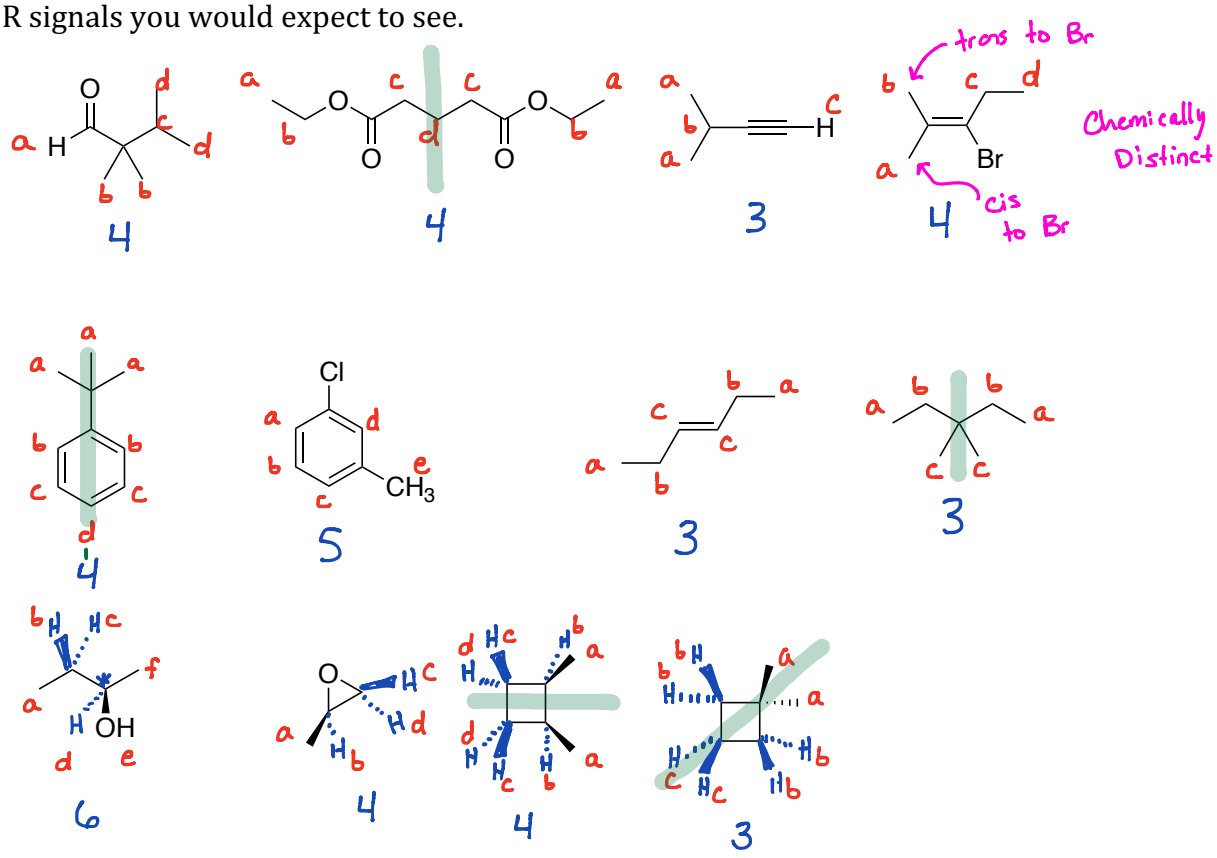
Answer Key

Chemistry 233

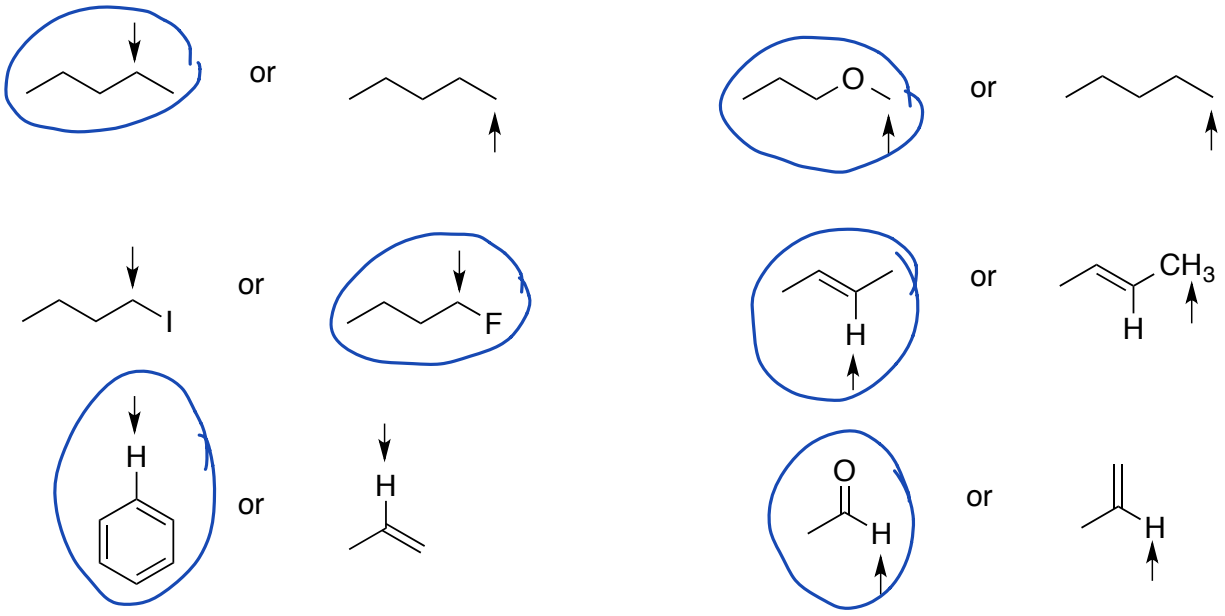
Chapter 13: NMR Spectroscopy Problem Set

1) For each compound below, identify each chemically distinct type of hydrogen. Specify the number of ^{1}H NMR signals you would expect to see.

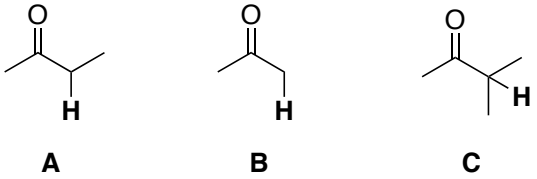


2) Which of the indicated protons in each pair shows up farther downfield?

Tips: For H-C-Z, H moves further downfield as Z becomes more electronegative
For C_{sp^3}-H, H moves further downfield as C becomes more substituted (3°>2°>1°)



3) Consider the indicated protons in each of the three compounds below. Arrange in order of increasing chemical shift of the indicated proton. *See tips in Q2.*

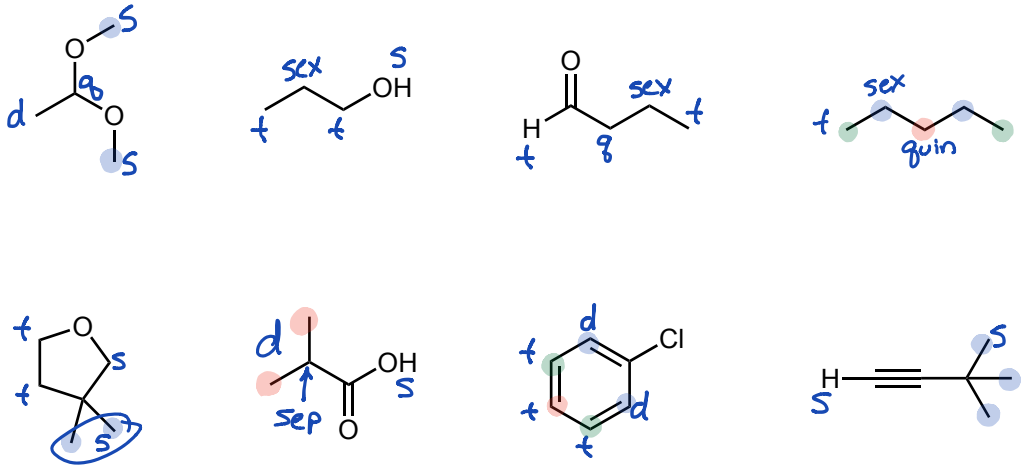


lowest δ highest δ

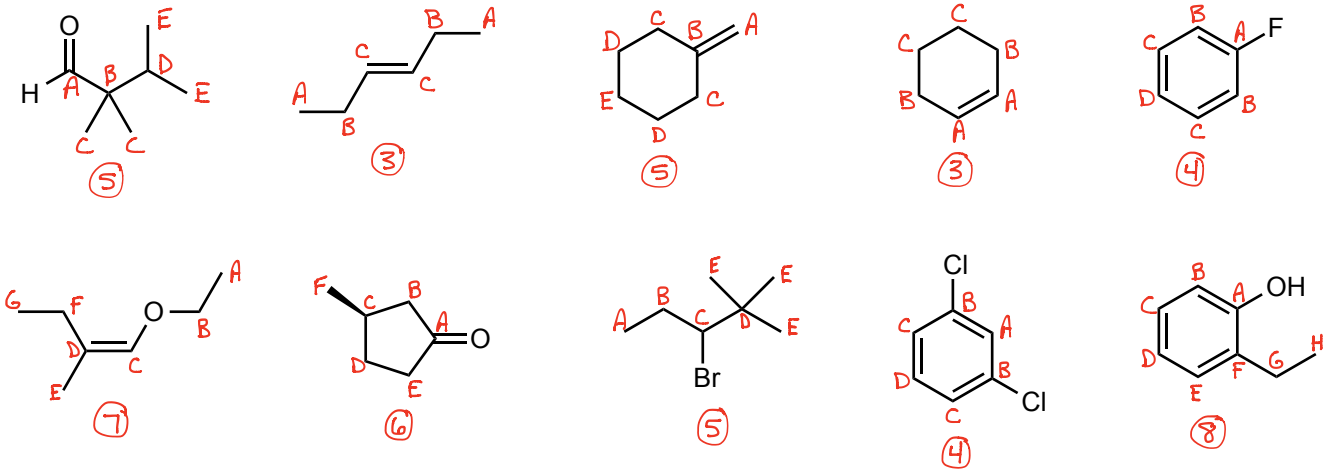
B < A < C

4) For each of the compounds below, determine the expected splitting for all protons.

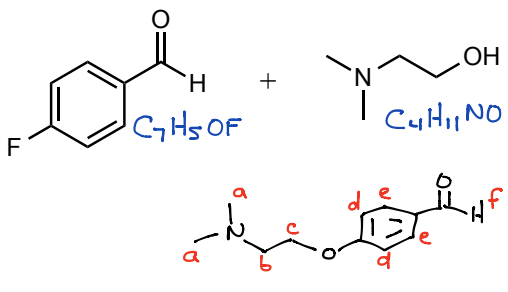
2 doublet (d)
3 triplet (t)
4 quartet (q)
5 quintet (quin)
6 sextet (sex)
7 septet (sep)



5) How many ^{13}C signals would you expect each compound below to exhibit? (i.e. How many chemically distinct C atoms are present in each molecule?)



6) The reaction shown below was carried out in a laboratory to give a compound with the indicated spectral data. Determine the structure of this compound.



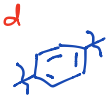
$C_{11}H_{15}NO_2$ – lost H and F

IR stretch at 1730 cm^{-1} – retain aldehyde

Eight signals in the ^{13}C NMR

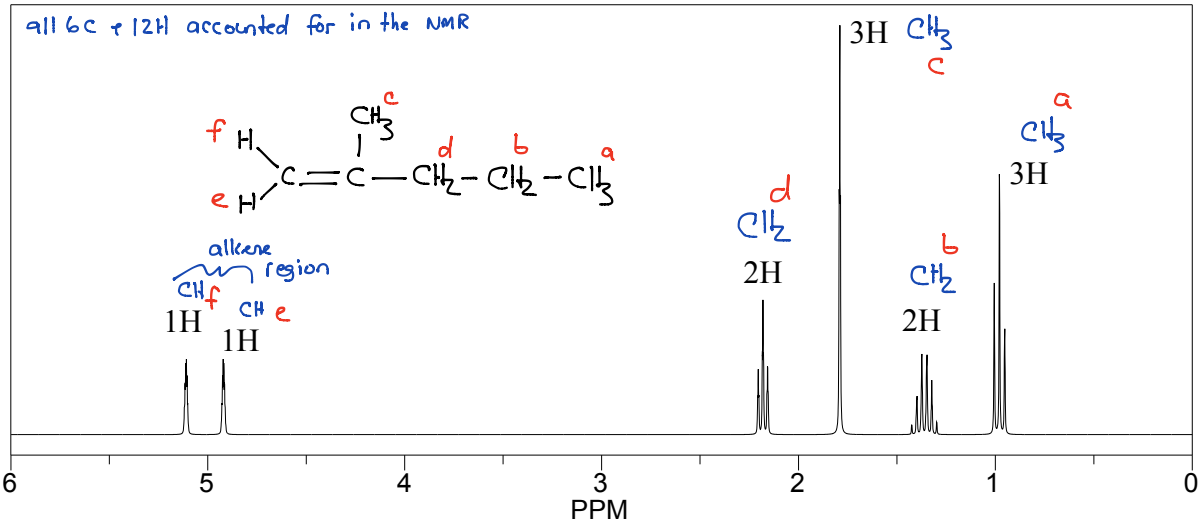
^1H NMR Data: 2.32 (s, 6H), 3.05 (t, 2H), 4.20 (t, 2H), 6.97 (d, 2H), 7.82 (d, 2H), 9.97 (s, 1H)

aromatic region; o=CH (ald)

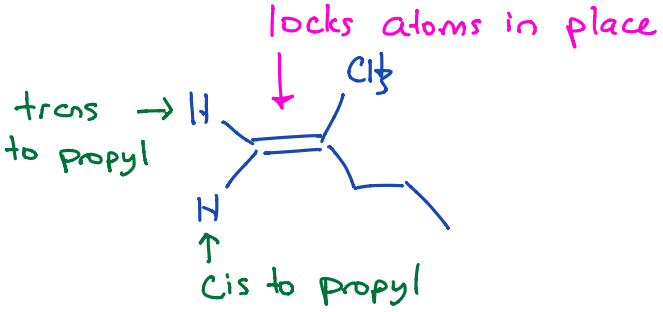


7) For each of the following, use the data provided to deduce an appropriate structure.

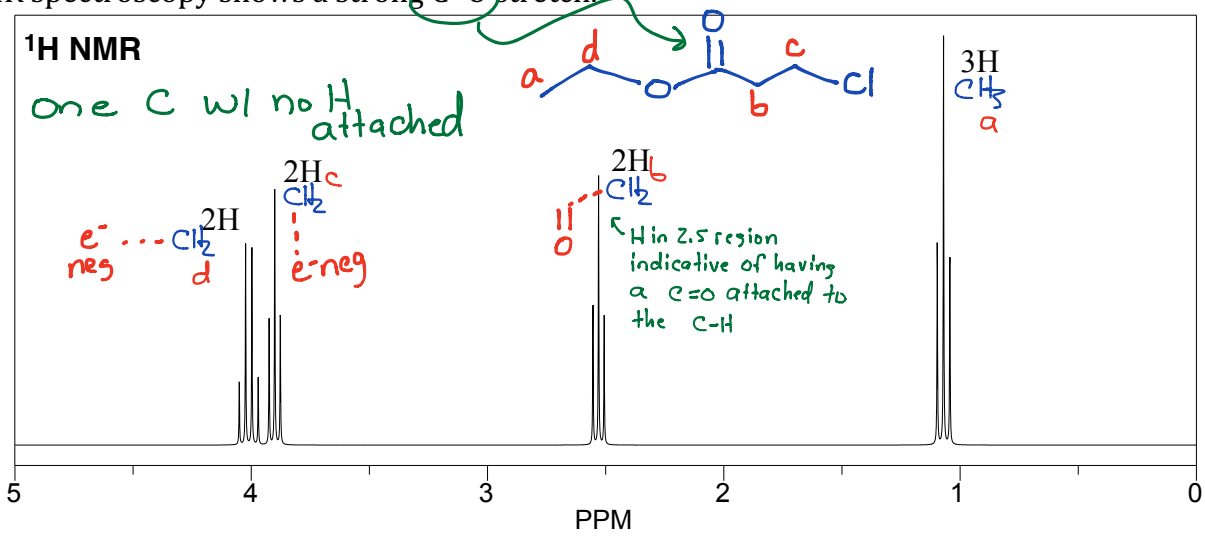
A. C_6H_{12} → 1 unsat

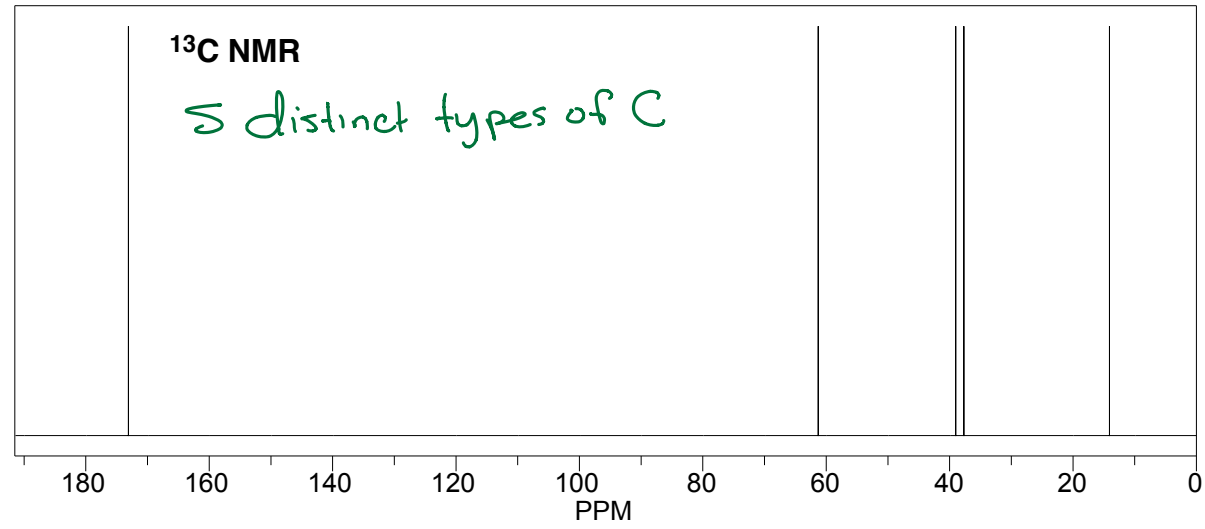


The alkene H are chemically distinct

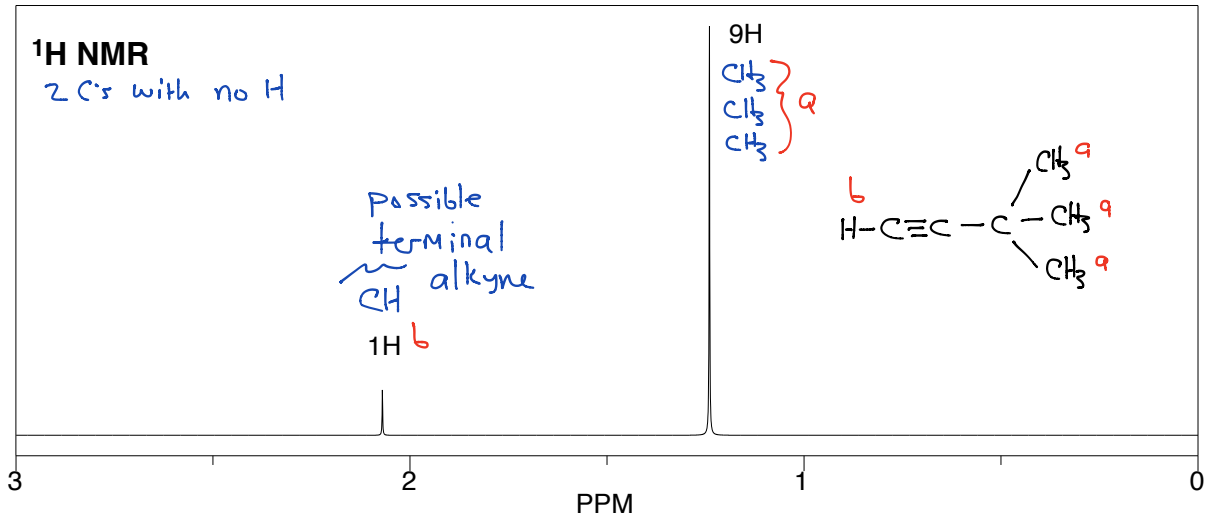


B. $C_5H_9ClO_2$ *Use the ^{13}C NMR to determine the number of distinct C atoms.*
IR spectroscopy shows a strong C=O stretch.



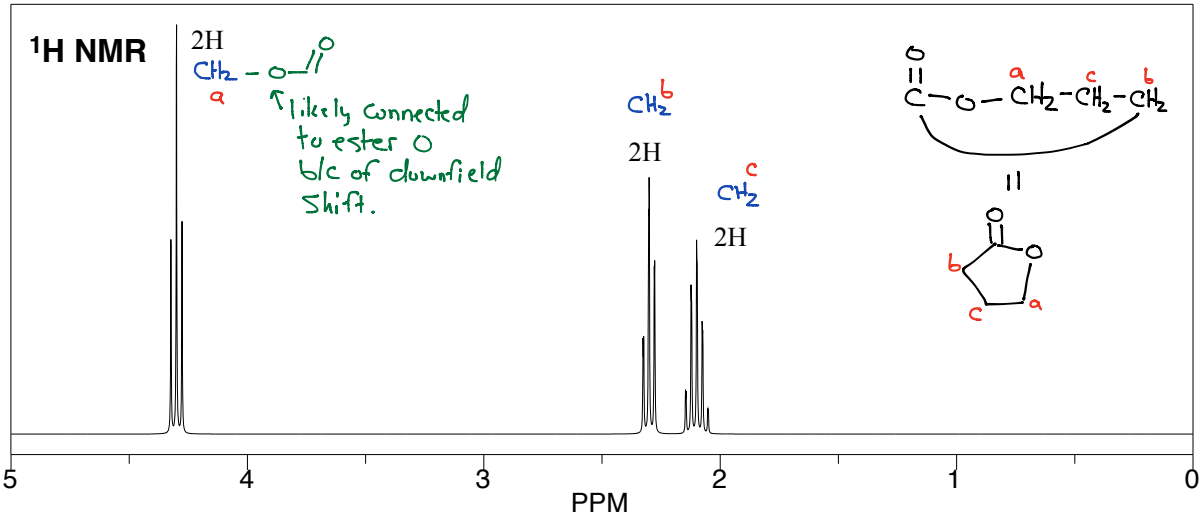


C. C_6H_{10} – 2 unsat

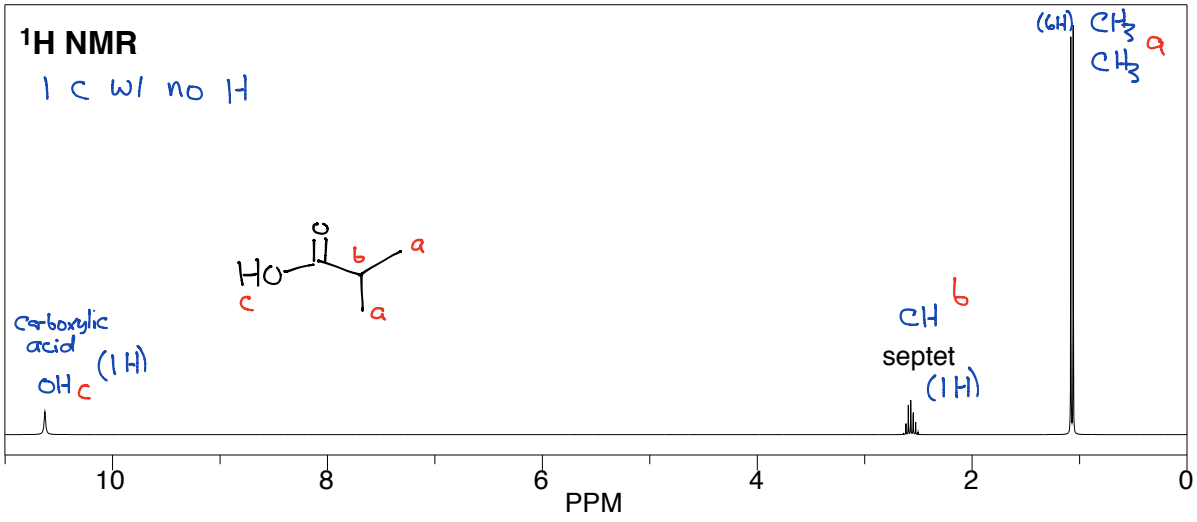


D. $C_4H_6O_2$ - 2 unsat ⌐ester  No indications of C=C so other unsat is likely a ring.

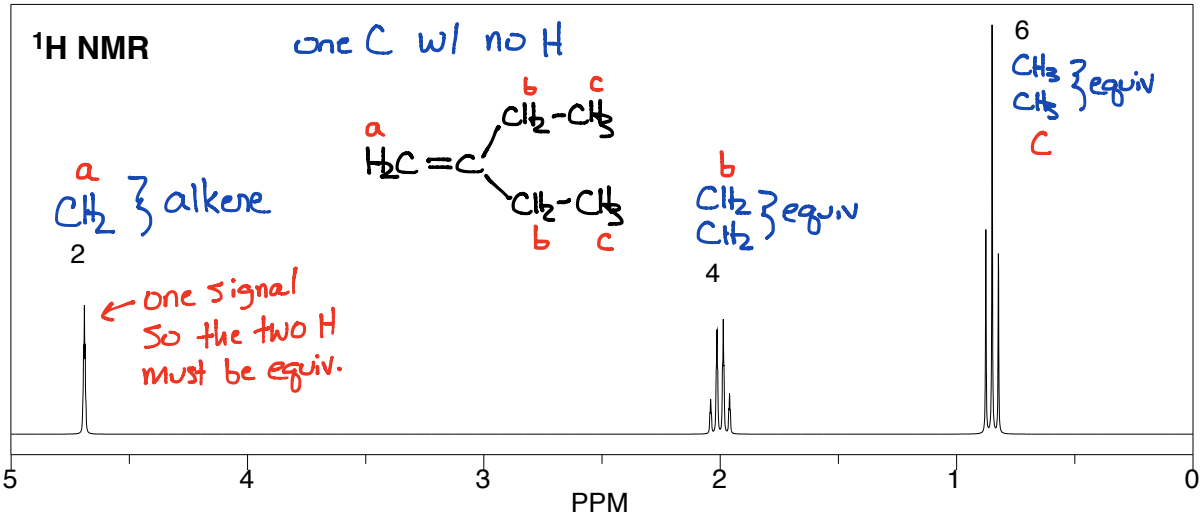
IR shows a strong stretch at 1740 cm^{-1}



E. $C_4H_8O_2$ – 1 unsat

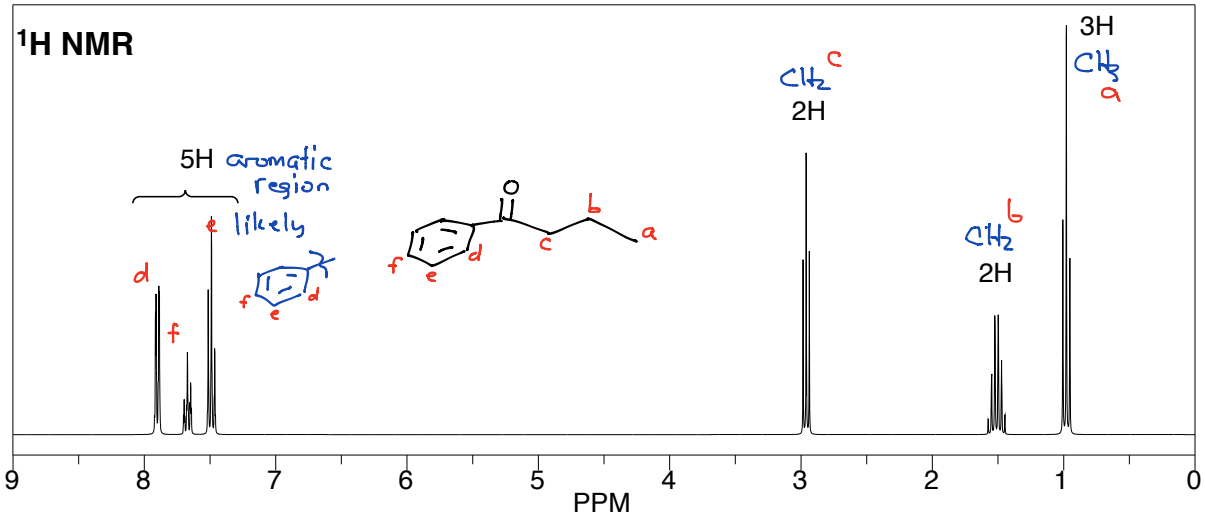


F. C_6H_{12} – 1 unsat.

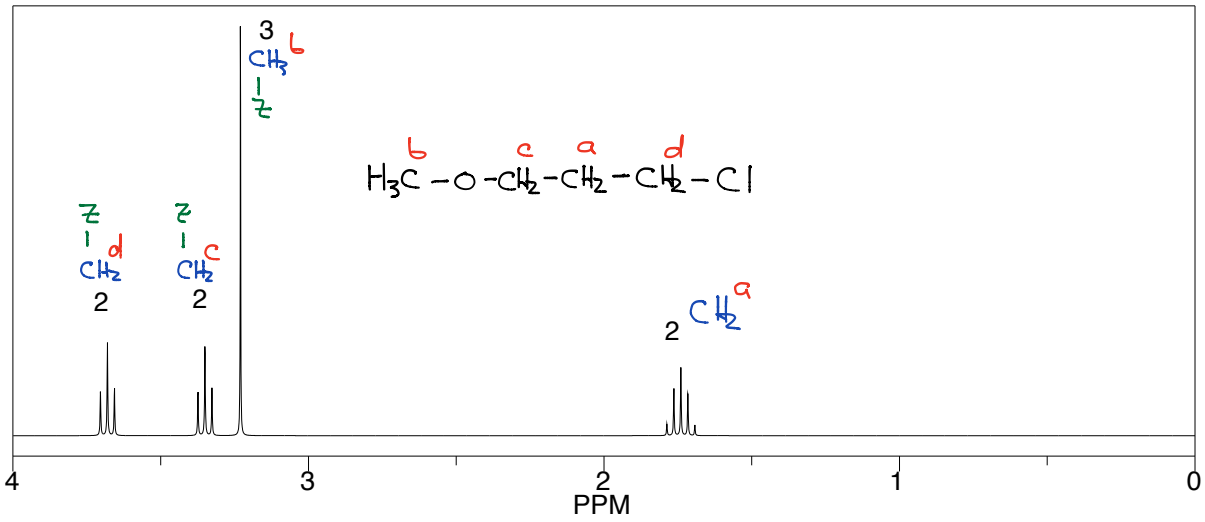


↳ Conjugated C=O

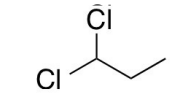
G. Compound contains 10C and IR shows a strong stretch around 1690 cm^{-1}

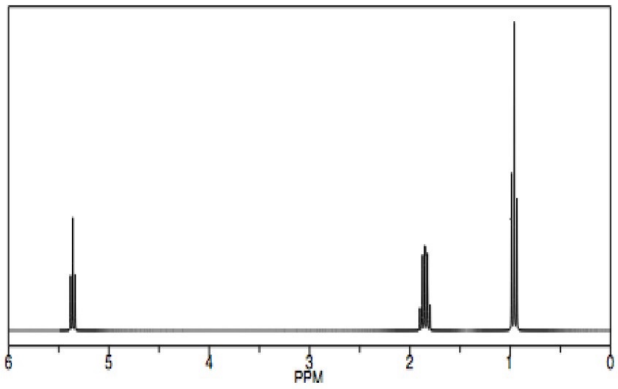


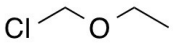
H. C_4H_9OCl – no unsat.

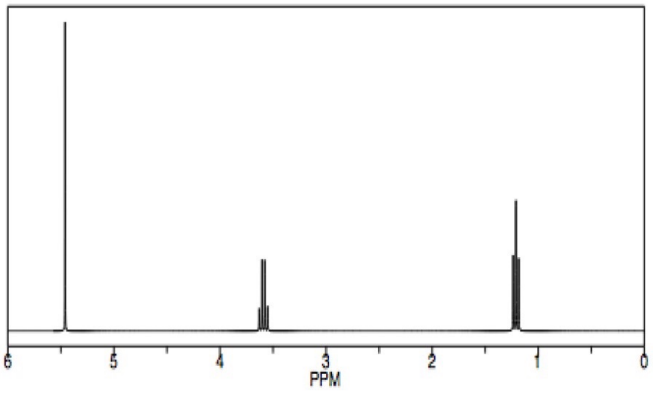


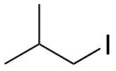
8) For each of the compounds below, draw a rough estimation of its expected ^{1}H NMR spectrum.

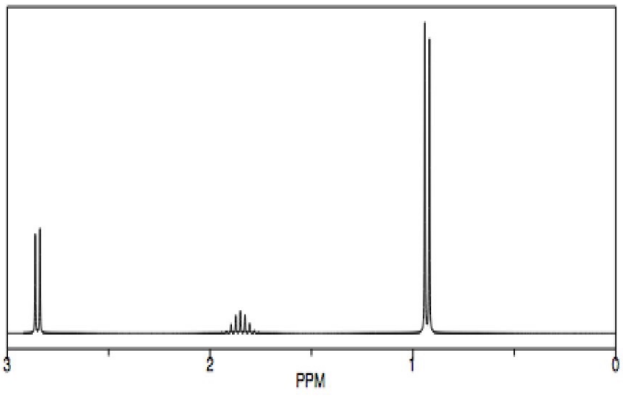


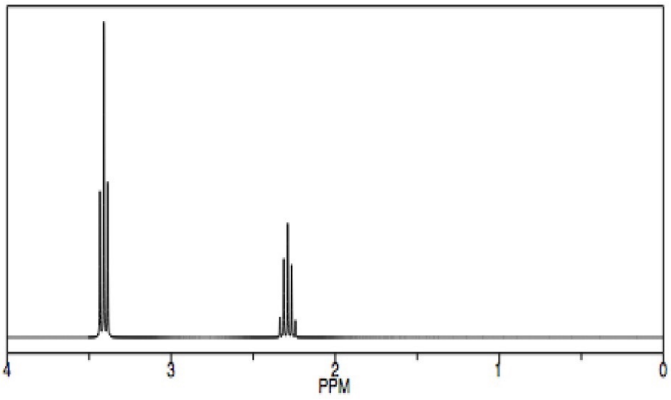




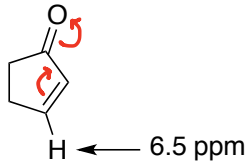


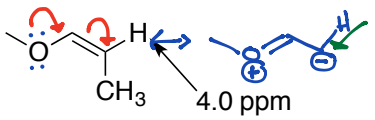






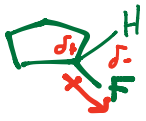
9) The vinyl proton chemical shift in the two compounds shown below is substantially different. Explain why the shift in these two compounds is so different. *Hint: think about resonance.*





⊖ on this C ↑ its e- density which has a shielding effect.

← ⊕ on this C ↓ e- density which has a deshielding effect.



Think of this in terms of how an attached halogen deshields a H by inductively withdrawing e- density