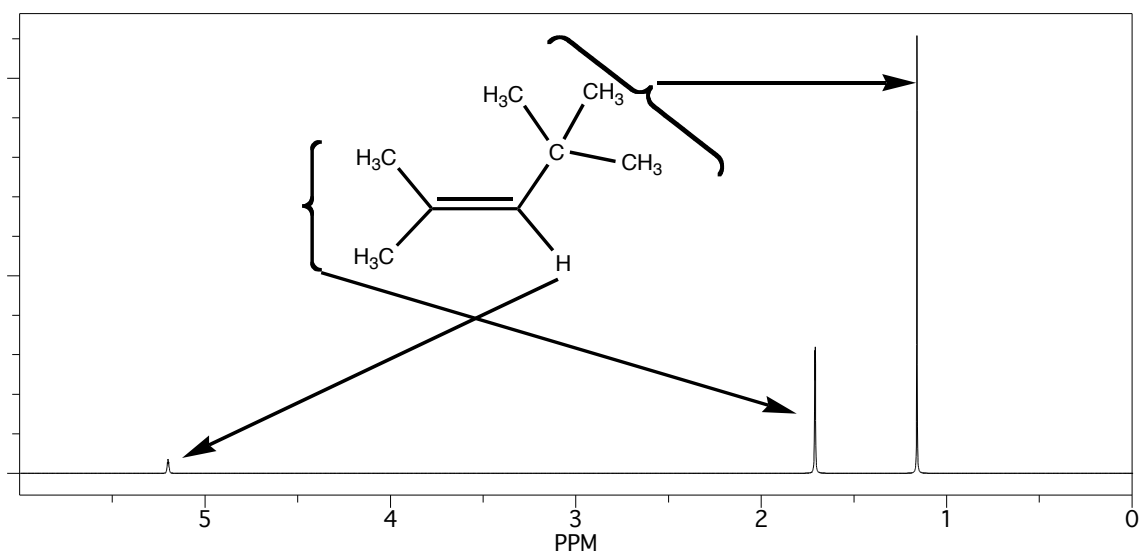
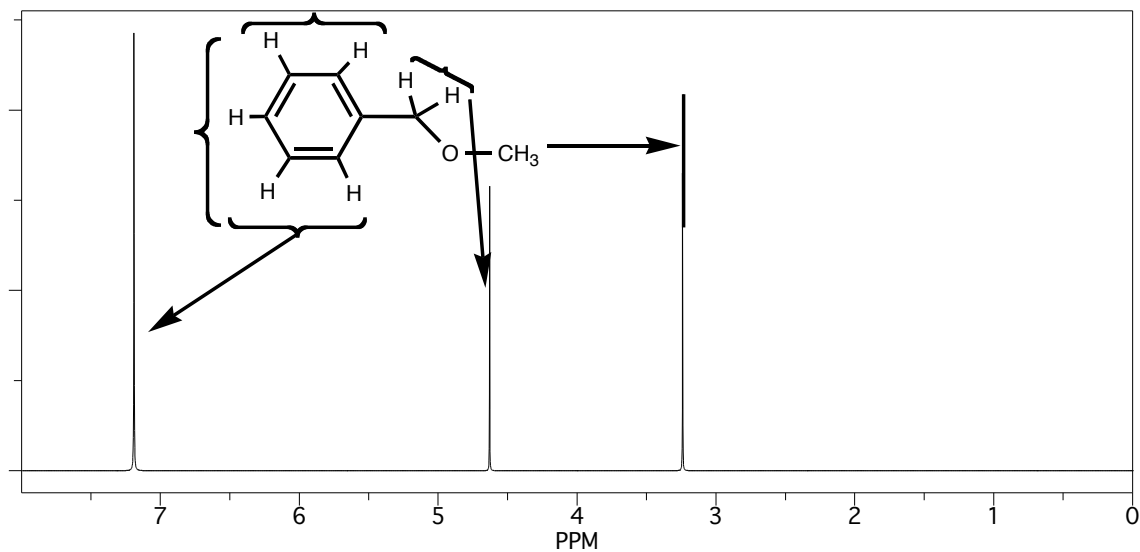


Additional Problems for practice.  
Assign the resonances in the following spectra:

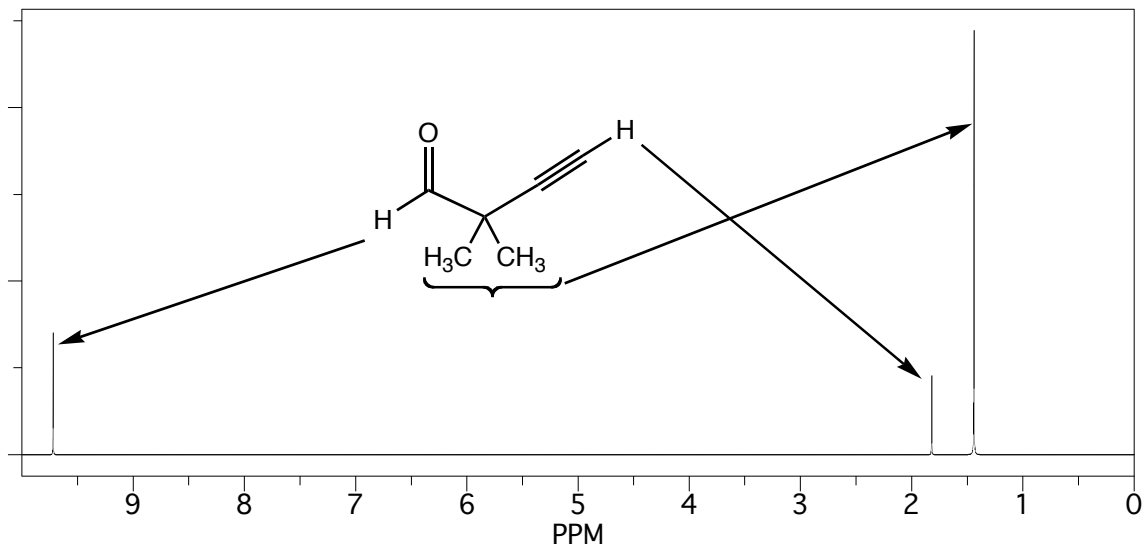
a.



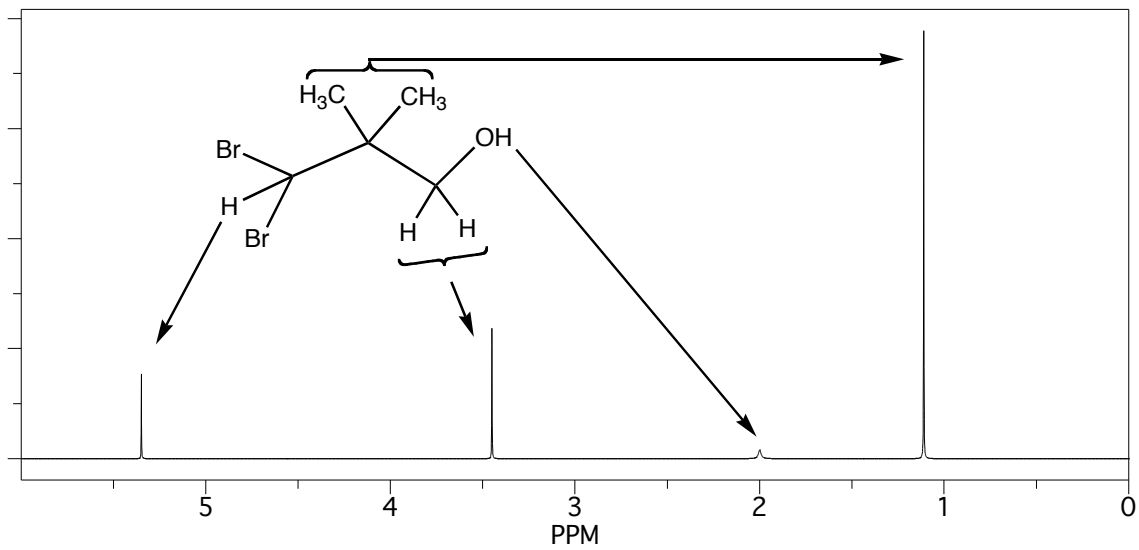
b.



c.



d.



Additional Problems for practice:

1. match the following IR spectra with the compounds listed below:  
1,3-cyclohexadiene spectrum D → conjugated double bond lowers stretching frequency to  $1641\text{ cm}^{-1}$

Diphenylacetylene spectrum A => aromatic indicated by  $1600\text{cm}^{-1}$  absorption; absence of a  $\text{C}\equiv\text{C}$  stretch indicates symmetrical internal alkyne.

1-octene Spectrum C  $1657\text{ cm}^{-1}$  absorption indicates ordinary  $\text{C}=\text{C}$  stretch

2-pentene Spectrum B very weak  $\text{C}=\text{C}$  absorption in 1600-1700 range indicates low dipole moment of an internal alkene.

2. match the following IR spectra with the compounds listed below

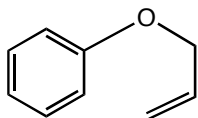
butyl acetate:  $\text{CH}_3\text{C}(=\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$  : Spectrum E: the ester  $\text{C}=\text{O}$  stretch at  $1740\text{ cm}^{-1}$  is indicative.

Butyramide:  $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(=\text{O})\text{NH}_2$ : Spectrum H we see an intense carbonyl absorption at  $1630\text{-}1640\text{ cm}^{-1}$  characteristic of an amide (lower frequency due to resonance with the nitrogen lone pairs) and also a large two-spike peak between  $3300$  and  $3400\text{ cm}^{-1}$ , which indicates two  $\text{NH}$  stretches.

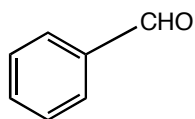
isobutyl amine:  $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{NH}_2$ : Spectrum I: two small spikes in  $3300\text{-}3400\text{ cm}^{-1}$  are characteristic of two  $\text{N-H}$  bond stretches; no intense carbonyl so this is not an amide.

lauric acid:  $\text{CH}_3(\text{CH}_2)_{12}\text{COOH}$ : Spectrum F: Broad  $\text{OH}$  stretch from  $3000$  to  $3400\text{ cm}^{-1}$  is indicative, as well as the intense  $\text{C}=\text{O}$  stretch at  $1705\text{ cm}^{-1}$ .

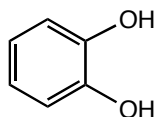
3. Match the following IR spectra with the compounds listed below



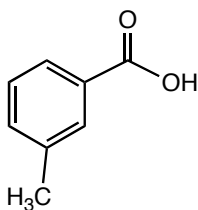
Spectrum L:  $1650\text{ cm}^{-1}$  weak spike indicates a C=C;  $1600\text{ cm}^{-1}$  spike indicates aromatic C-C stretch.



Spectrum M: intense absorption at  $1700\text{ cm}^{-1}$  indicates a conjugated carbonyl; aldehyde C-H stretch apparent at between  $2700\text{--}2800\text{ cm}^{-1}$ ;  $1600\text{ cm}^{-1}$  spike indicates aromatic C-C stretch

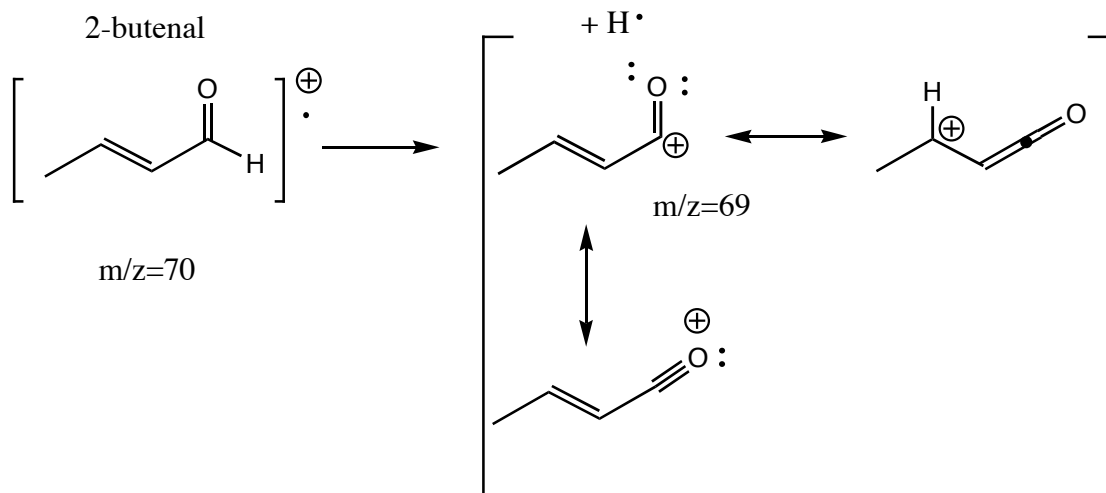


Spectrum K Broad OH stretch around  $3400\text{ cm}^{-1}$ , as well as  $1600\text{ cm}^{-1}$  spike indicates aromatic C-C stretch. no C=O evident.



Spectrum J:  $1600\text{ cm}^{-1}$  spike indicates aromatic C-C stretch;  $1690\text{ cm}^{-1}$  intense C=O absorption is a conjugated carbonyl; the broad OH stretch around  $3000\text{ cm}^{-1}$  is indicative.

4. The mass spectrum of 2-butenal shows a peak at  $m/z$  69 that is 28.9% as intense as the base peak. Propose at least one fragmentation route to account for this peak, and explain why this fragment would be reasonably stable.

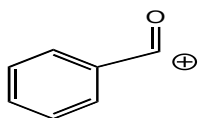


loss of a hydrogen atom from the radical cation leads to a resonance-stabilized positive charge

5. The exact mass of a compound determined by high-resolution mass spectra is 212.0833. Given the following table, what is the molecular formula? Given the spectrum, what is the structure?

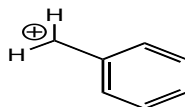
From the table, we see that an exact mass of 212.0833 is closest in molecular formula to  $C_{14}H_{12}O_2$

The mass spectrum has diagnostic fragments at  $m/z=105$  and  $m/z=91$ . These fragments arise from the benzyl cation and the phenacyl cation:



$m/z = 105$

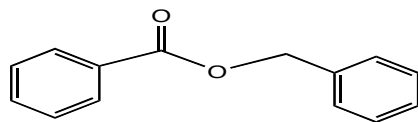
fragment ion



$m/z = 91$

fragment ion

putting these two fragments together with an additional oxygen as suggested by the correct molecular formula gives the following structure:



$C_{14}H_{12}O_2$   
 Exact Mass: 212.08  
 Mol. Wt.: 212.24  
 $m/e$ : 212.08 (100.0%), 213.09 (15.4%), 214.09 (1.5%)  
 C, 79.22; H, 5.70; O, 15.08