NMR Problem Set# 1

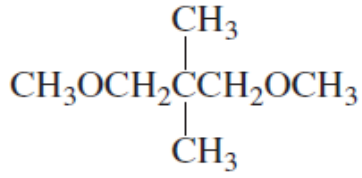
1. What frequency (in MHz) is required to cause a proton to flip its spin when it is exposed to a magnetic field of 1 tesla?

2.

How could you distinguish the ^{1}H NMR spectra of the following compounds?

a. $CH_3OCH_2OCH_3$

b. CH_3OCH_3

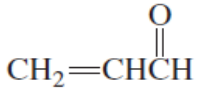
c. 

How many signals would you expect to see in the ^{1}H NMR spectrum of each of the following compounds?

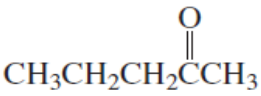
a. $CH_3CH_2CH_2CH_3$

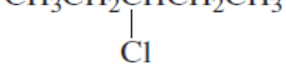
b. $BrCH_2CH_2Br$

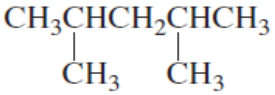
c. $CH_2{=}CHCl$

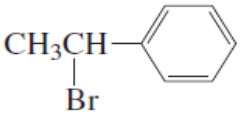
d. 

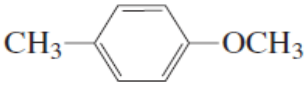
e. 

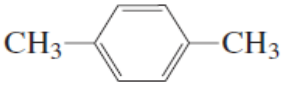
f. 

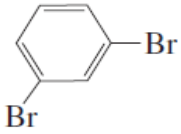
g. 

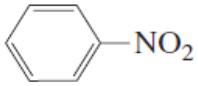
h. 

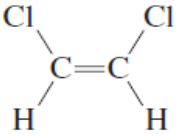
i. 

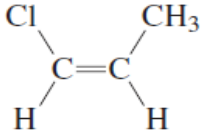
j. 

k. 

l. 

m. 

n. 

o. 

3.

4. A signal has been reported to occur at 600 Hz downfield from TMS in an NMR spectrometer with a 300-MHz operating frequency.

a. What is the chemical shift of the signal?

b. What would its chemical shift be in an instrument operating at 100 MHz?

c. How many hertz downfield from TMS would the signal be in a 100-MHz spectrometer?

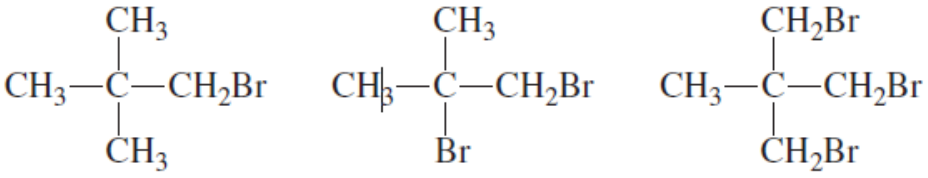
5.

a. If two signals differ by 1.5 ppm in a 300-MHz spectrometer, by how much do they differ in a 100-MHz spectrometer?

b. If two signals differ by 90 hertz in a 300-MHz spectrometer, by how much do they differ in a 100-MHz spectrometer?

6.

How would integration distinguish the ^{1}H NMR spectra of the following compounds?



7.

a. Calculate the ratios of the different kinds of protons in a compound with an integral ratio of 6 : 4 : 18.4 (going from left to right across the spectrum).

b. Determine the structure of a compound that would give these relative integrals in the observed order.

8.

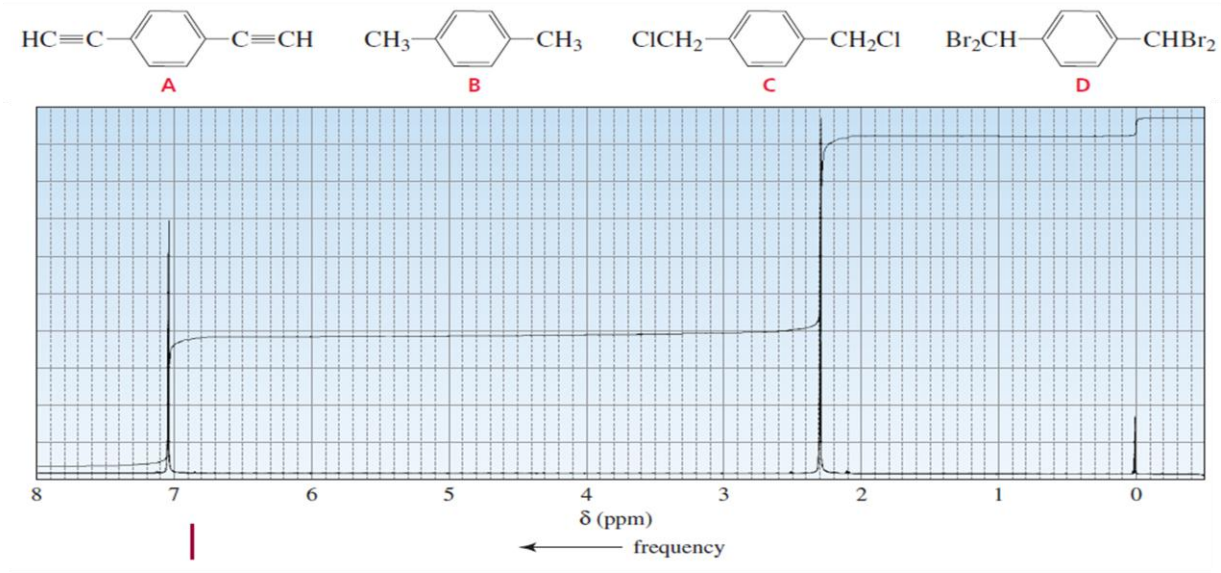
a. Which set of protons in each of the following compounds is the least shielded?

1. $CH_3CH_2CH_2Cl$ 2. $CH_3CH_2\overset{\overset{O}{\|}}{C}OCH_3$ 3. $CH_3\underset{Br}{\underset{|}{C}}H\underset{Br}{\underset{|}{C}}HBr$

b. Which set of protons in each compound is the most shielded?

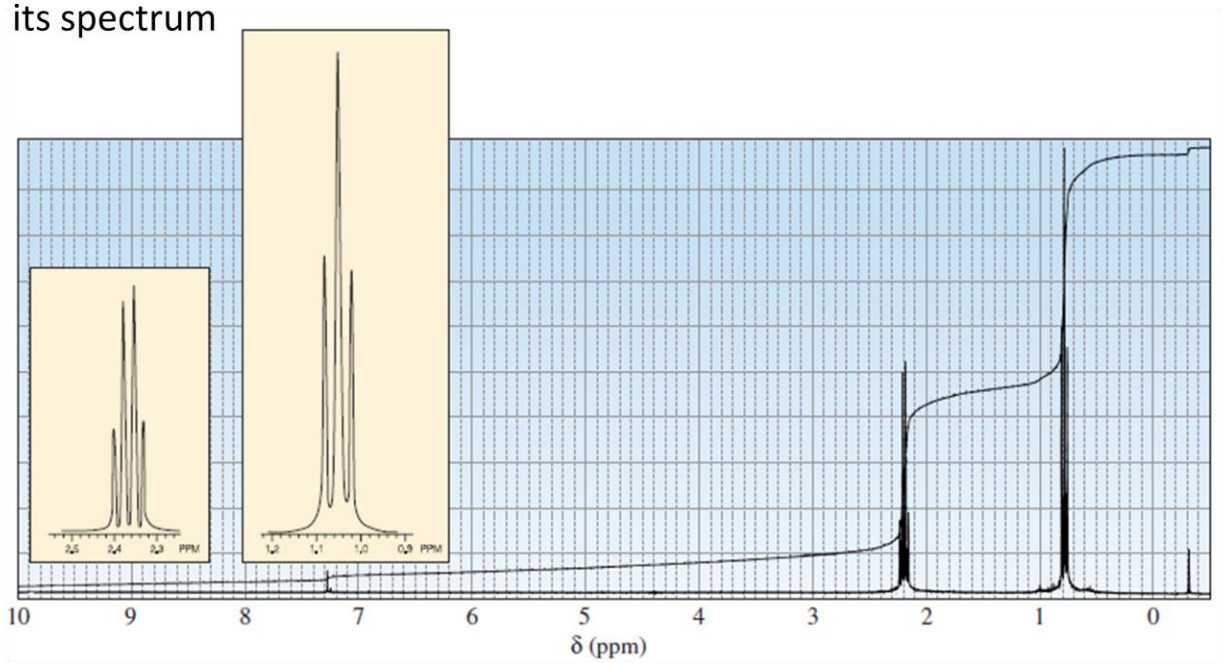
9.

The ^{1}H NMR spectrum shown below corresponds to one of the following compounds. Which compound is responsible for this spectrum?



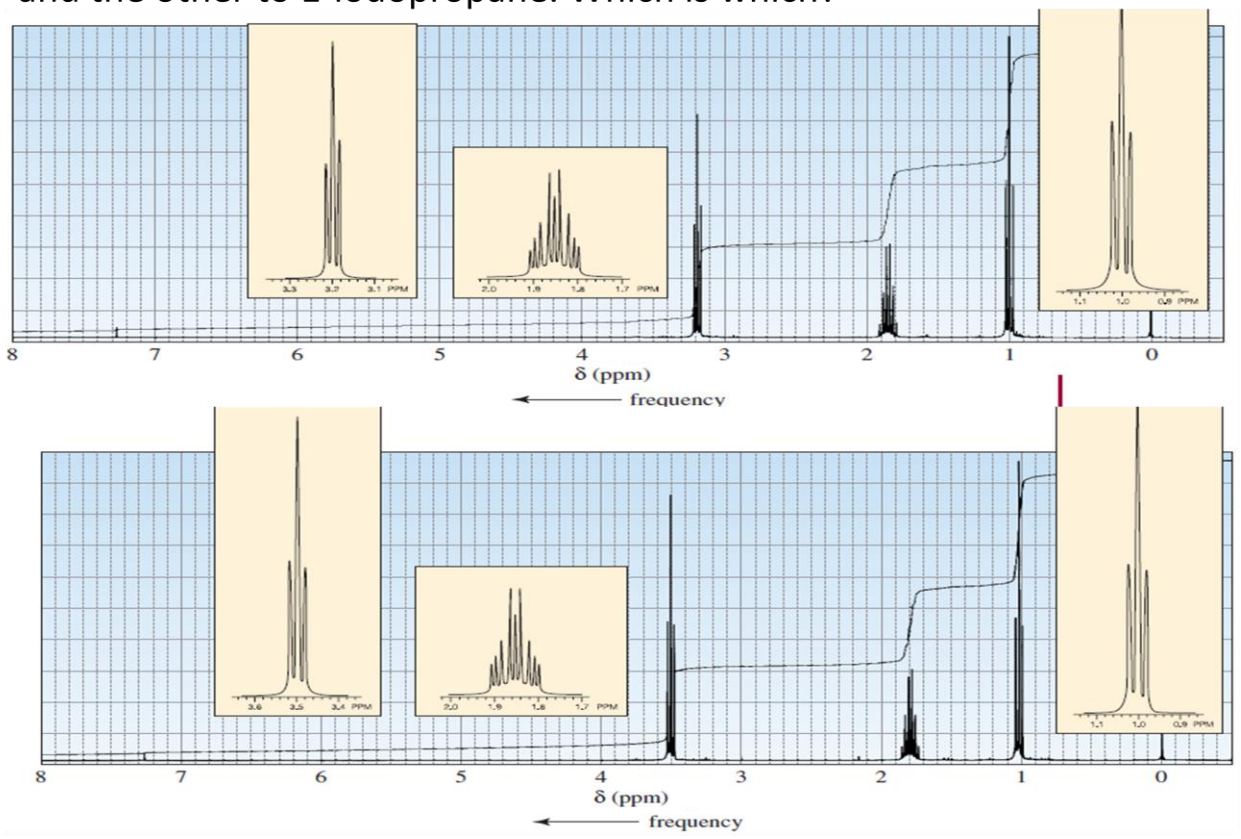
10.

Identify the following compound from its molecular formula $C_5H_{10}O$ and its spectrum



11.

One of the spectra in the following Figure is due to 1-chloropropane, and the other to 1-iodopropane. Which is which?



12.

In each of the following compounds, which of the underlined protons has the greater chemical shift (i.e., the farther downfield signal or the higher frequency signal)?

a. $CH_3\underline{C}H\underline{C}H\underline{B}r$ (Br, Br)

b. $\underline{C}H_3CHO\underline{C}H_3$ (CH_3)

c. $CH_3\underline{C}H_2CH\underline{C}H_3$ (Cl)

d. $CH_3\underline{C}H\underline{C}(=O)\underline{C}H_2CH_3$ (CH_3)

e. $CH_3\underline{C}H_2CH=\underline{C}H_2$

13.

In each of the following pairs of compounds, which of the underlined protons has the greater chemical shift (i.e., the farther downfield signal or the higher frequency signal)?

a. $CH_3CH_2\underline{C}H_2Cl$ or $CH_3CH_2\underline{C}H_2Br$

b. $CH_3CH_2\underline{C}H_2Cl$ or $CH_3CH_2\underline{C}H(Cl)CH_3$

c. $CH_3CH_2\overset{O}{\overset{\|}{C}}\underline{H}$ or $CH_3CH_2\overset{O}{\overset{\|}{C}}OCH_3$

14.

Label the protons in the following compounds: The proton that gives the signal at the lowest frequency should be labeled *a*, the next *b*, etc.

a. $CH_3CH_2\overset{O}{\overset{\|}{C}}H$

b. $CH_3CH_2CH(OCH_3)CH_3$

c. $ClCH_2CH_2CH_2Cl$

d. $CH_3CH_2CH_2\overset{O}{\overset{\|}{C}}OCH_3$

e. $CH_3CH_2CH(OCH_3)CH_2CH_3$

f. $CH_3CH_2CH_2OCH(CH_3)CH_3$

g. $CH_3CH_2CH_2\overset{O}{\overset{\|}{C}}CH_3$

h. $CH_3CH(CH_3)CH_2OCH_3$

i. $CH_3CH(CH_3)CH(Cl)CH_3$

15.

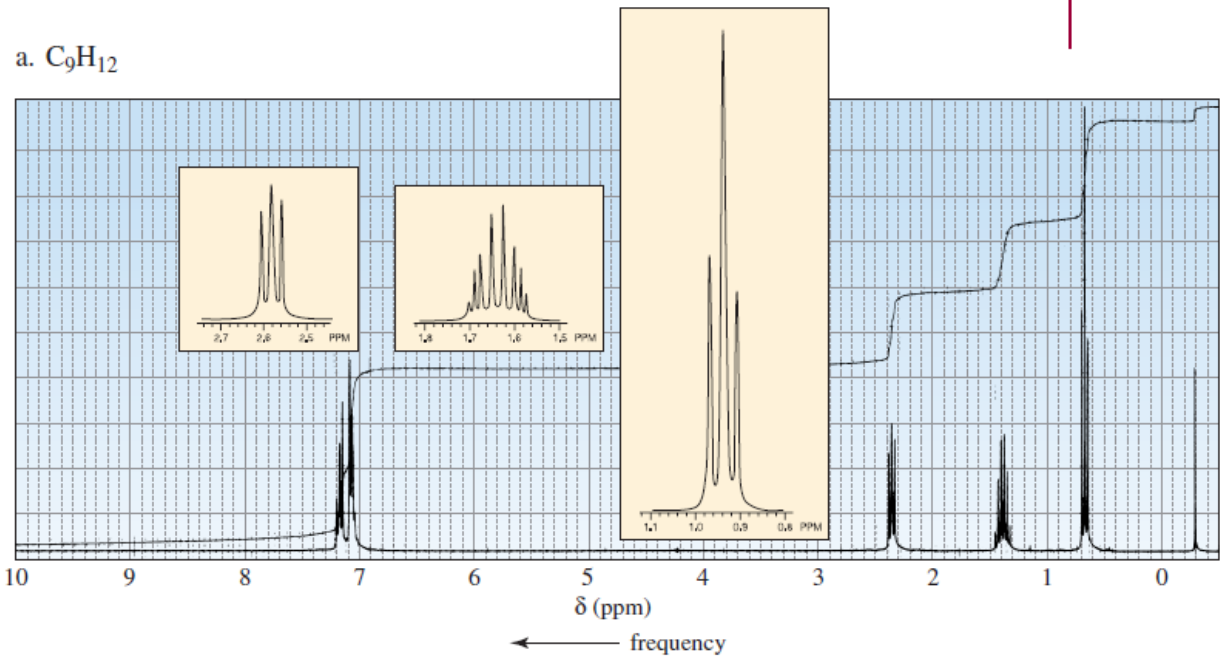
A 300-MHz spectrometer records a proton that absorbs at a frequency 2130 Hz downfield from TMS.

(a) Determine its chemical shift.

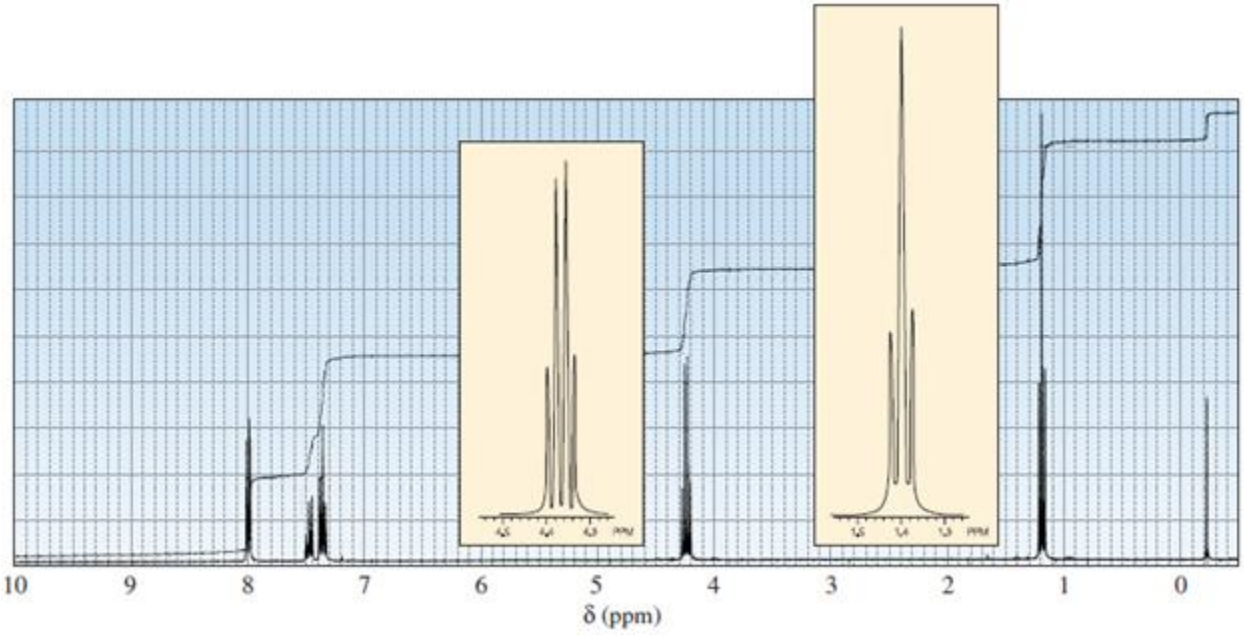
(b) Predict this proton's chemical shift at 60 MHz.

16. Identify each compound from its molecular formula and its ^{1}H NMR spectrum:

a. C_9H_{12}



b. $C_9H_{10}O_2$



17.

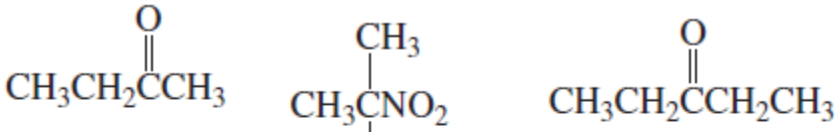
Identify the following compounds. (Relative integrals are given from left to right across the spectrum.)

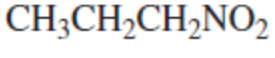
a. The ^{1}H NMR spectrum of a compound with molecular formula $C_4H_{10}O_2$ has two singlets with an area ratio of 2 : 3.

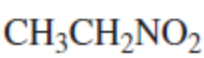
b. The ^{1}H NMR spectrum of a compound with molecular formula $C_6H_{10}O_2$ has two singlets with an area ratio of 2 : 3.

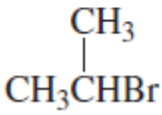
c. The ^{1}H NMR spectrum of a compound with molecular formula $C_8H_6O_2$ has two singlets with an area ratio of 1 : 2.

18. Match each spectrum with one of the following compounds:

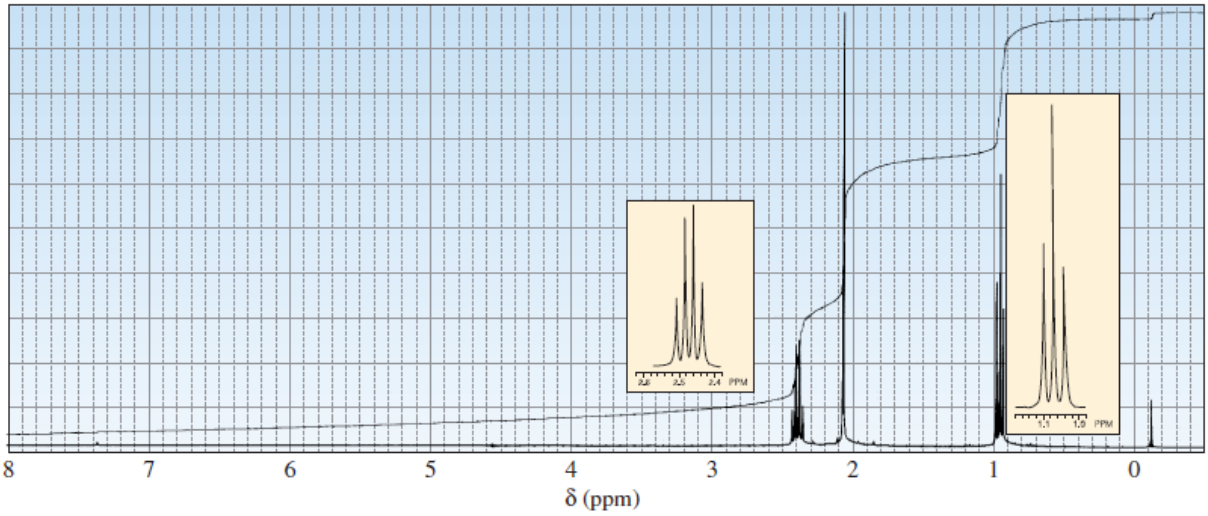


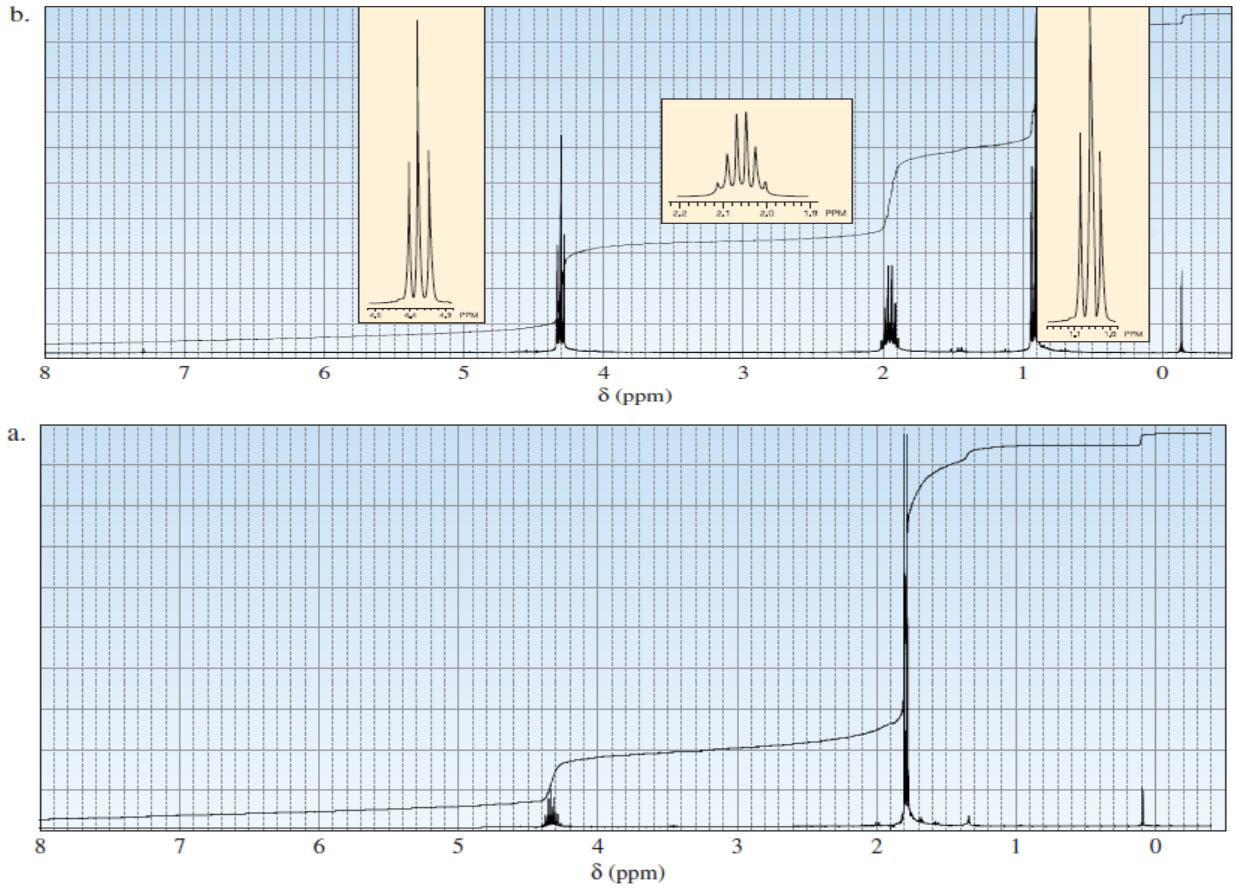






c.





19.

Determine the structure of the compound with molecular formula C10H14O2