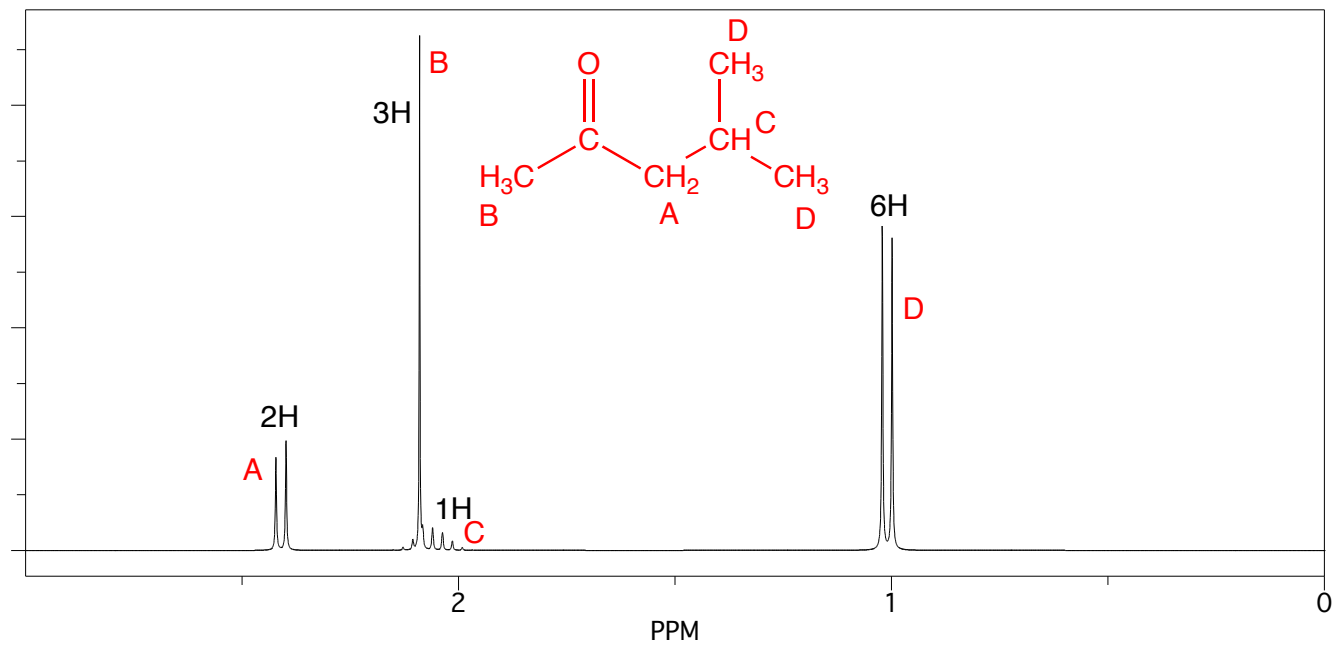
C



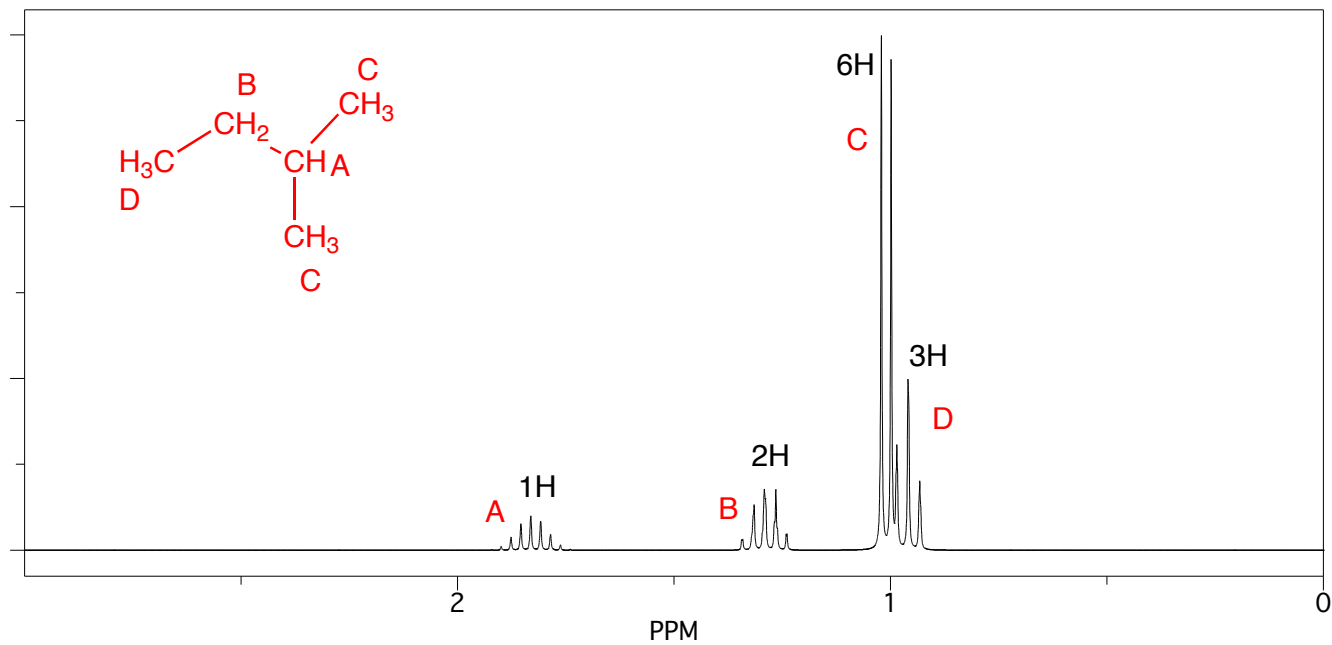
D



E



F



G

