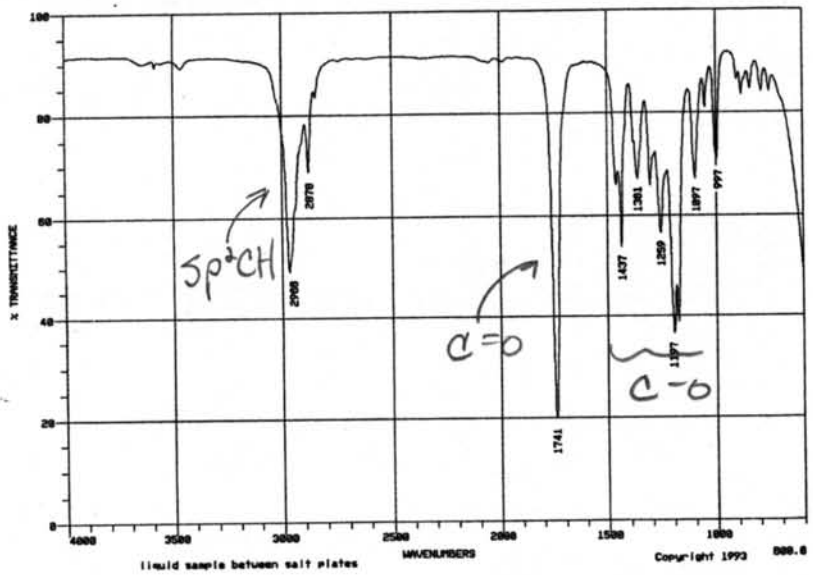
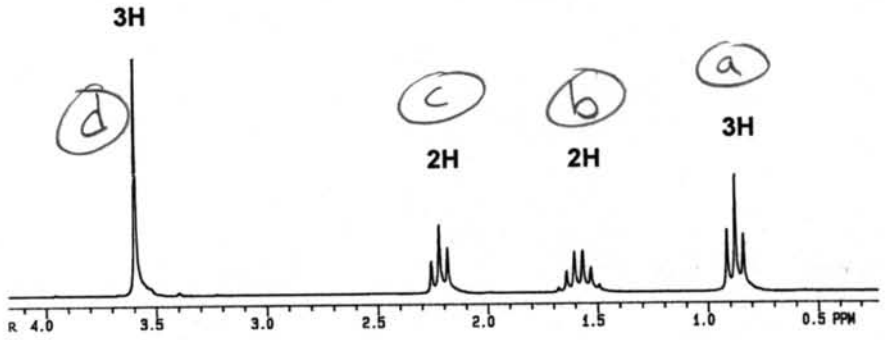
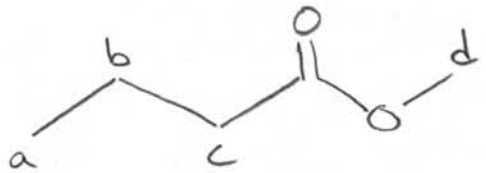
Problem 1: Provide a structure of a compound having a molecular formula of $C_5H_{10}O_2$ that is consistent with the following spectra. **SHOW your work** and assign all relevant peaks in the IR and ^1H NMR spectra. To confirm your choice, predict the splitting patterns for the protons in your proposed structure and estimate and/or calculate their chemical shifts.

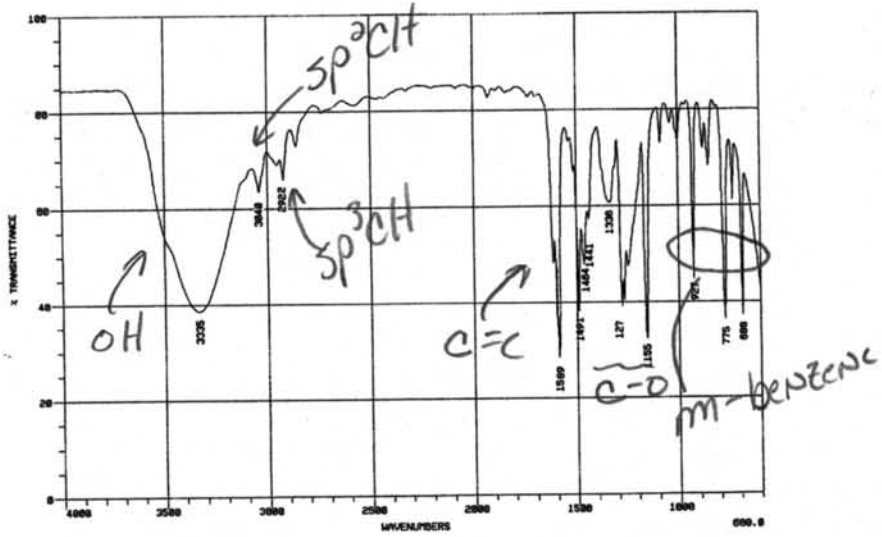


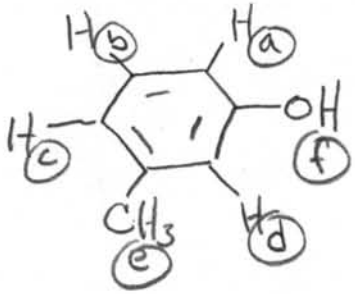


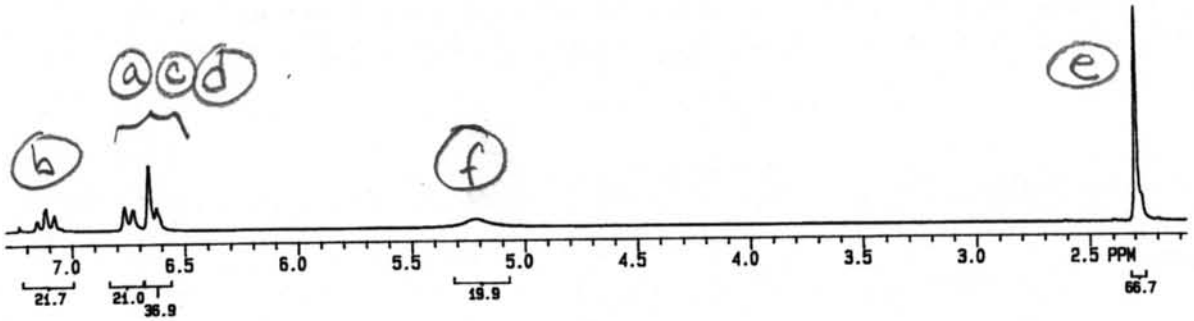


Proton	#H/splitting	δ (ppm)
(a)	3H / d	0.9
(b)	2H / sextet	$\delta = 1.2 + \Delta(R) + \Delta(R)$ $= 1.2 + 0 + 0$ $= 1.2$
(c)	2H / t	$\delta = 1.2 + \Delta(R) + \Delta(C(=O)R)$ $= 1.2 + 0 + 1.2$ $= 2.4$
(d)	3H / s	3.8

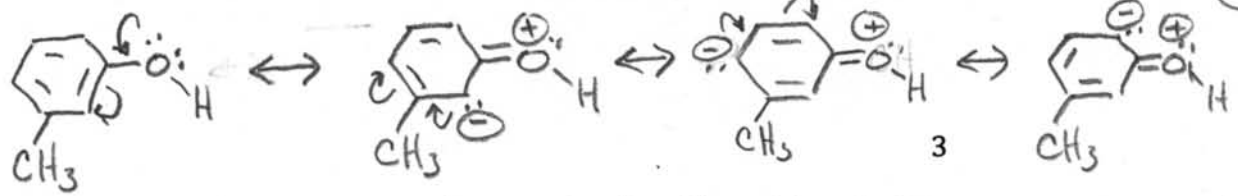
Problem 2: Provide a structure of a compound having a molecular formula of C_7H_8O that is consistent with the following spectra. **SHOW your work** and assign all relevant peaks in the IR and ^1H NMR spectra. To confirm your choice, predict the splitting patterns for the protons in your proposed structure and estimate and/or calculate their chemical shifts.



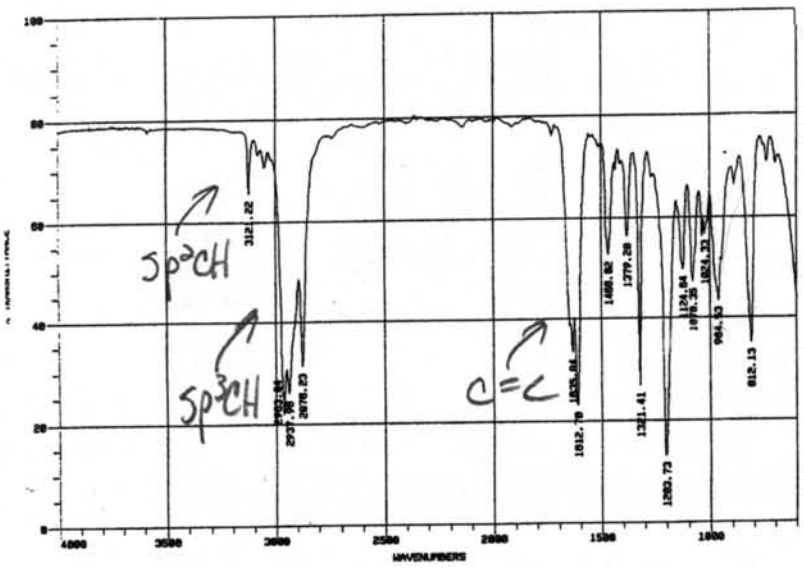


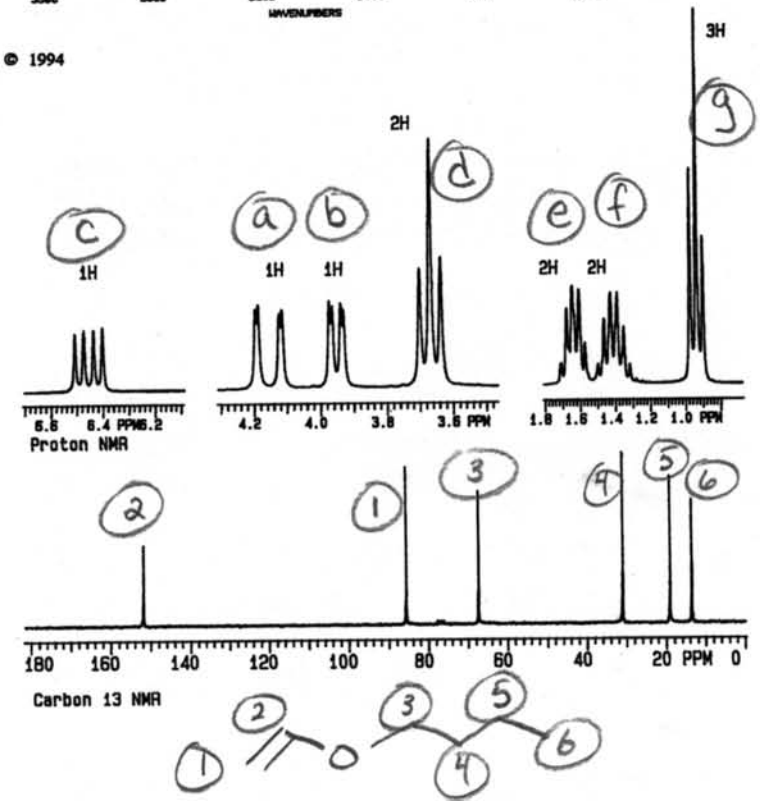


Proton	#H/splitting	δ (ppm)
a	1H/d	7.3
b	1H/t	7.3
c	1H/d	7.3
d	1H/s	7.3
e	3H/s	2.3
f	1H/s	4-7

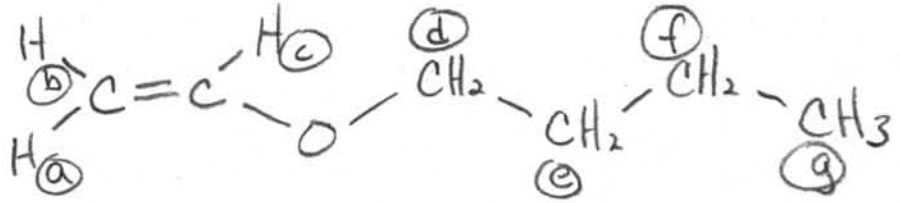


Resonance structures show that Ha, Hc, & Hd will be shielded (lower ppm value)



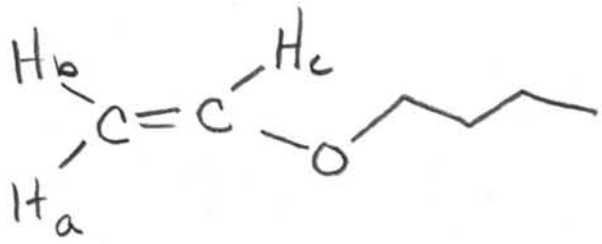


Problem 3: Provide a structure of a compound having a molecular formula of $C_6H_{12}O$ that is consistent with the following spectra. **SHOW your work** and assign all relevant peaks in the IR, ^1H NMR, and ^{13}C NMR spectra. To confirm your choice, predict the splitting patterns for the protons in your proposed structure and estimate and/or calculate their chemical shifts.



Proton	#H/Splitting	δ (ppm)
(a)	1H/dd	5-5.3
(b)	1H/dd	5-5.3
(c)	1H/dd	5-5.3
(d)	2H/t	$\delta = 1.2 + \Delta(OR) + \Delta(R)$ $= 1.2 + 2.1 + 0$ $= 3.3$
(e)	2H/pentet	$\delta = 1.2 + \Delta(R) + \Delta(R)$ $= 1.2 + 0 + 0$ $= 1.2$
(f)	2H/sextet	$\delta = 1.2 + \Delta(R) + \Delta(R)$ $= 1.2 + 0 + 0$ $= 1.2$
(g)	3H/t	0.9

Problem 3 (cont)

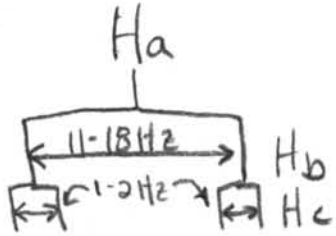


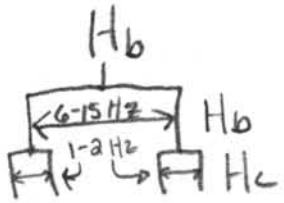
Ha is trans to Hc
Ha is gem to Hb

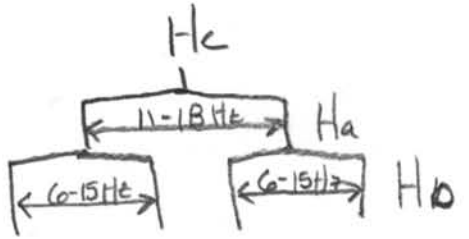
Hb is cis to Hc
Hb is gem to Ha

Hc is trans to Ha
Hc is cis to Hb

signal splitting







signal shape

The signal for Ha will be wider than that for Hb

Alkene Coupling Constants

gem (geminal) → 1-2 Hz
cis → 6-15 Hz
trans → 11-18 Hz