Structure Determination using NMR and IR Spectral Data

Click on a number to view the spectral data for each compound.

Data for each unknown includes: ^{1}H NMR (splitting patterns included)
^{13}C NMR
IR spectrum (KBr pellet or film)

Solvent peaks due to $CDCl_3$ are present at 7.2 ppm in the proton spectra and 77.0 ppm in the carbon spectra.

In the ^{1}H NMR spectra, the phrase "exchanges" means that shaking the NMR solution with D_2O resulted in loss of the signal due to hydrogen/deuterium exchange.

Click here to learn about interpretation of spectral data.

#1 C_4H_6O	#6 $C_8H_{19}N$	#11 $C_5H_{12}O_2$
#2 $C_3H_5O_2Br$	#7 C_3H_7OCl	#12 C_3H_7OCl
#3 C_9H_{12}	#8 $C_6H_6O_2$	#13 $C_6H_{11}O_2Br$
#4 C_6H_{10}	#9 $C_6H_4Cl_2$	#14 $C_{10}H_{12}O_2$
#5 $C_8H_6O_2$	#10 $C_{16}H_{35}N$	#15 $C_9H_{13}NO$

Interpretation of Data

back to problems

Use the **molecular formula** to determine the degrees of unsaturation or double bond equivalents (rings or multiple bonds).

Most of the ^{1}H spectra contain first-order **splitting patterns**; in cases where some peaks do not follow the *N+1* rule, by process of elimination of other peaks, you can solve the problem. Look for the obvious first-order splitting patterns:

- ethyl pattern (triplet and quartet)
- isopropyl pattern (double and multiplet, which may resolve into a discernable heptet)
- methoxy groups on esters (singlet downfield from alkane region, approx. 3.5 ppm)
- methyl group adjacent to a carbonyl (approximately 2.0 ppm)
- aromatic signals along with at least 4 degrees of unsaturation indicates a benzene ring.

back to problems

Examine the IR spectrum to determine the **functional groups** present in the unknown:

- For example, if the formula contains oxygen, you should be able to distinguish between an ether versus an alcohol (O-H stretch).
- If a carbonyl stretch is present, look for O-H stretch (acid) or N-H stretch (amide).
- Look for triple bonds at approximately 2200 cm^{-1}.
- Look for sp^2 carbon-hydrogen frequencies above 3000 cm^{-1} (alkenes, aromatic rings).

back to problems

Remember, the number of peaks in the ^{13}C spectrum indicates the number of different kinds of carbon atoms, the magnetically different carbon atoms. Some of the ^{13}C spectra contain carbon-hydrogen splitting information labeled as a **multiplet**.
For example, a peak listed as 38.6, t means the peak is at 38.6 ppm and exists as a triplet.

- A quartet indicates there are three hydrogens attached to that carbon atom (CH_3 group).
- A triplet indicates there are 2 hydrogens attached to that carbon atom (CH_2 group).
- A doublet indicates there is one hydrogen attached to that carbon atom (CH group).
- A singlet indicates a quaternary carbon group.

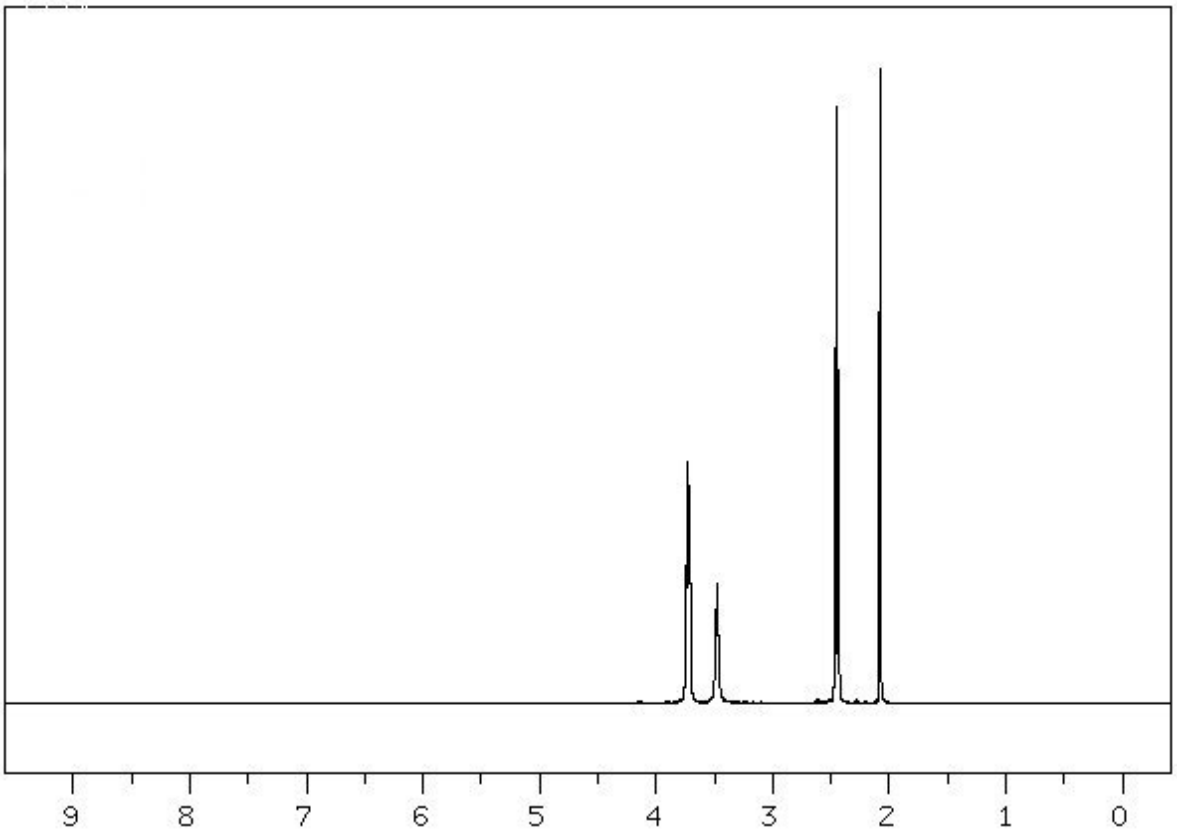
back to problems

^{1}H NMR spectrum **^{13}C NMR spectrum** **IR spectrum**

#1 C_4H_6O

back to problems

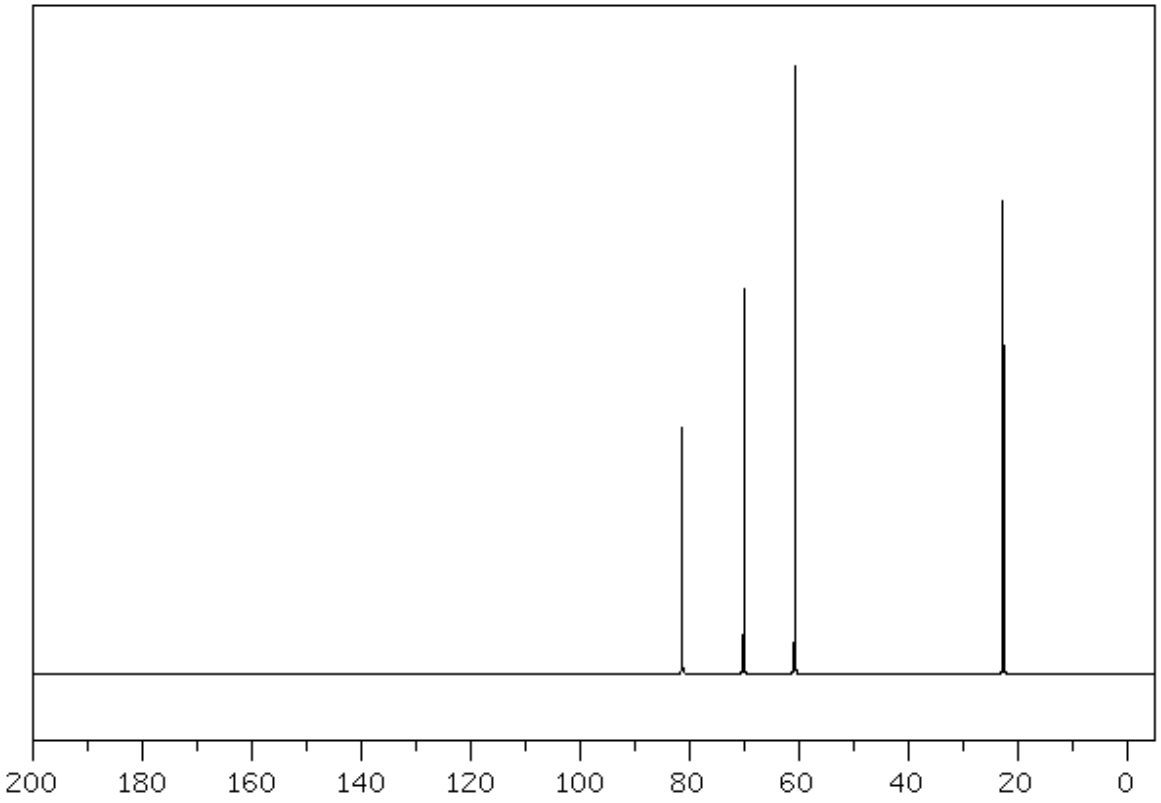
peak splitting below



3.72 t 2H
3.48 bs 1H (exchanges)
2.45 t 2H
2.08 s 1H

[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

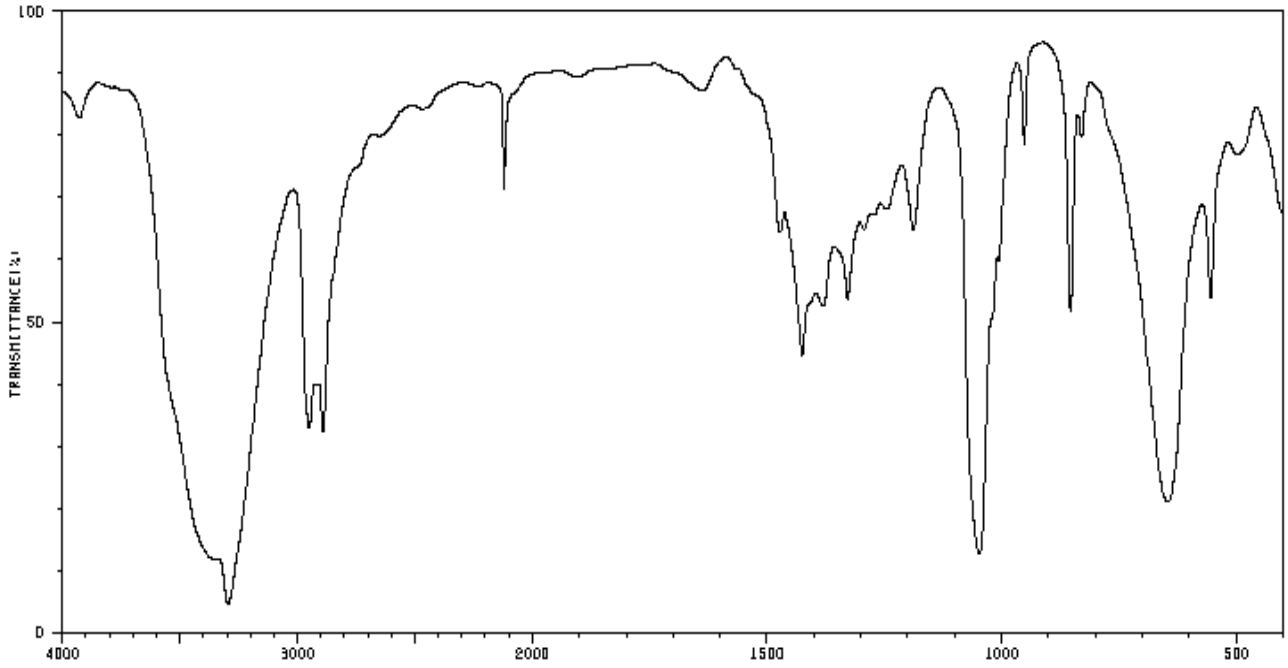
#1 C_4H_6O back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#1 C_4H_6O

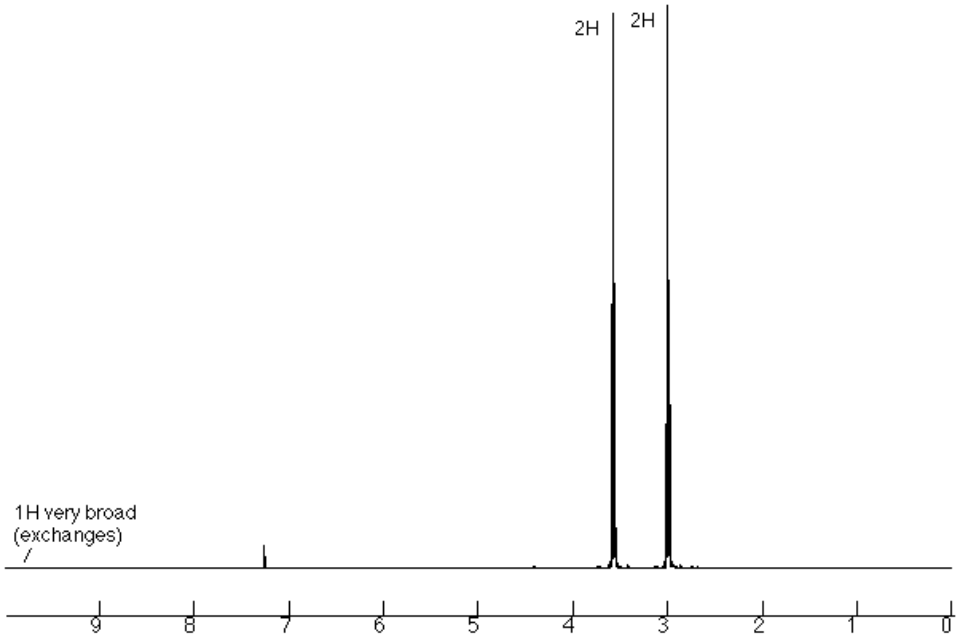
back to problems

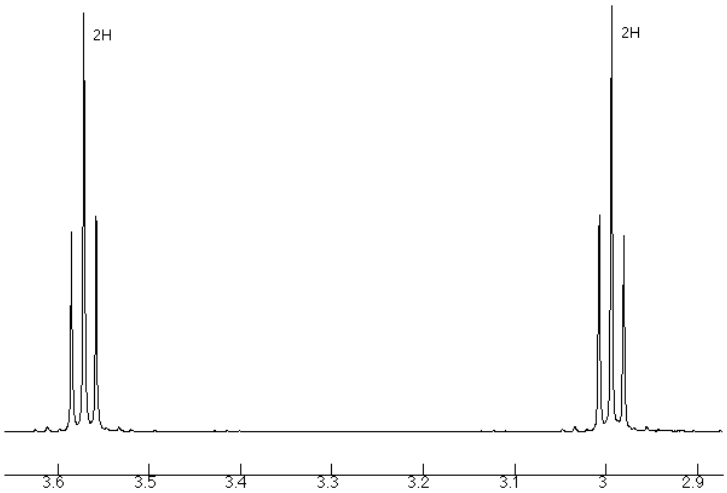


[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#2 $C_3H_5O_2Br$ back to problems

peak splitting below

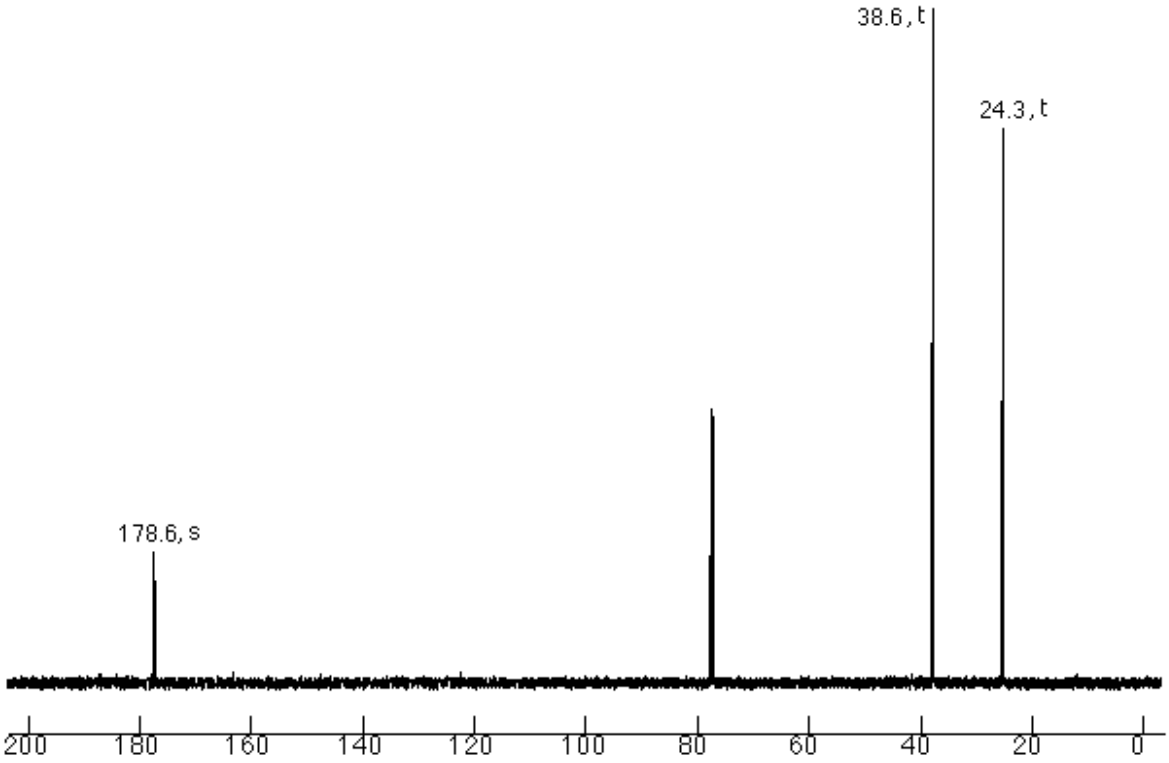




[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

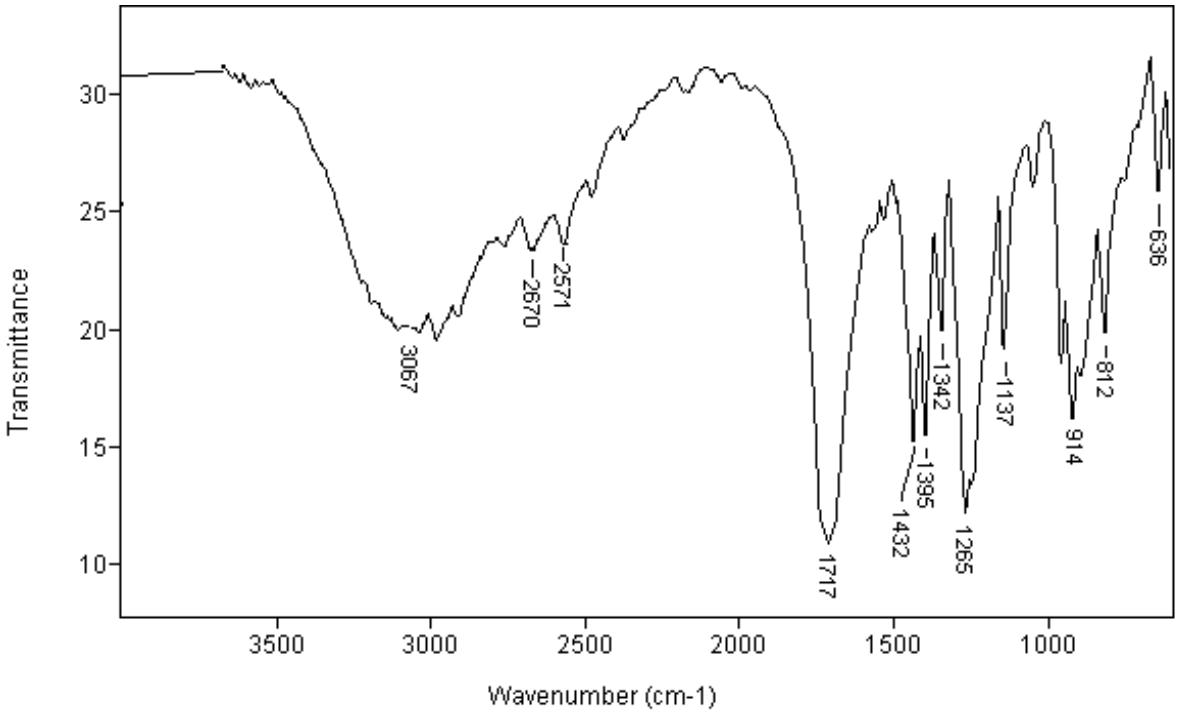
#2 $C_3H_5O_2Br$

back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

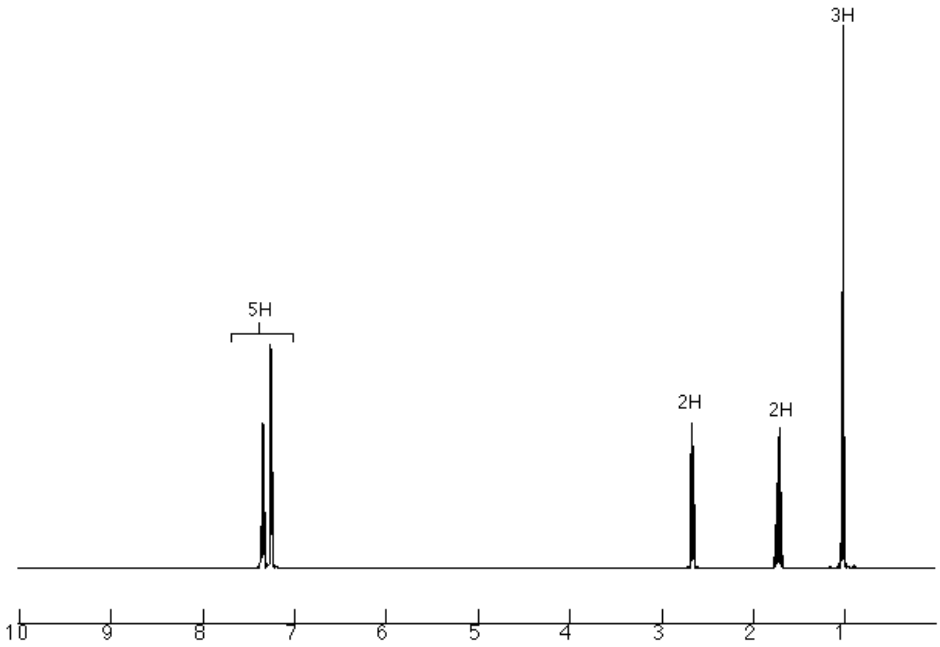
#2 $C_3H_5O_2Br$ back to problems

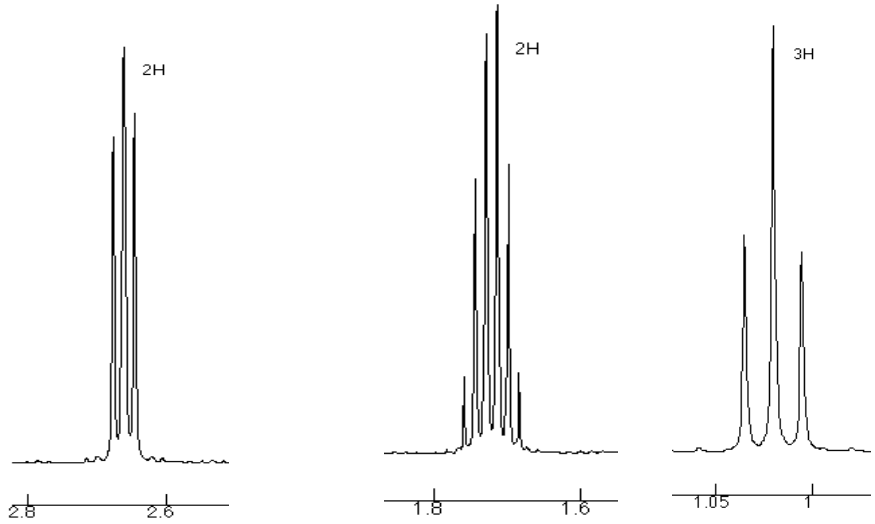


[^{1}H NMR spectrum] **[^{13}C NMR spectrum]** **[IR spectrum]**

#3 C_9H_{12} back to problems

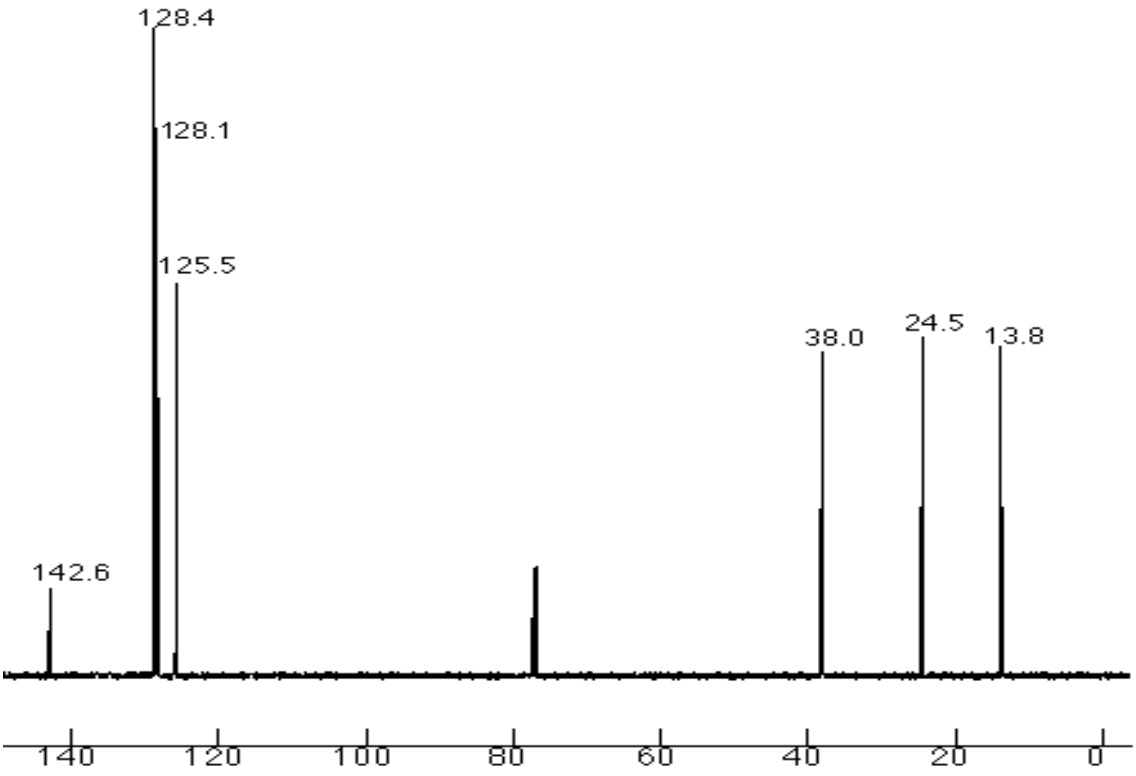
peak splitting below





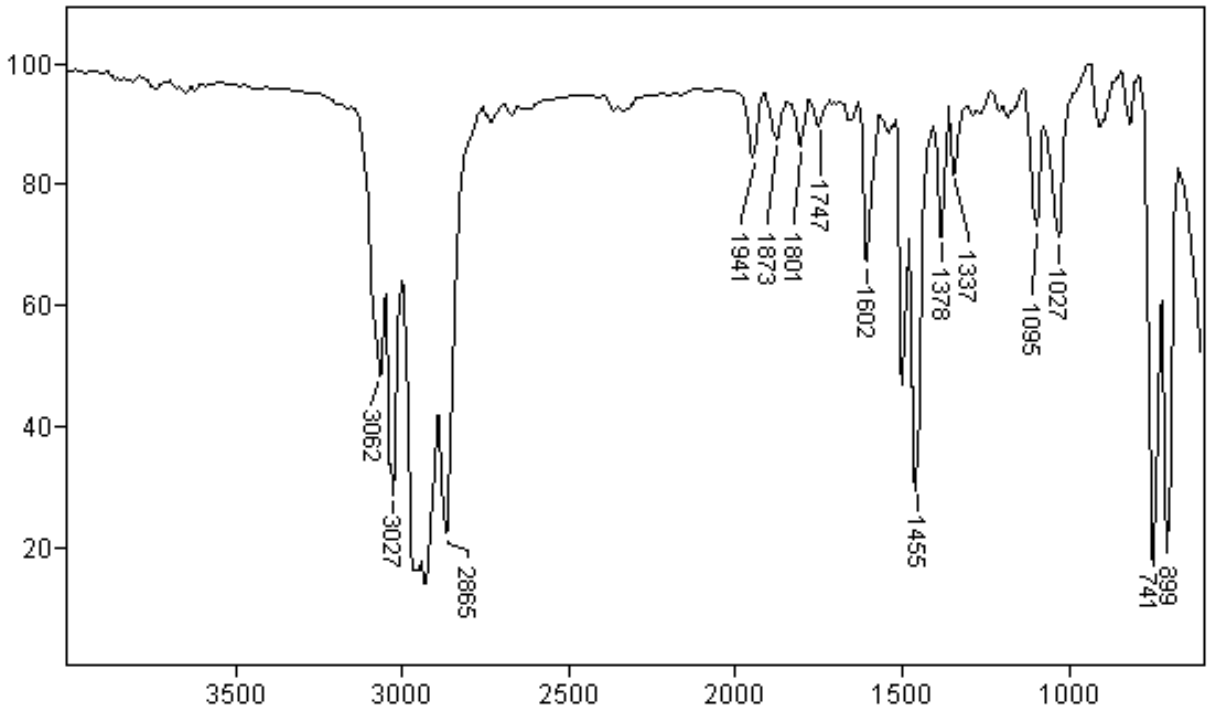
[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#3 C_9H_{12} back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

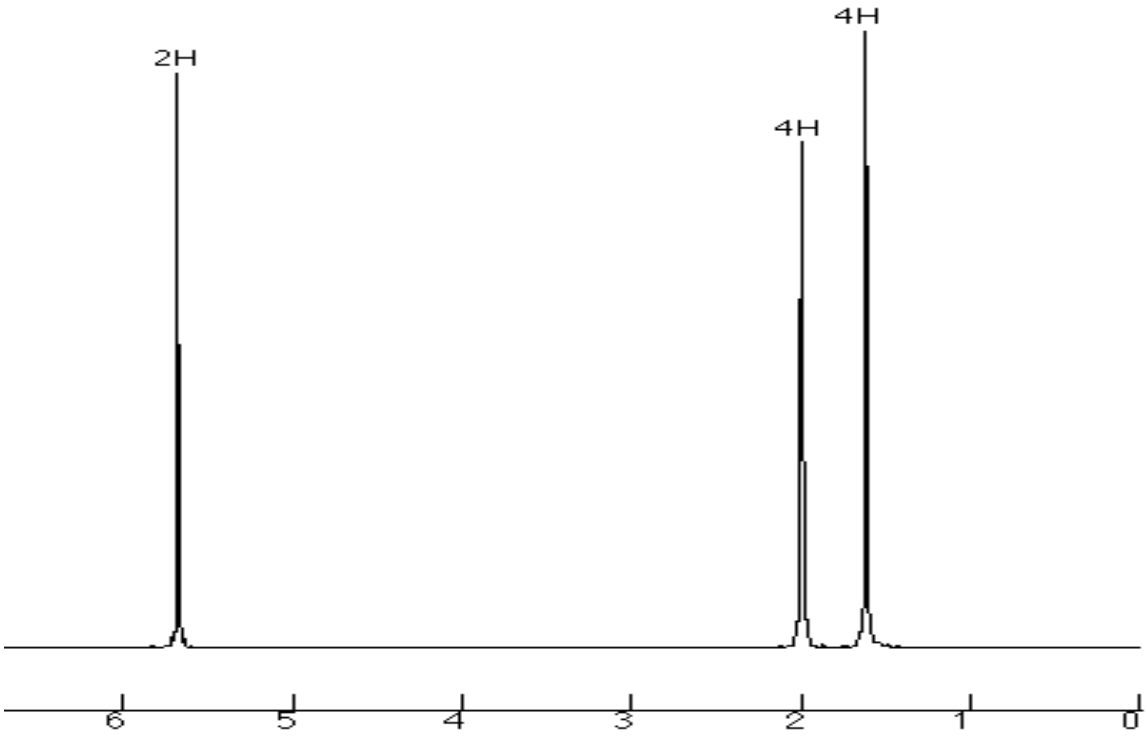
#3 C_9H_{12} back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

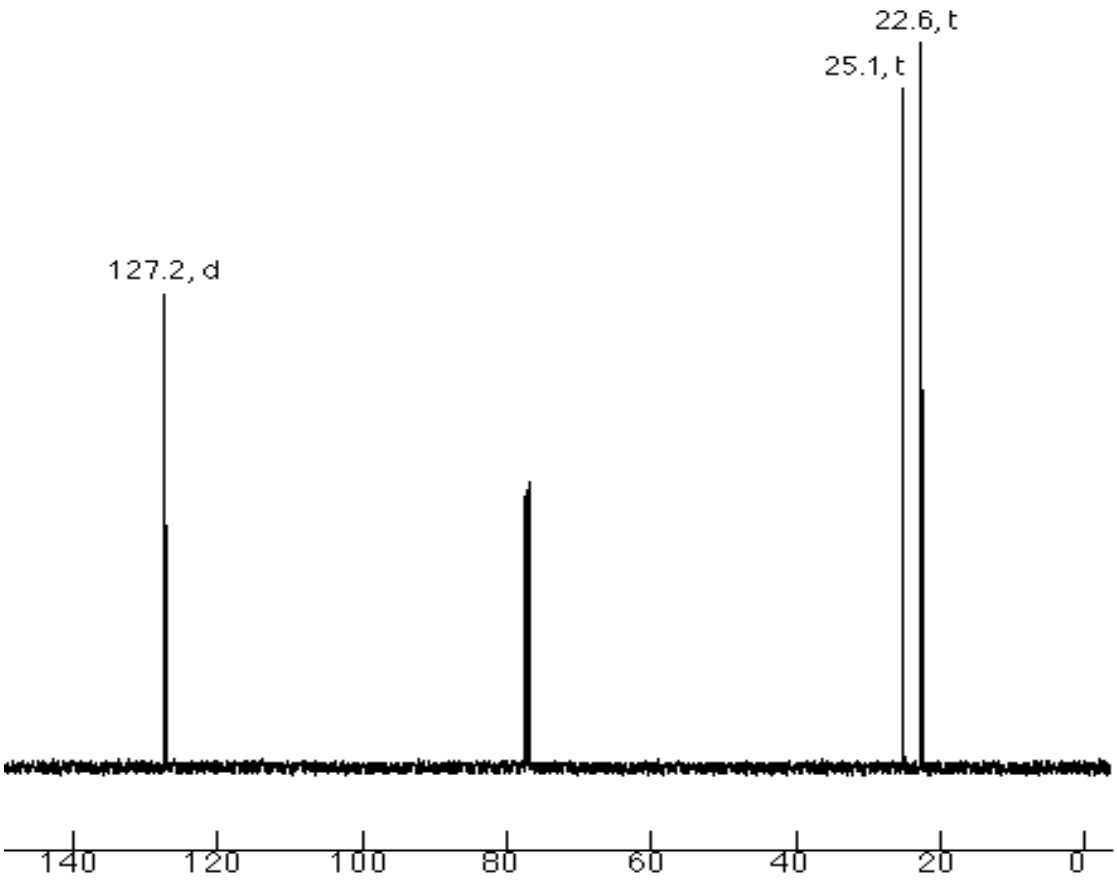
#4 C_6H_{10} back to problems

all singlets!



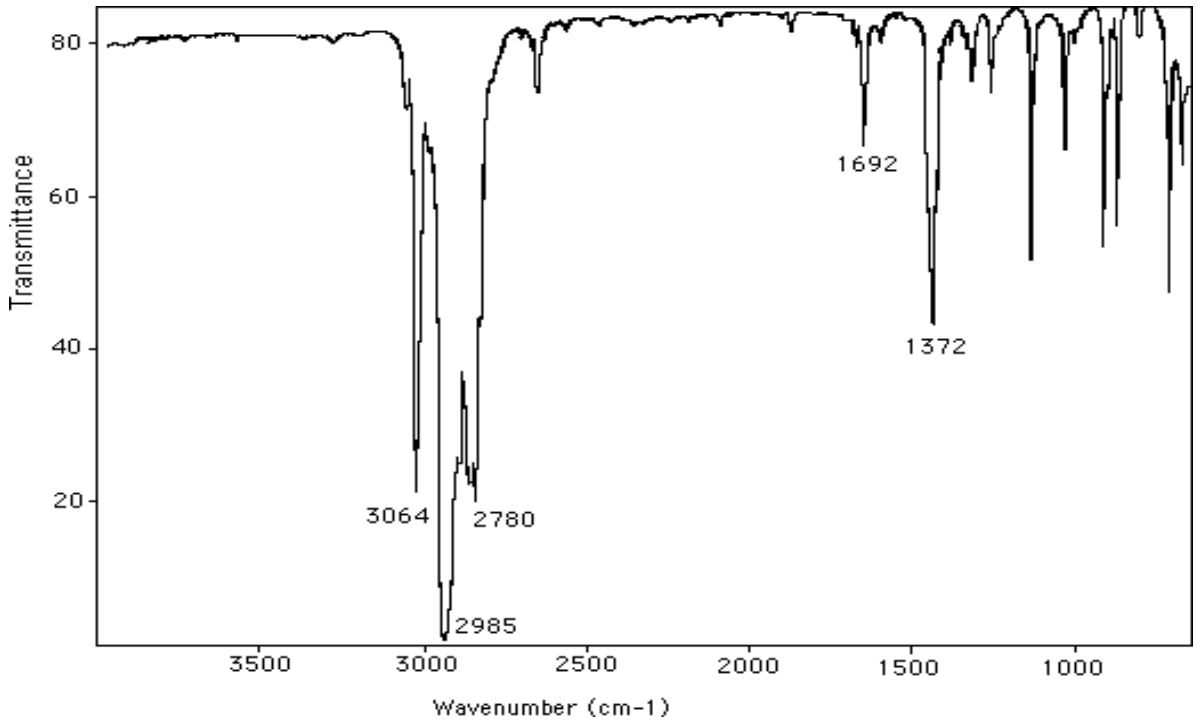
[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#4 C_6H_{10} back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

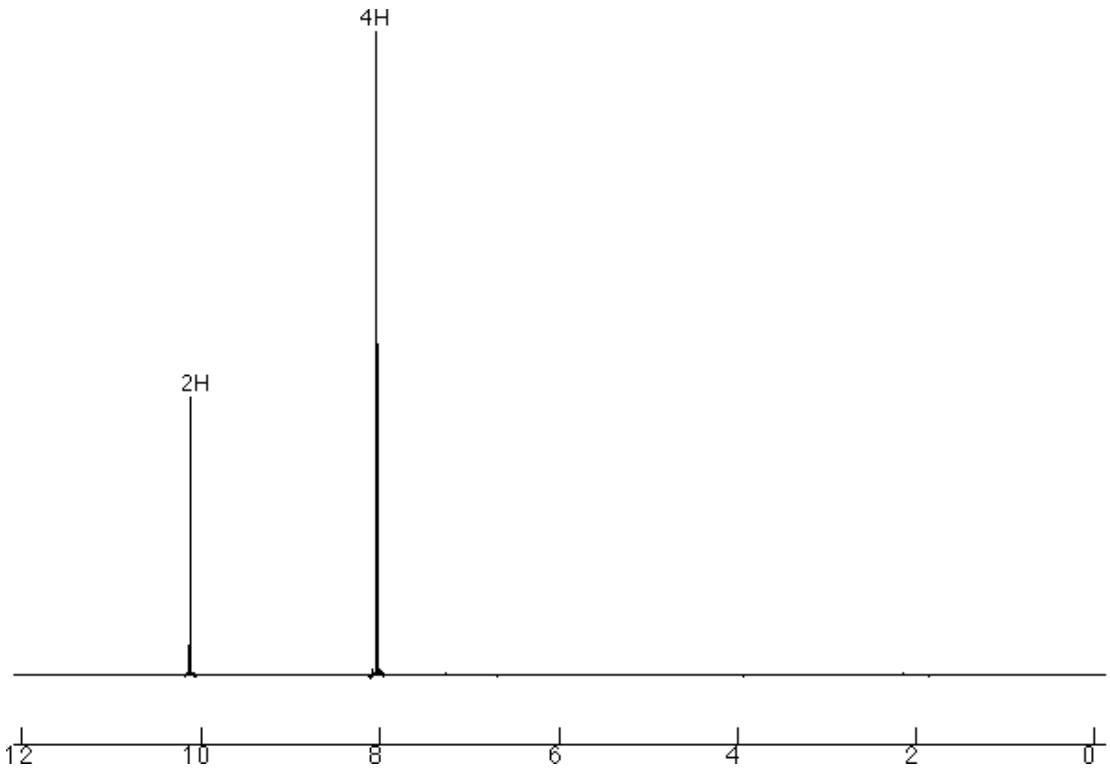
#4 C_6H_{10} back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

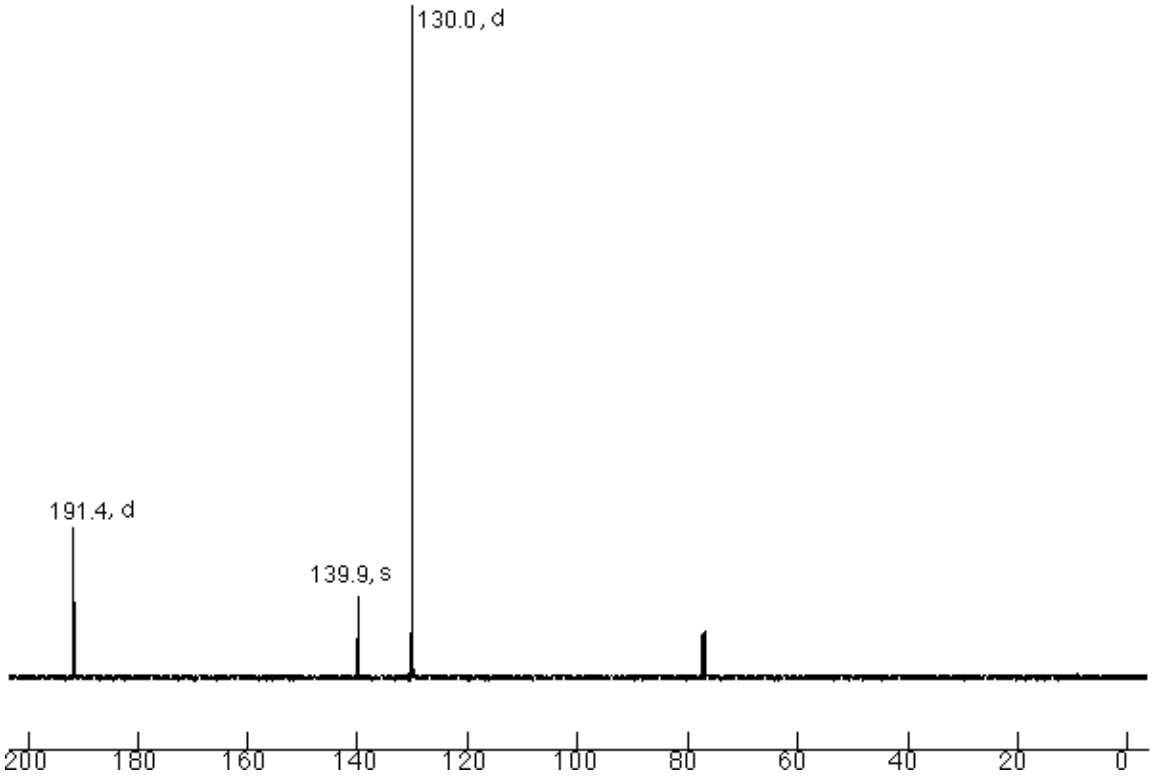
#5 $C_8H_6O_2$ back to problems

all singlets!



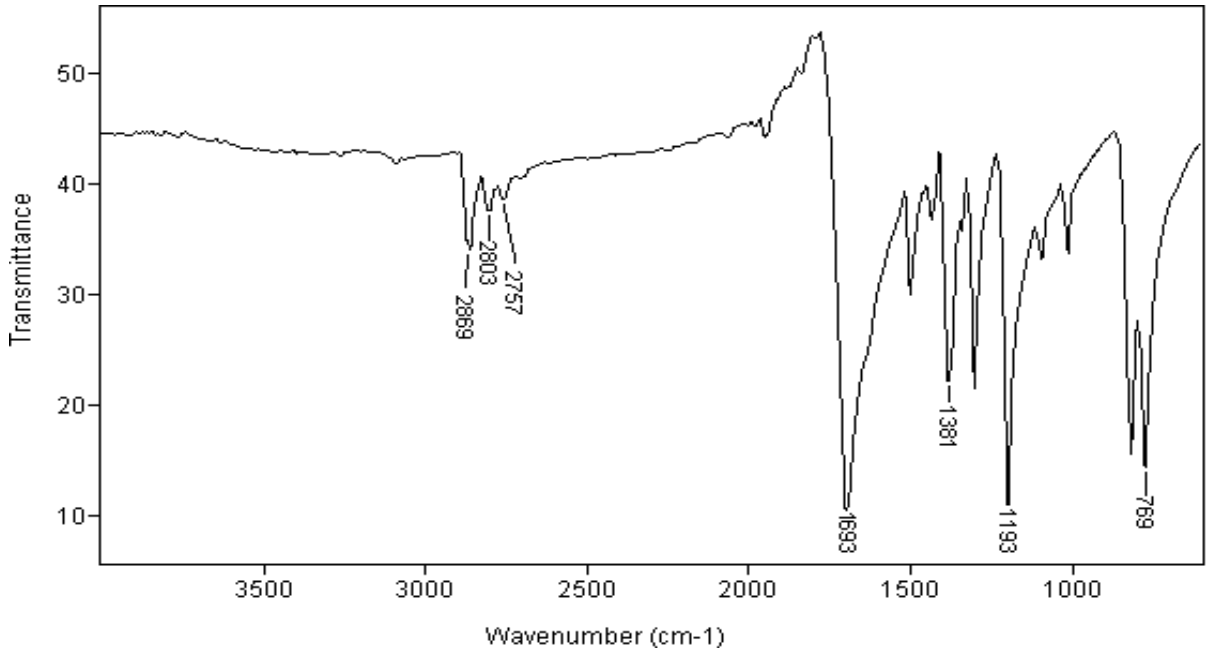
[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#5 $C_8H_6O_2$ back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

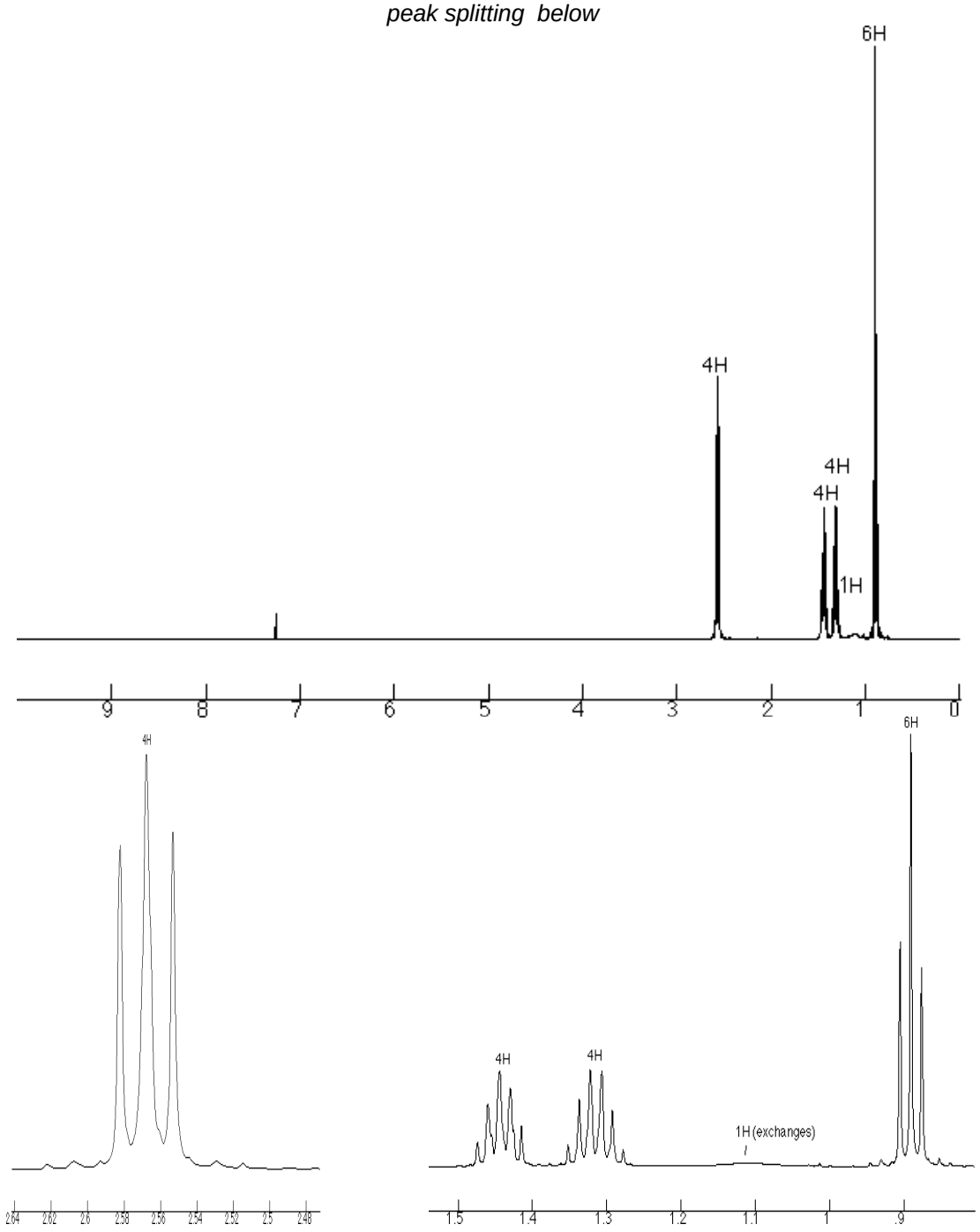
#5 $C_8H_6O_2$ back to problems



[^{1}H NMR spectrum] **[^{13}C NMR spectrum]** **[IR spectrum]**

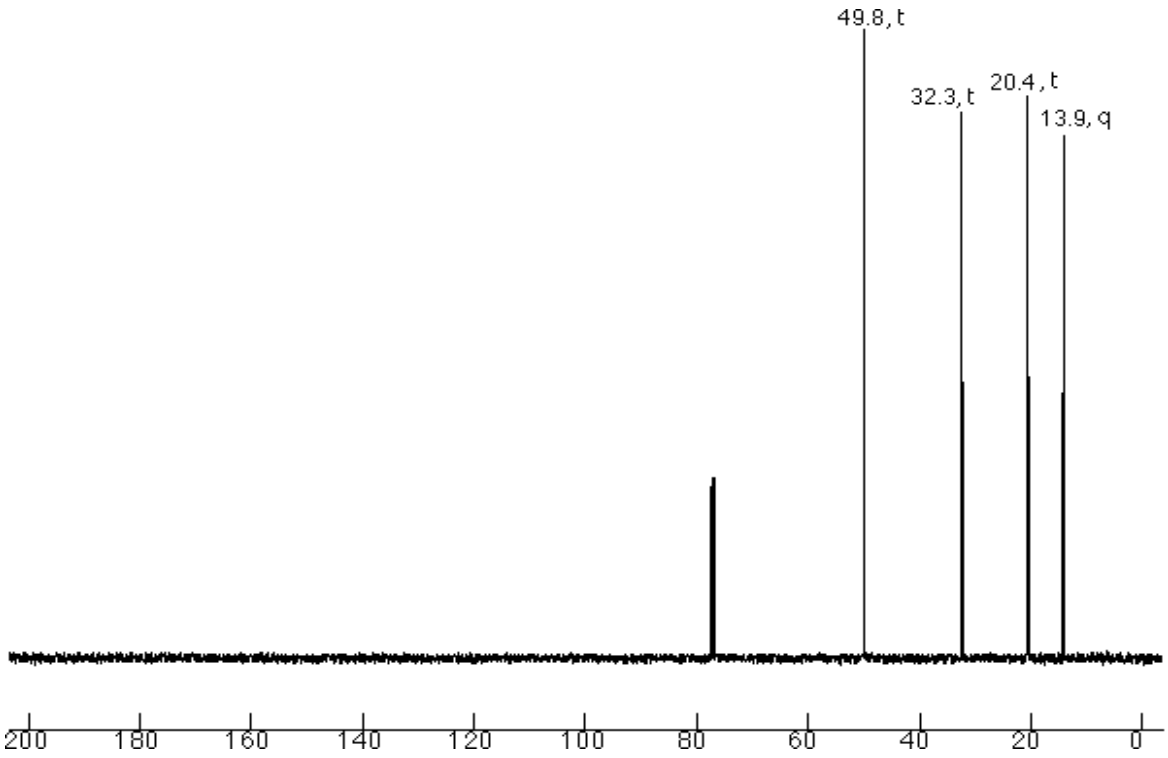
#6 $C_8H_{19}N$ back to problems

peak splitting below



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

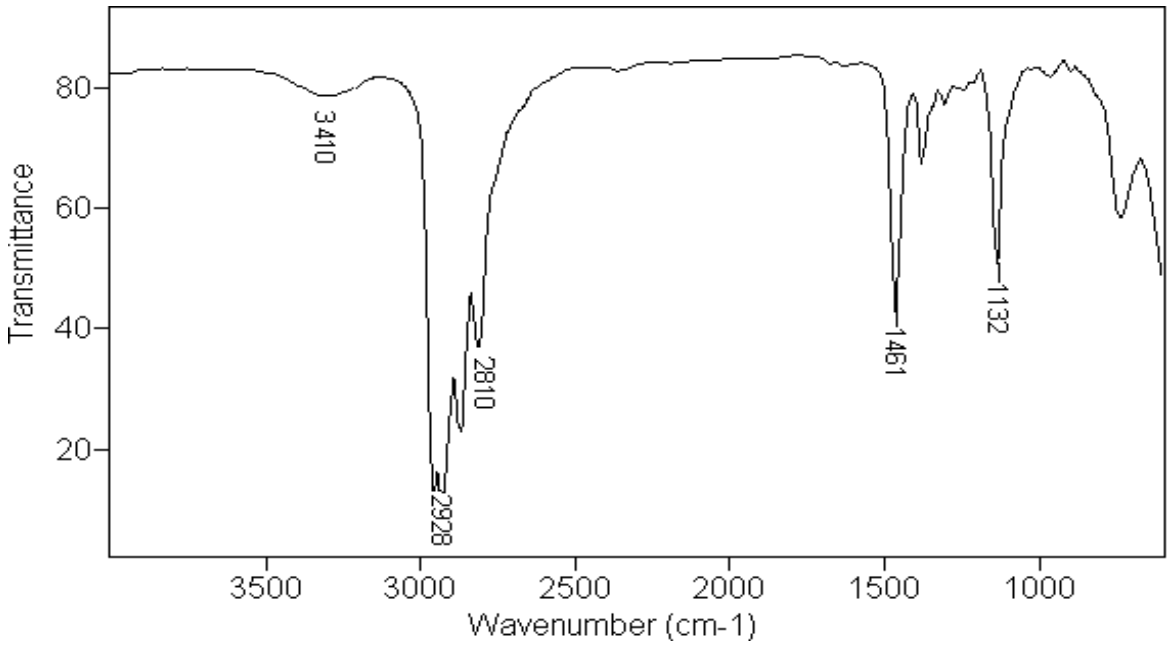
#6 $C_8H_{19}N$ back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#6 $C_8H_{19}N$

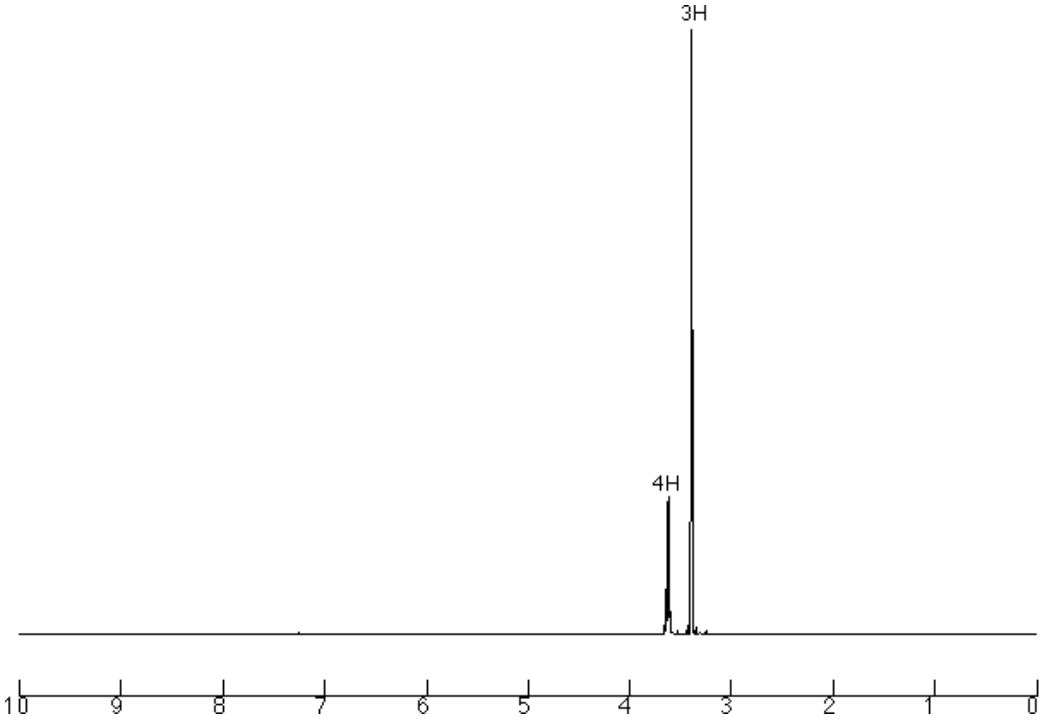
back to problems

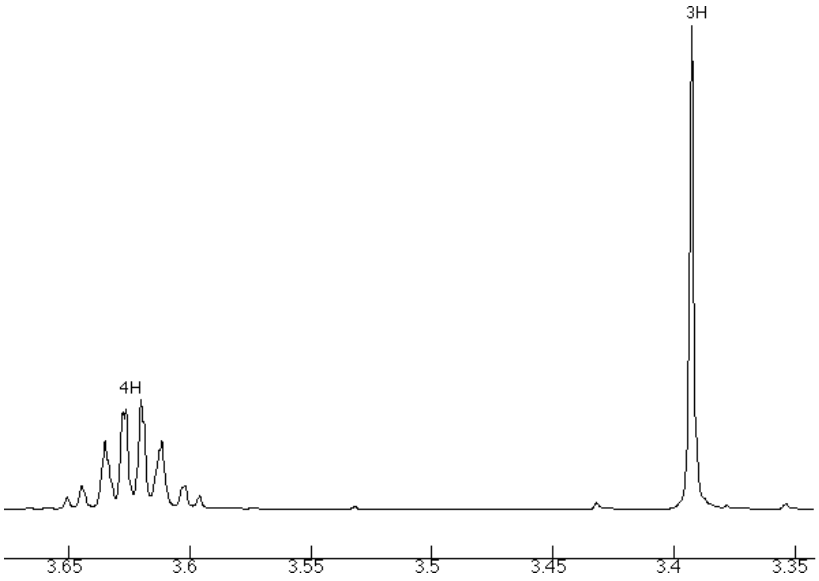


[^{1}H NMR spectrum] **[^{13}C NMR spectrum]** **[IR spectrum]**

#7 C_3H_7OCl back to problems

peak splitting below

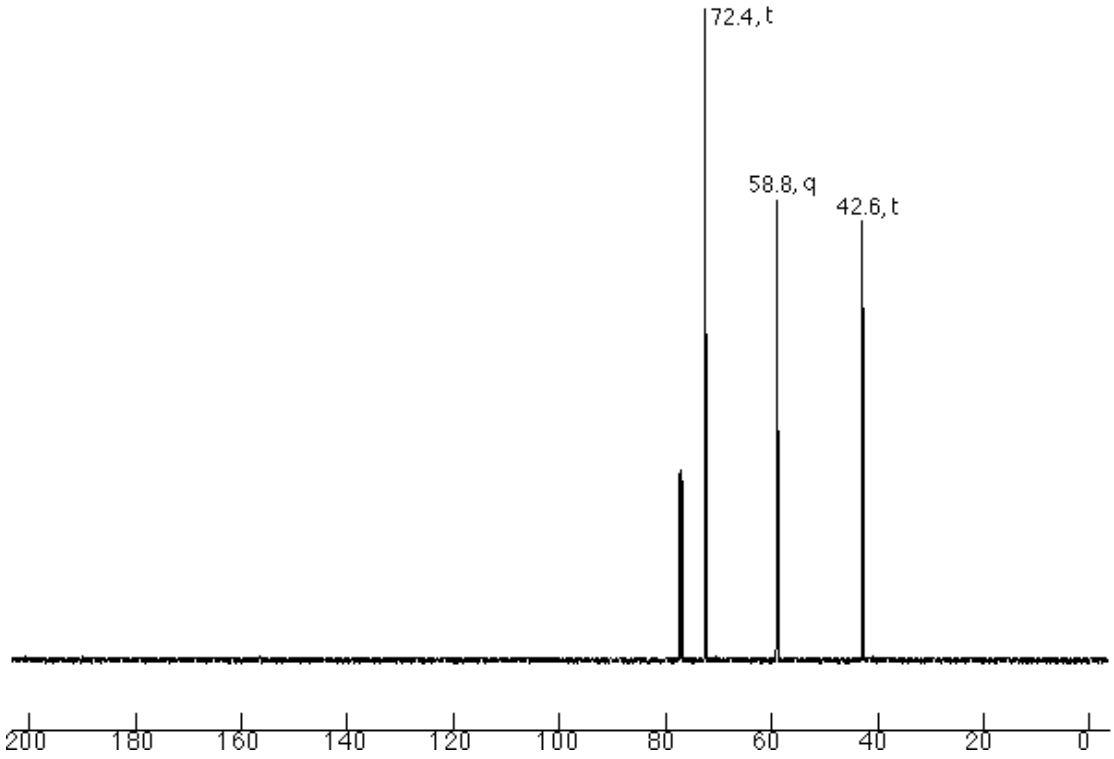




[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

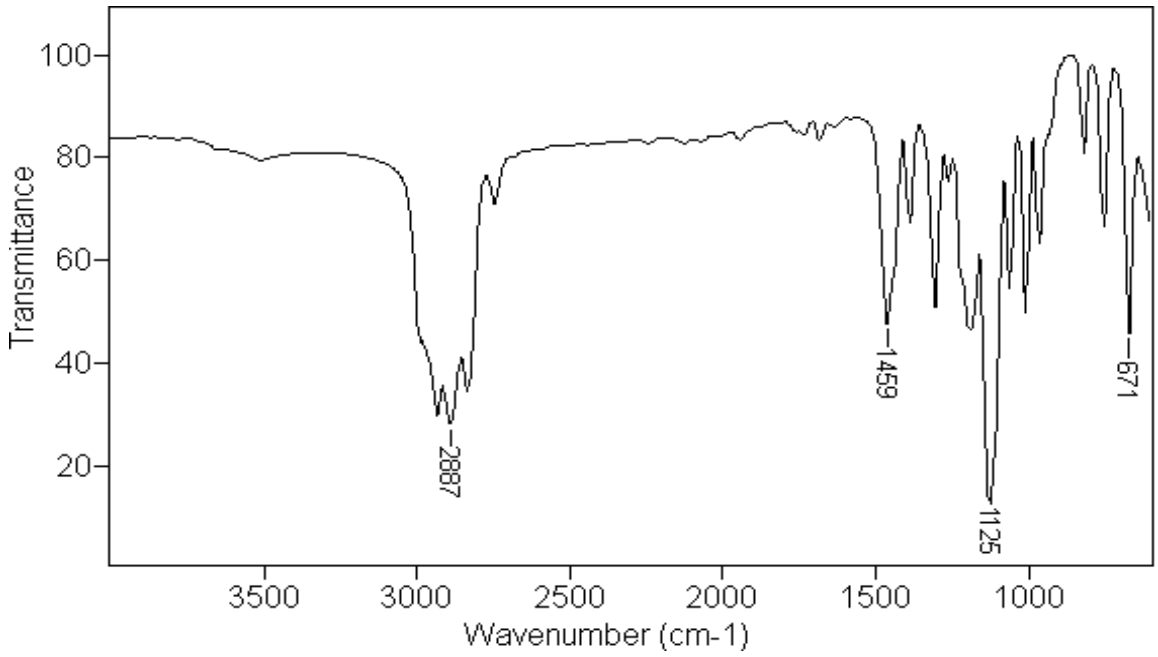
#7 C_3H_7OCl

back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

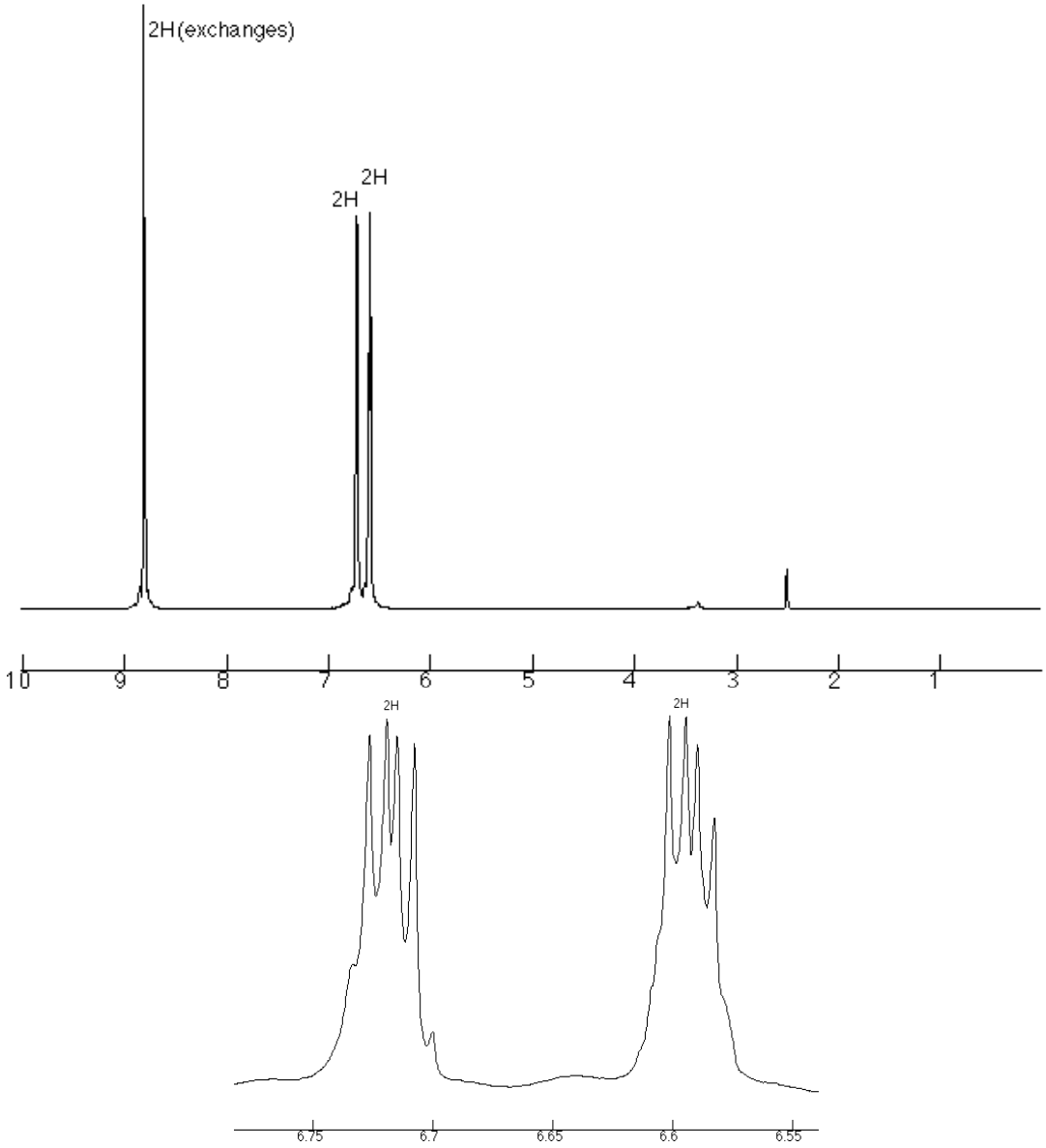
#7 C_3H_7OCl back to problems



^{1}H NMR spectrum **^{13}C NMR spectrum** **IR spectrum**

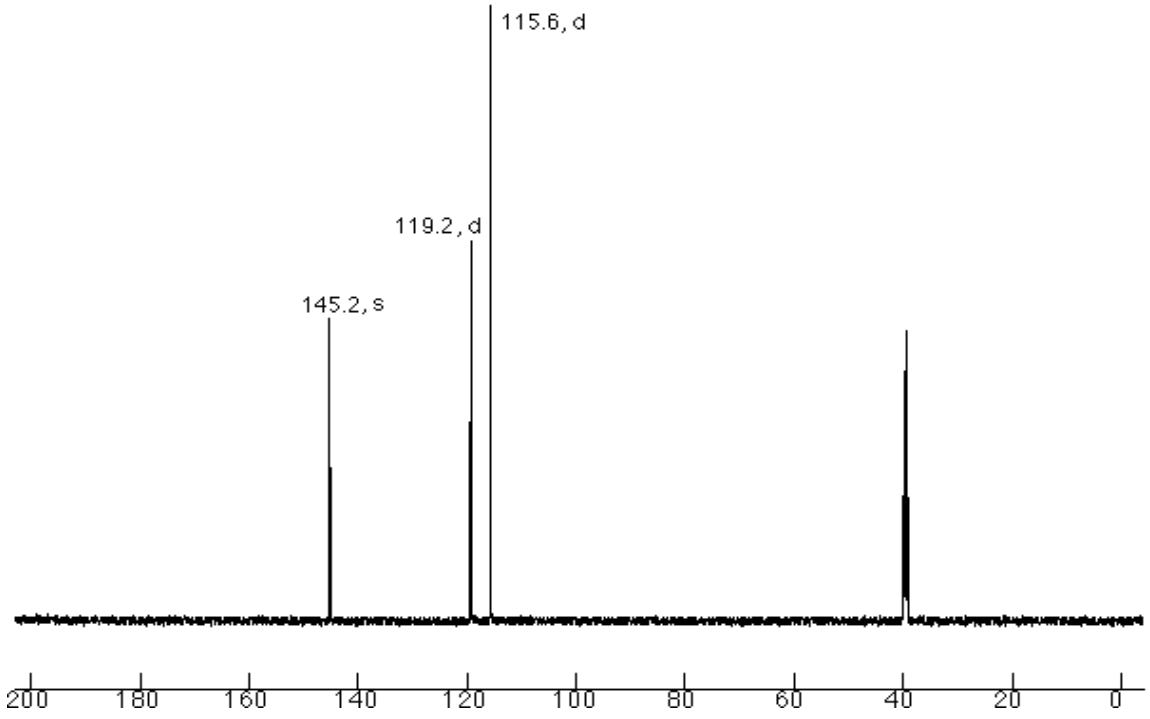
#8 $C_6H_6O_2$ back to problems

peak splitting below



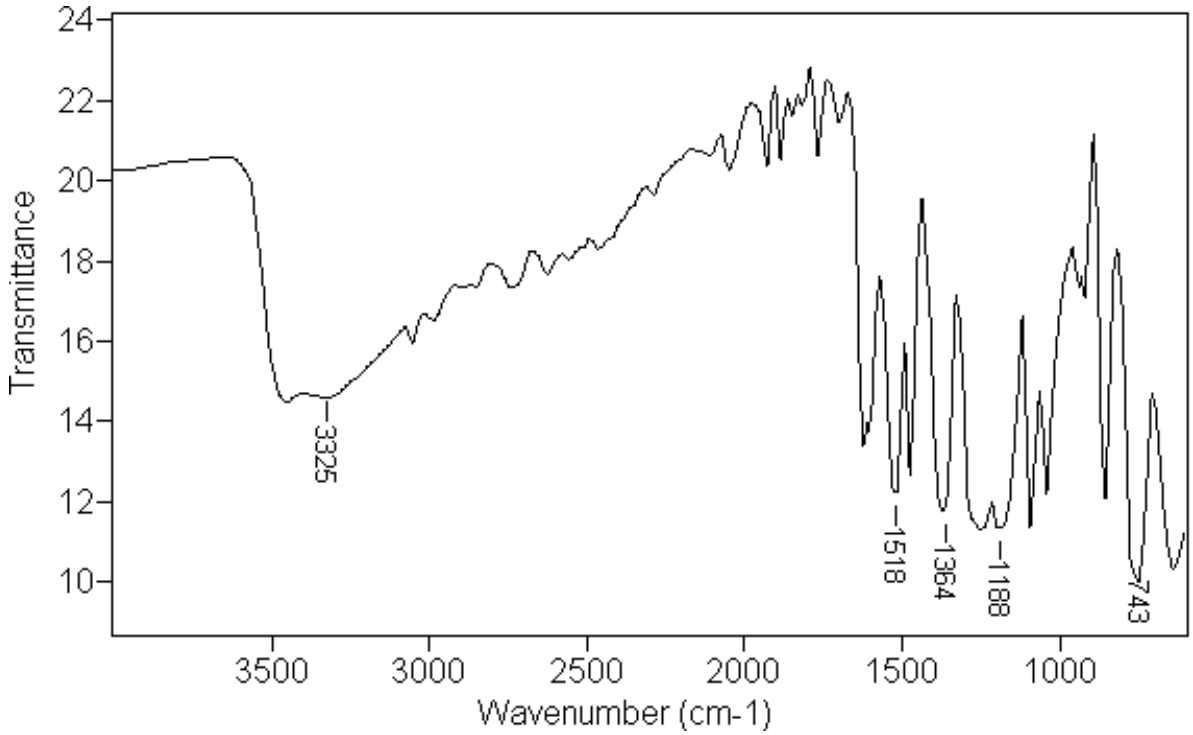
[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#8 $C_6H_6O_2$ back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

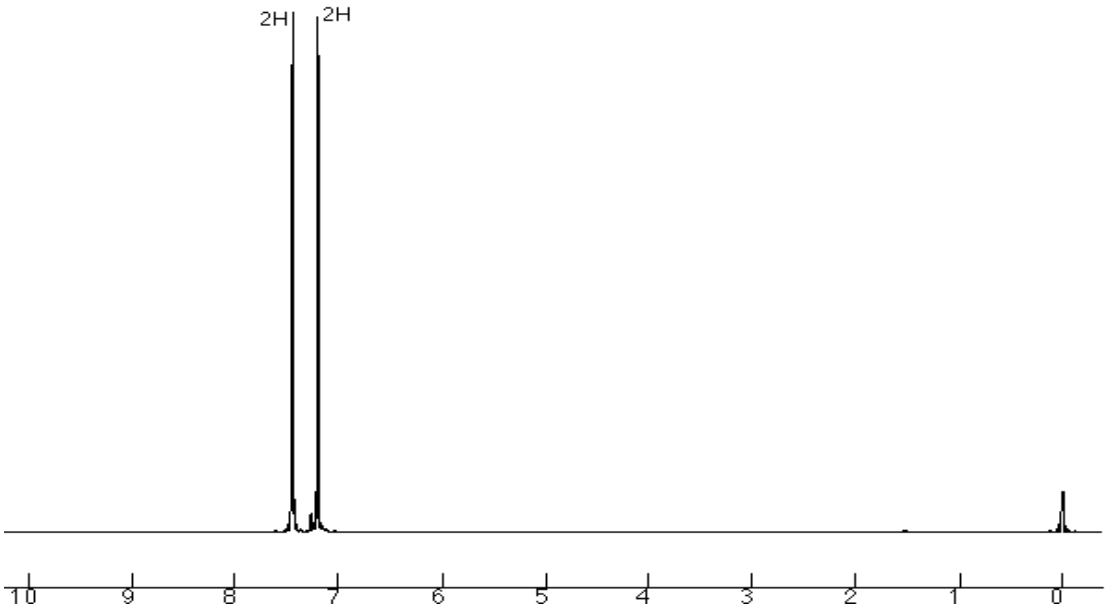
#8 $C_6H_6O_2$ back to problems

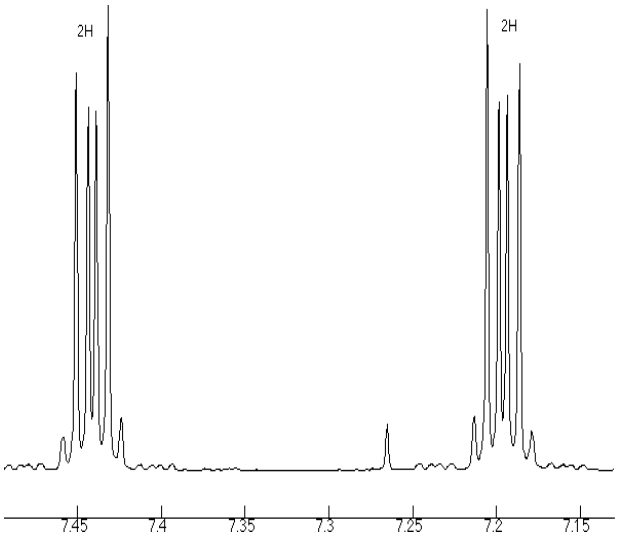


^{1}H NMR spectrum **^{13}C NMR spectrum** **IR spectrum**

#9 $C_6H_4Cl_2$ back to problems

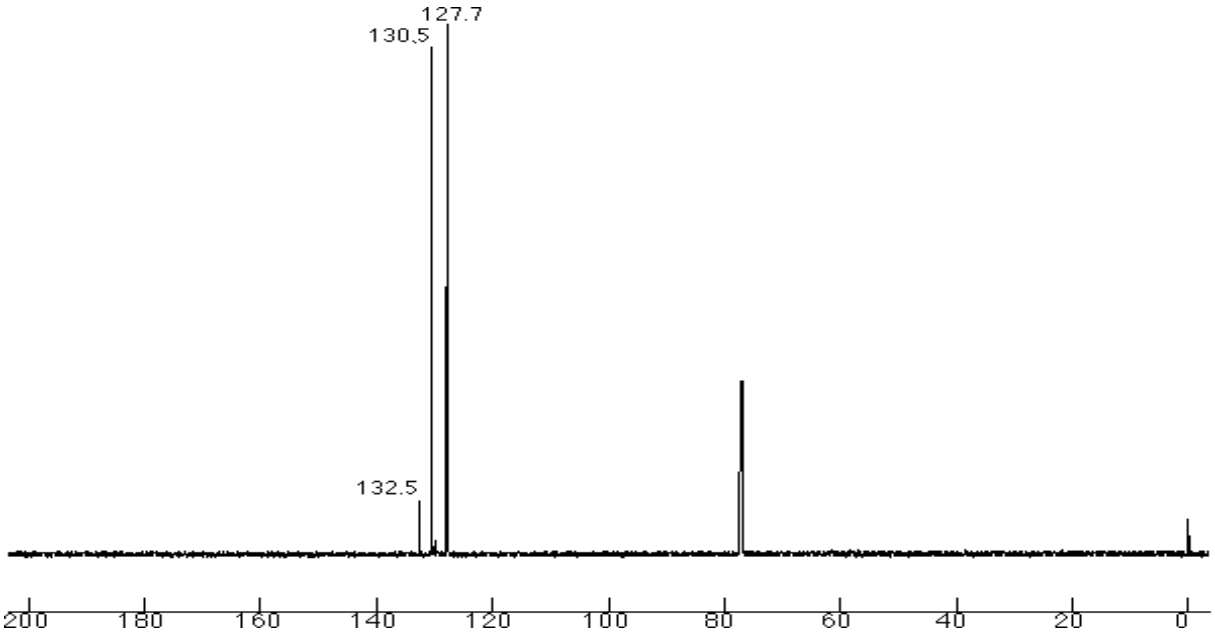
peak splitting below





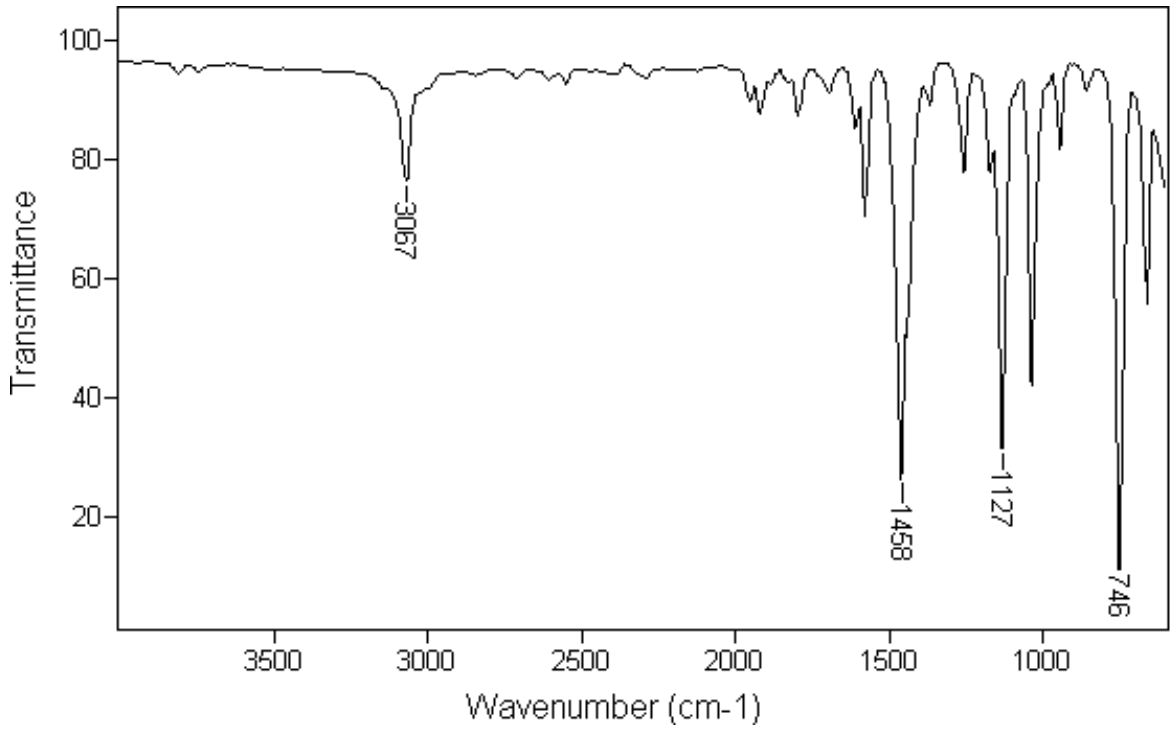
[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#9 $C_6H_4Cl_2$ back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

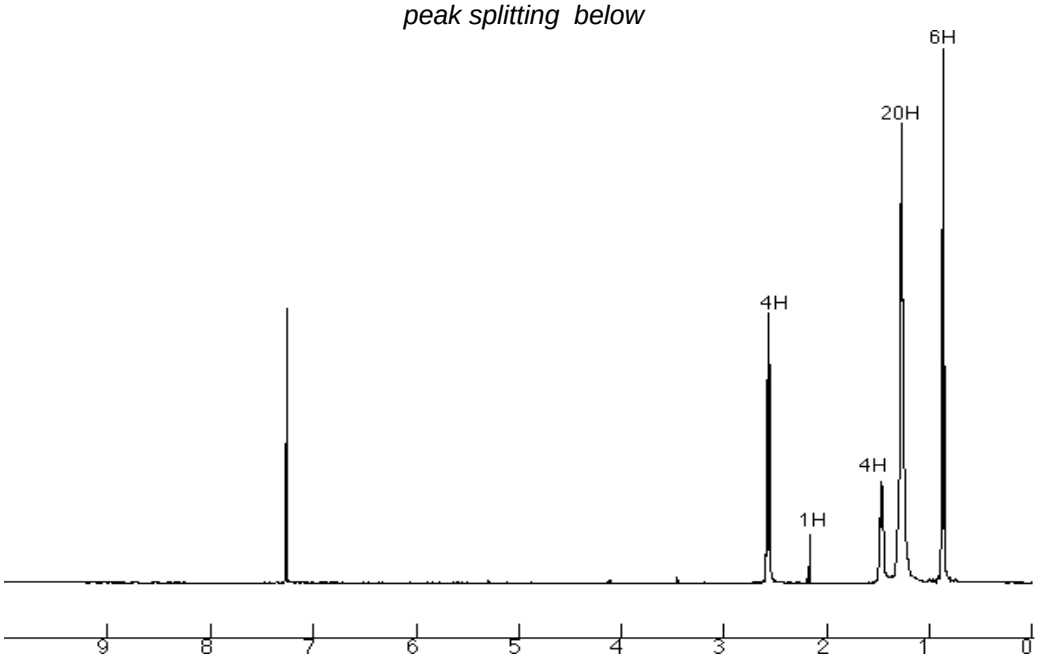
#9 $C_6H_4Cl_2$ back to problems

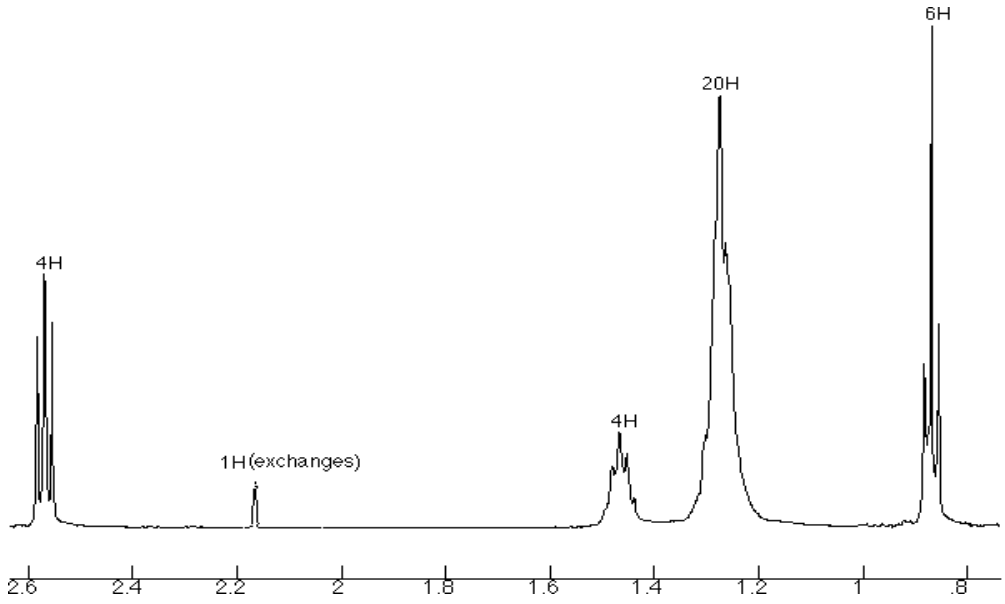


[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#10 $C_{16}H_{35}N$ back to problems

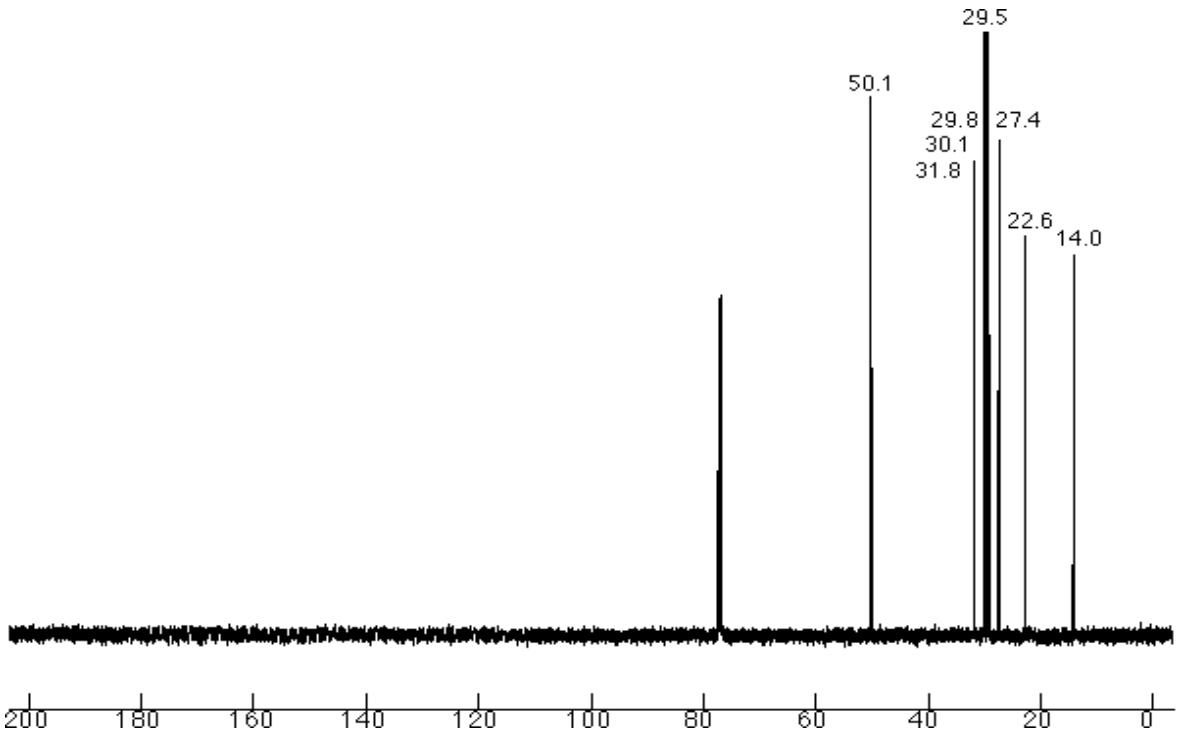
peak splitting below





[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

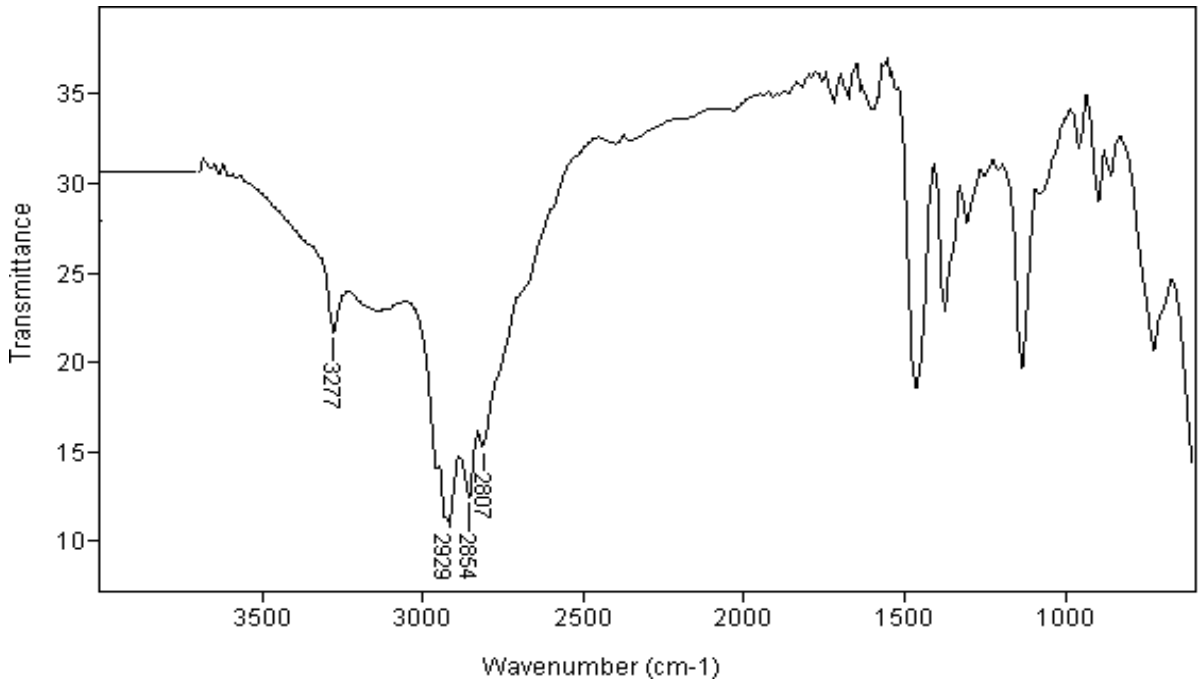
#10 $C_{16}H_{35}N$ back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#10 $C_{16}H_{35}N$

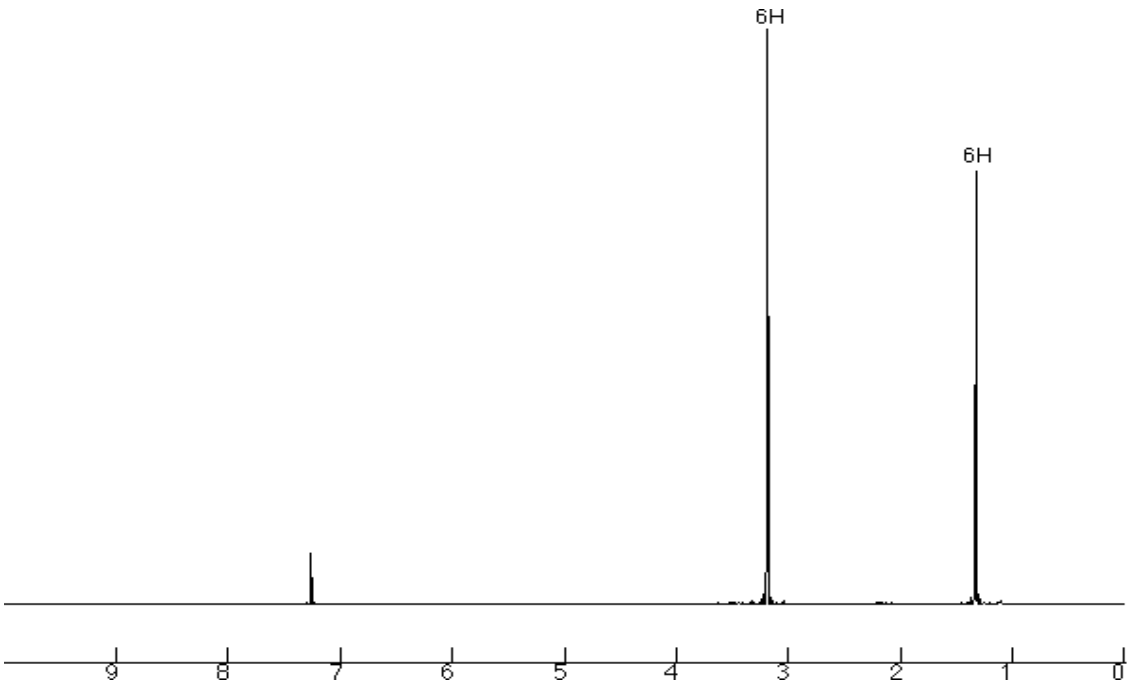
back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

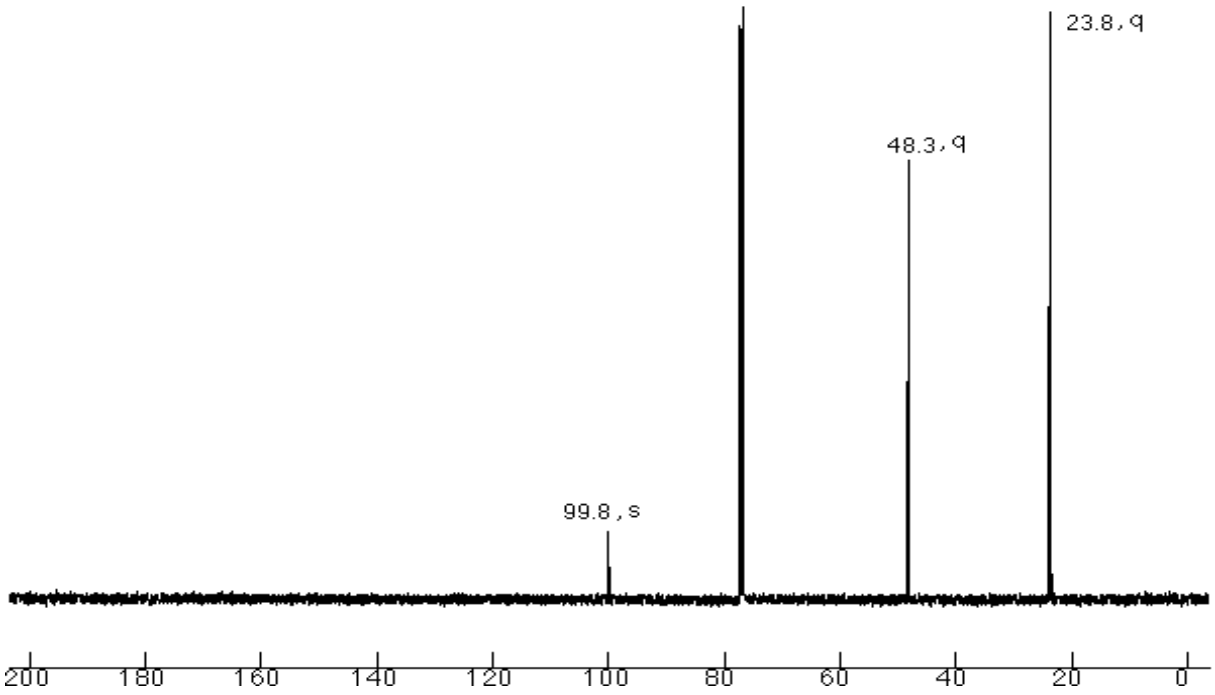
#11 $C_5H_{12}O_2$ back to problems

all singlets!



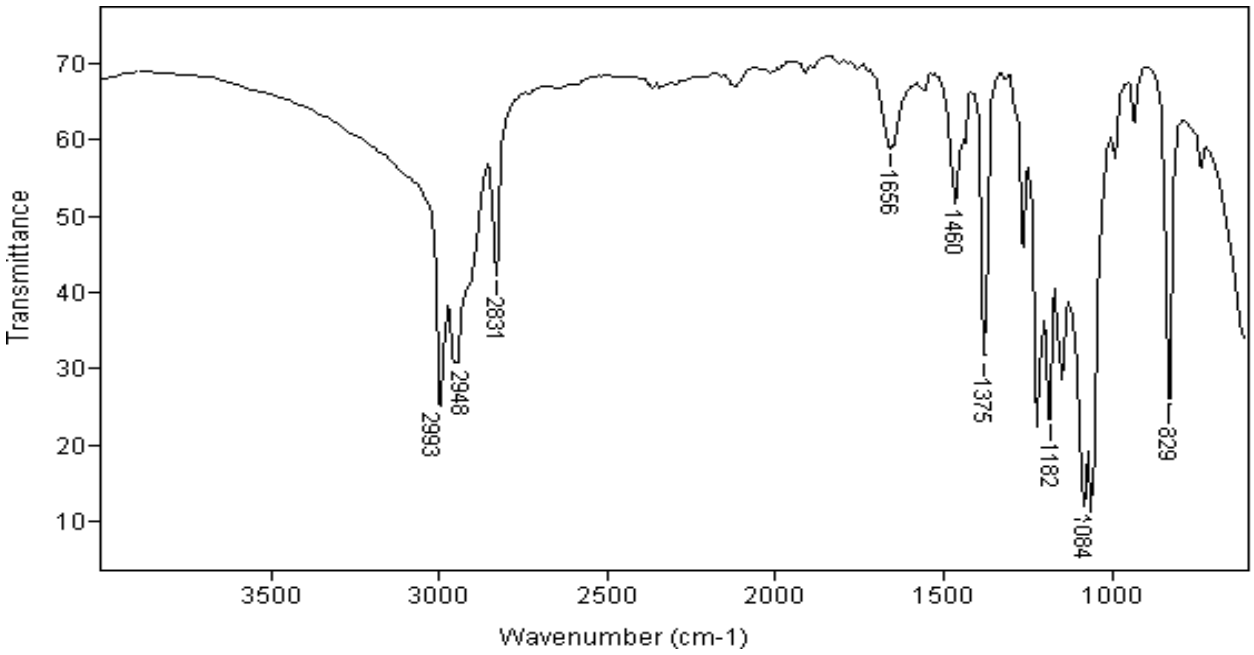
[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#11 $C_5H_{12}O_2$ back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

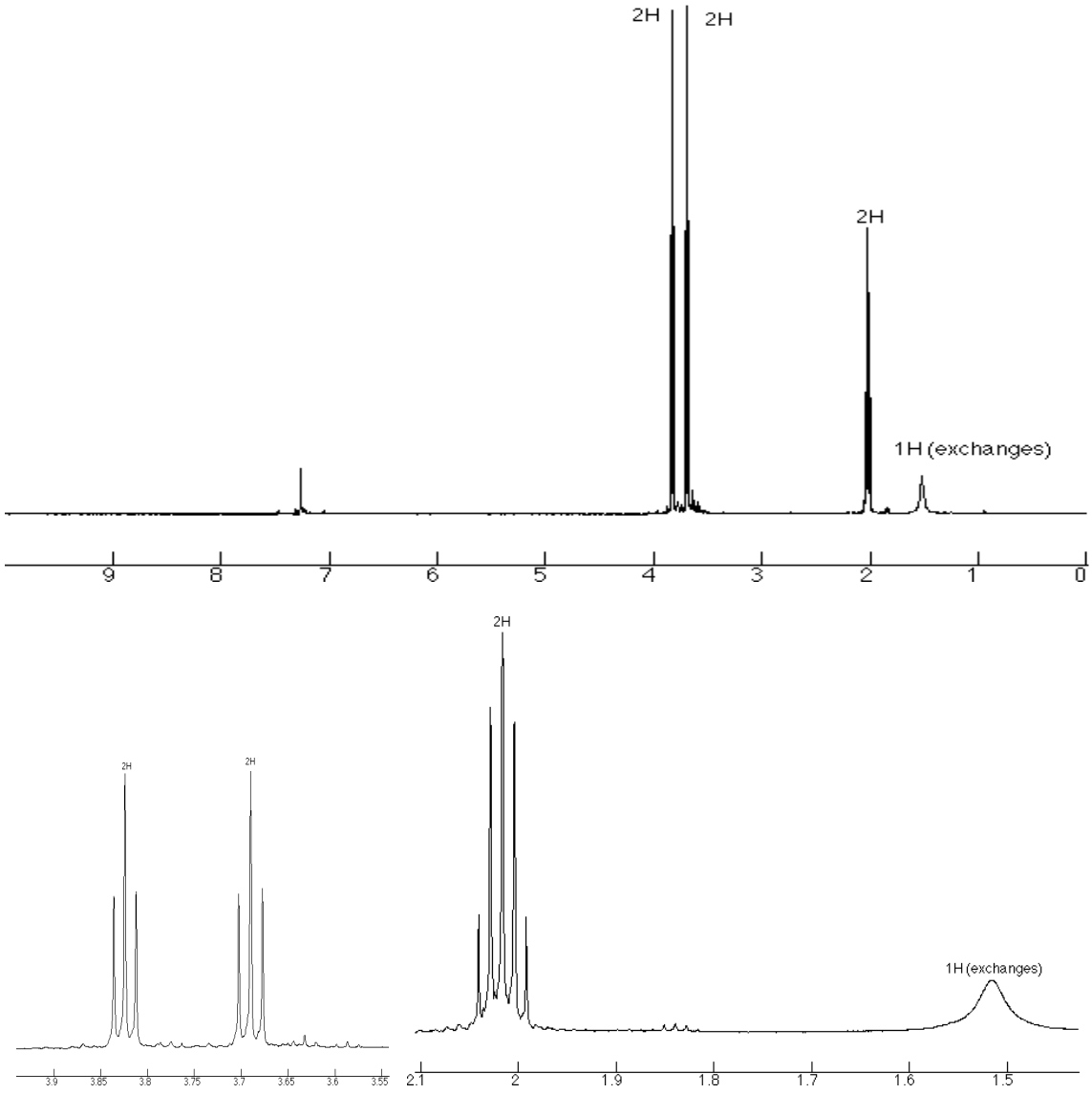
#11 $C_5H_{12}O_2$ back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

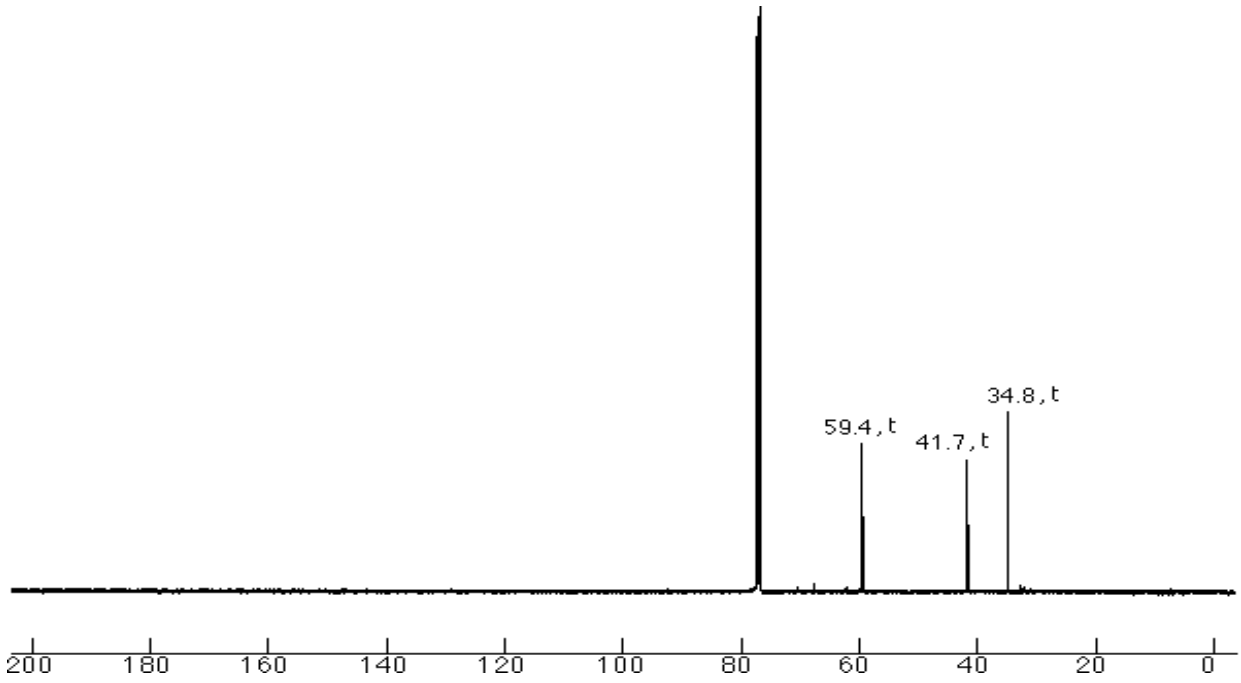
#12 C_3H_7OCl back to problems

peak splitting below



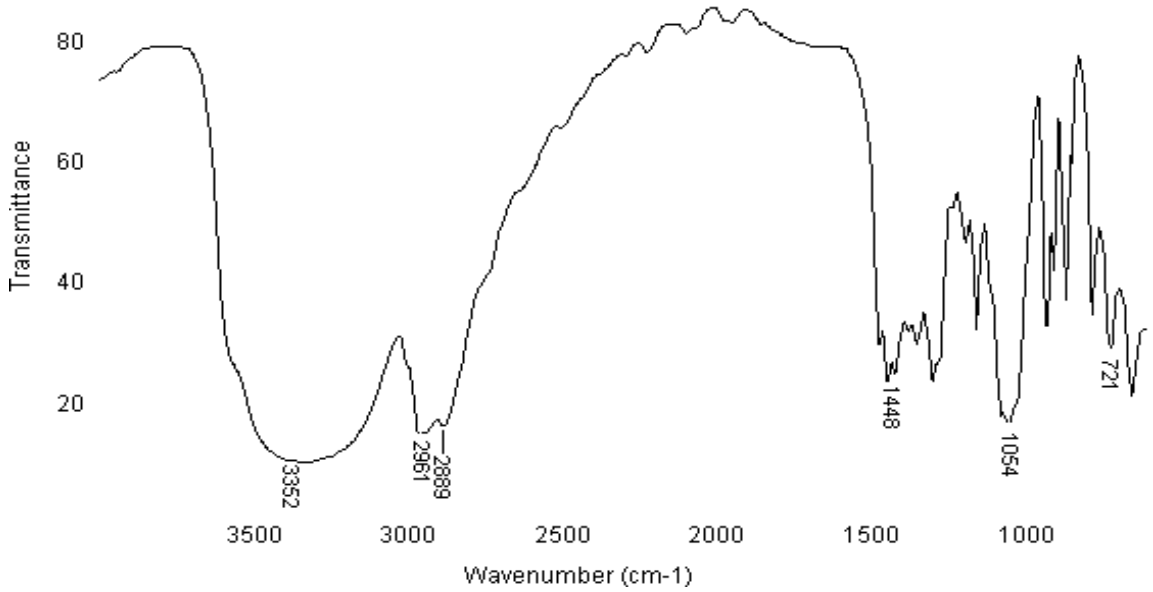
[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#12 C_3H_7OCl back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

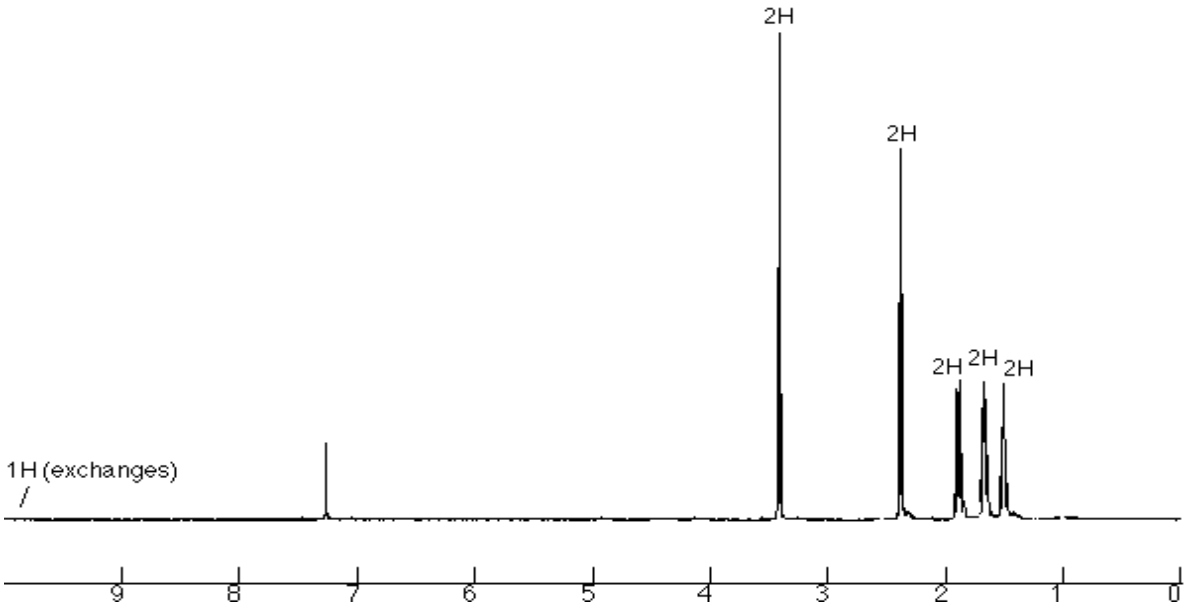
#12 C_3H_7OCl back to problems

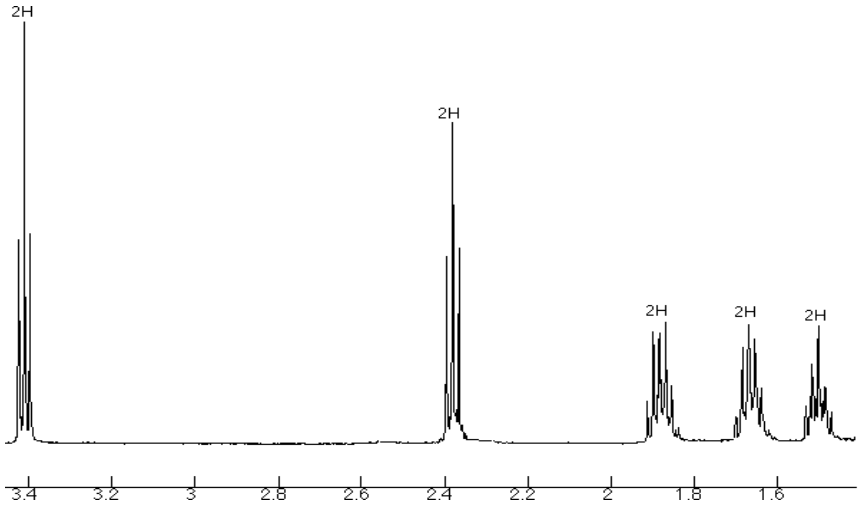


[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#13 $C_6H_{11}O_2Br$ back to problems

peak splitting below

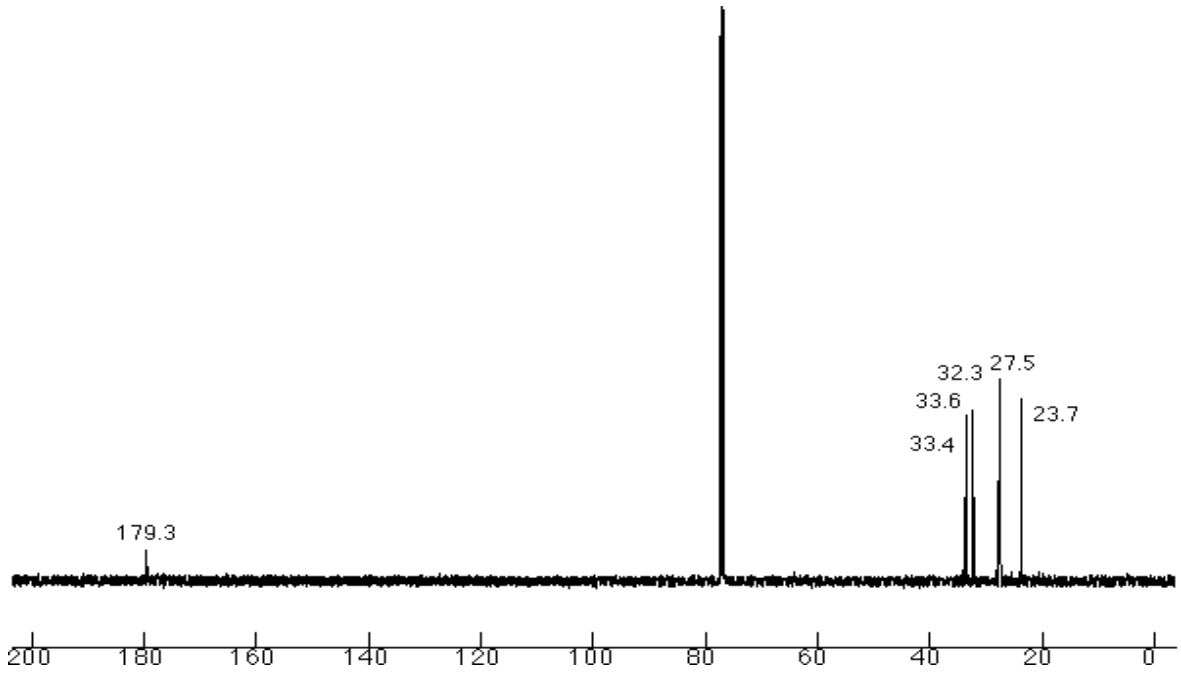




[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

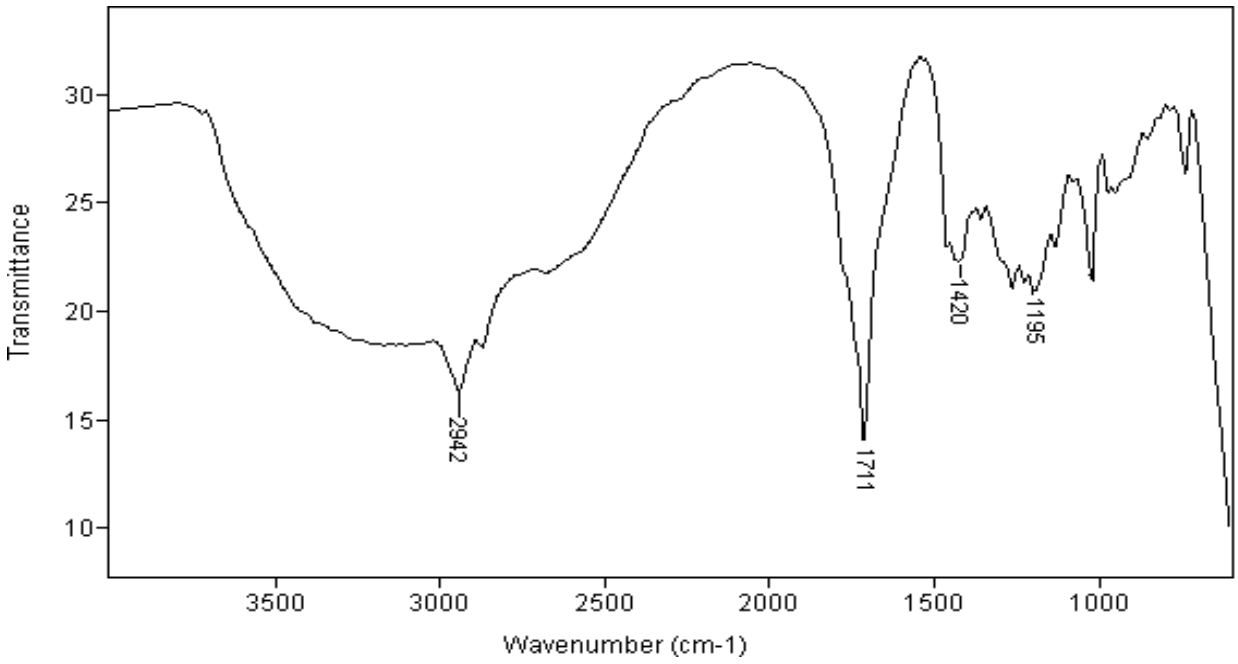
#13 $C_6H_{11}O_2Br$

back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

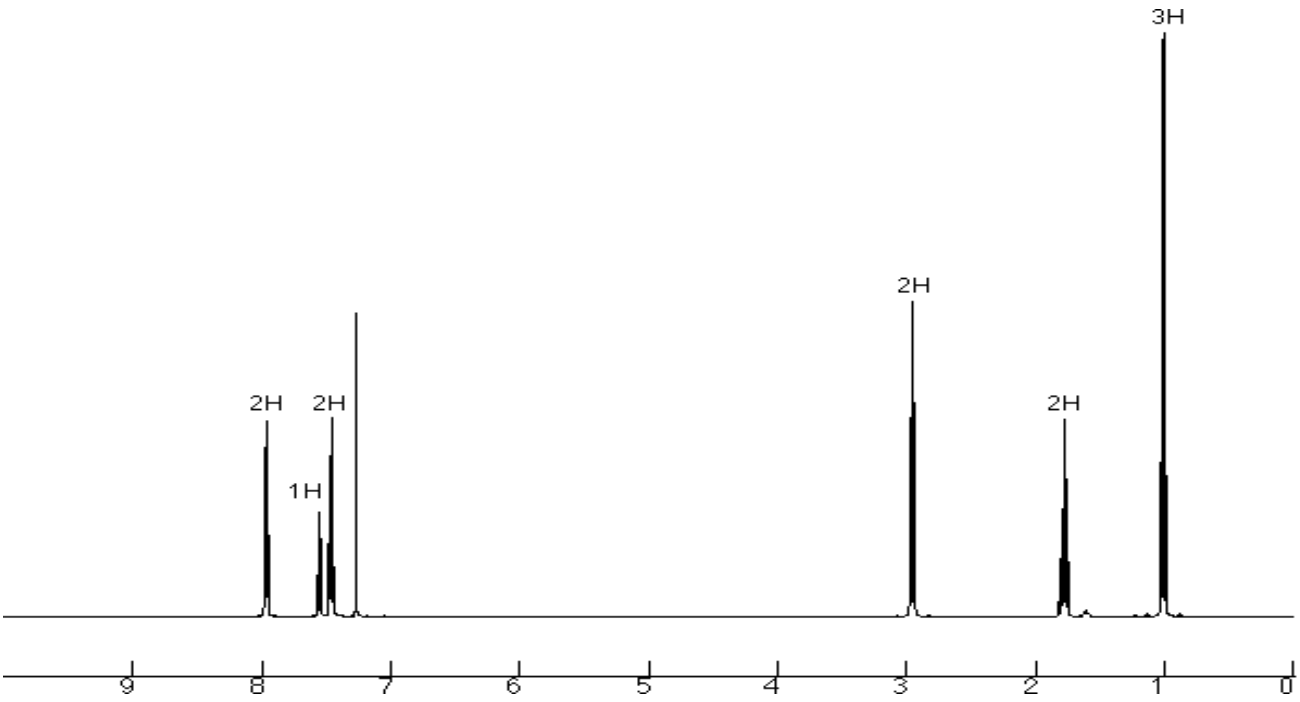
#13 $C_6H_{11}O_2Br$ back to problems

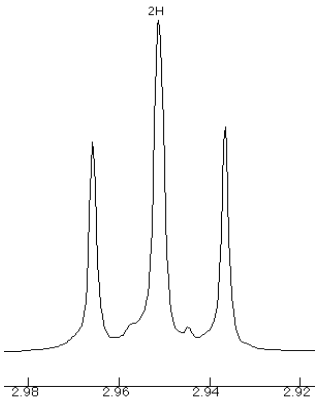


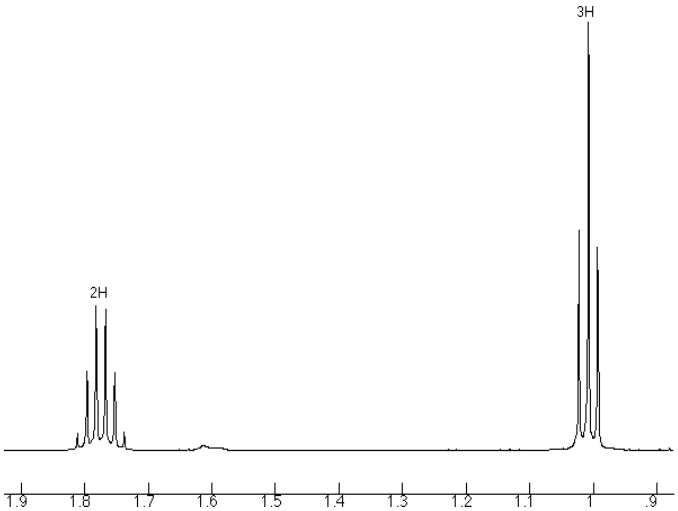
[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#14 $C_{10}H_{12}O_2$ back to problems

peak splitting below

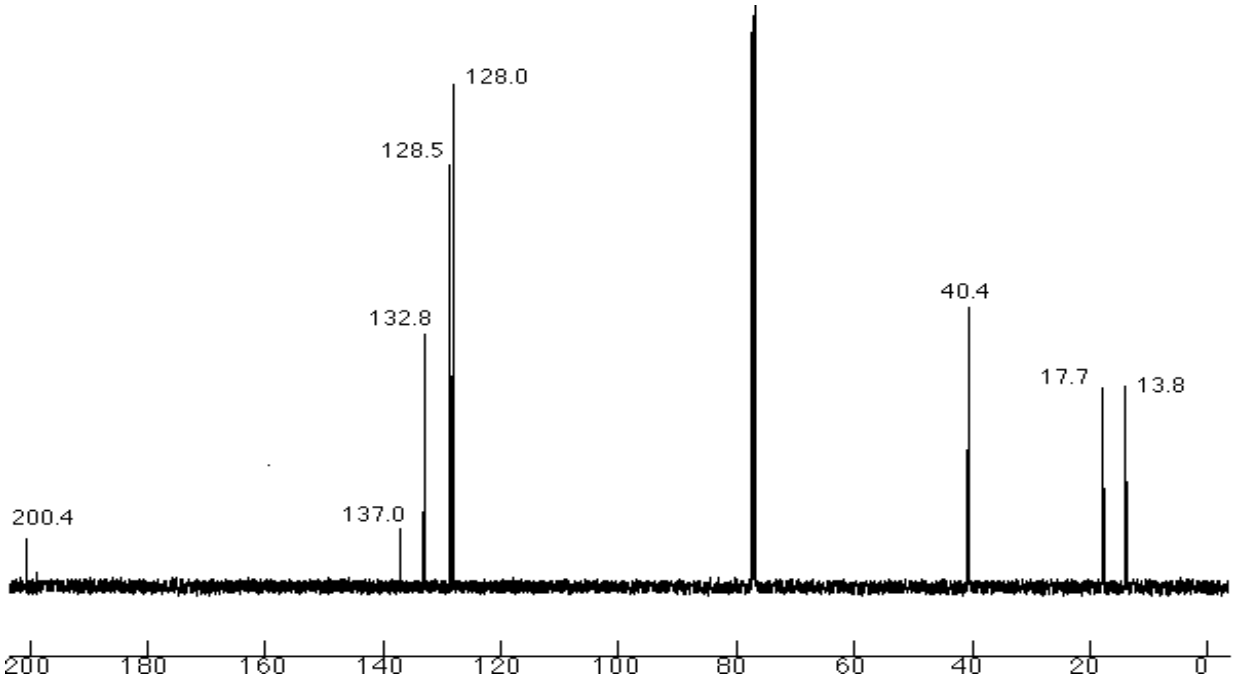






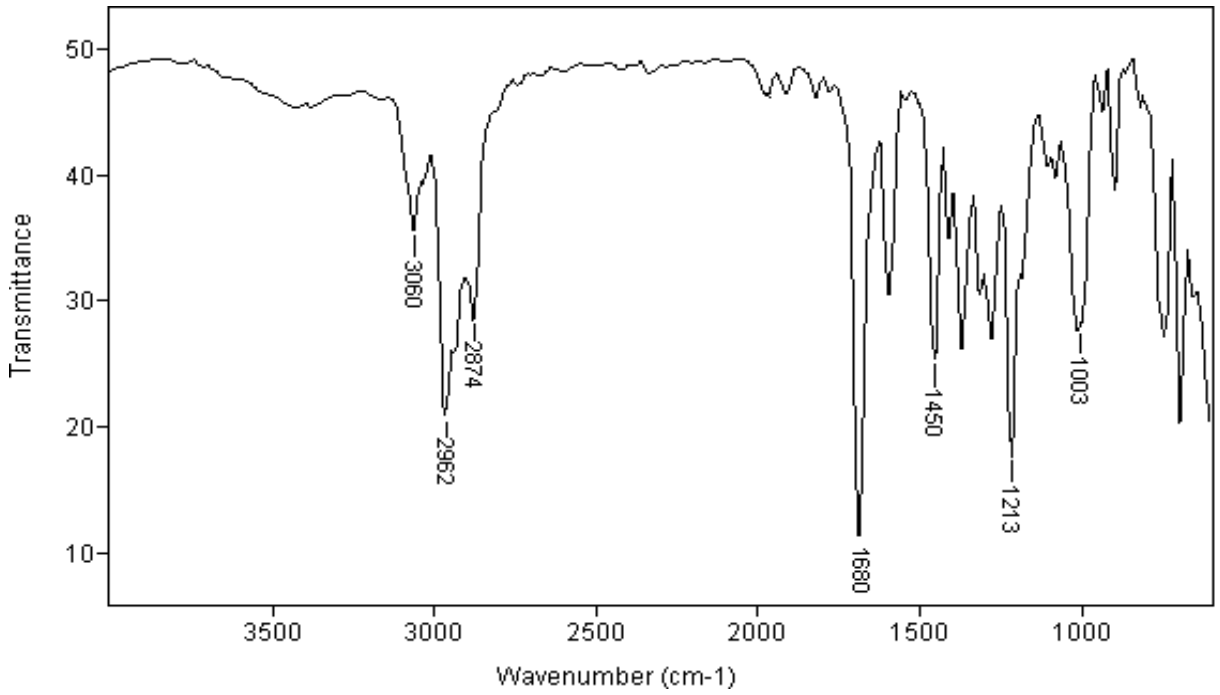
[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#14 $C_{10}H_{12}O_2$ back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

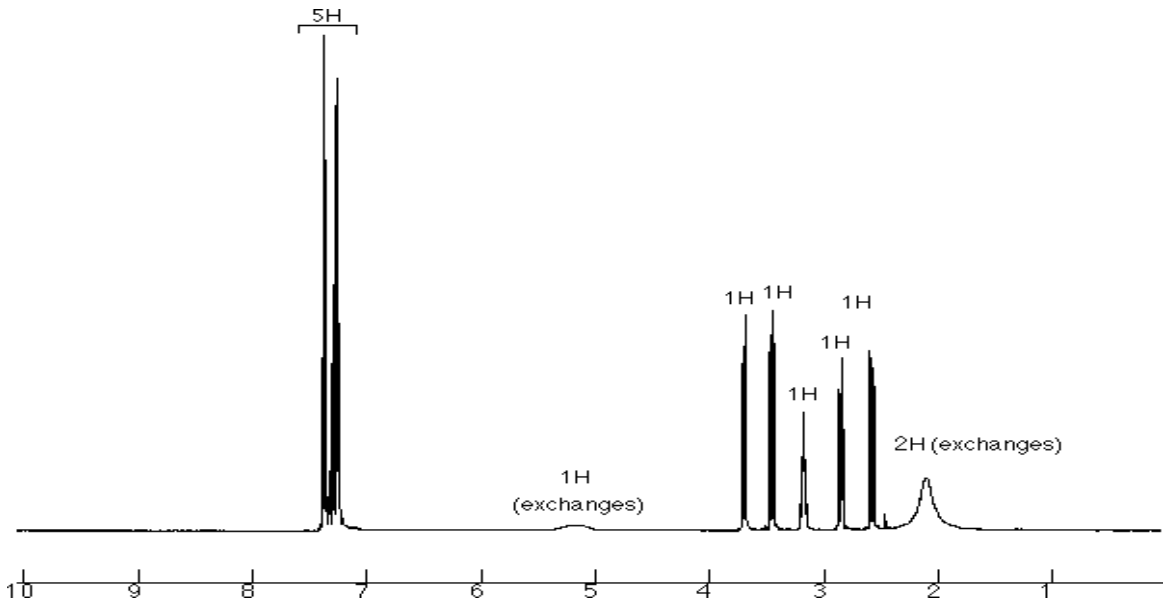
#14 $C_{10}H_{12}O_2$ back to problems

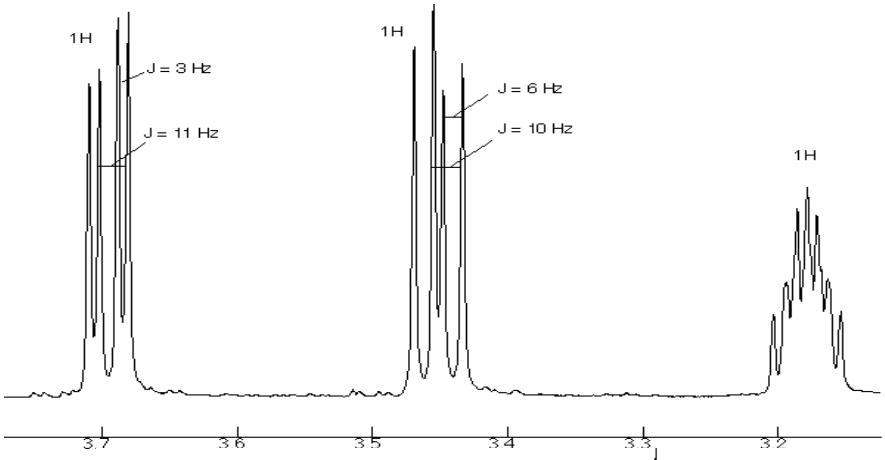


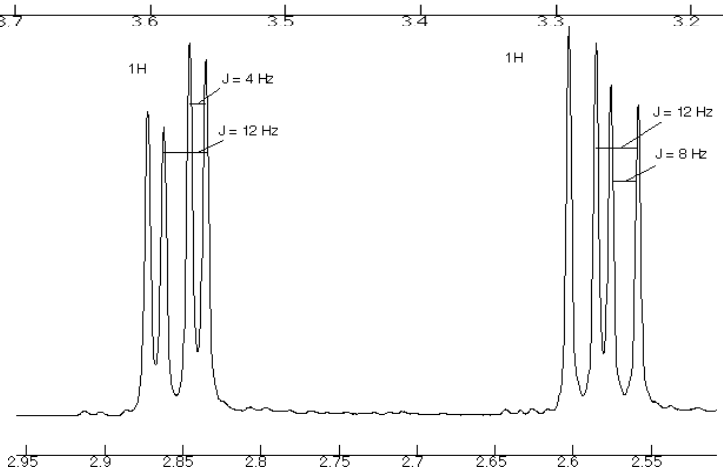
[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#15 $C_9H_{13}NO$ back to problems

peak splitting below

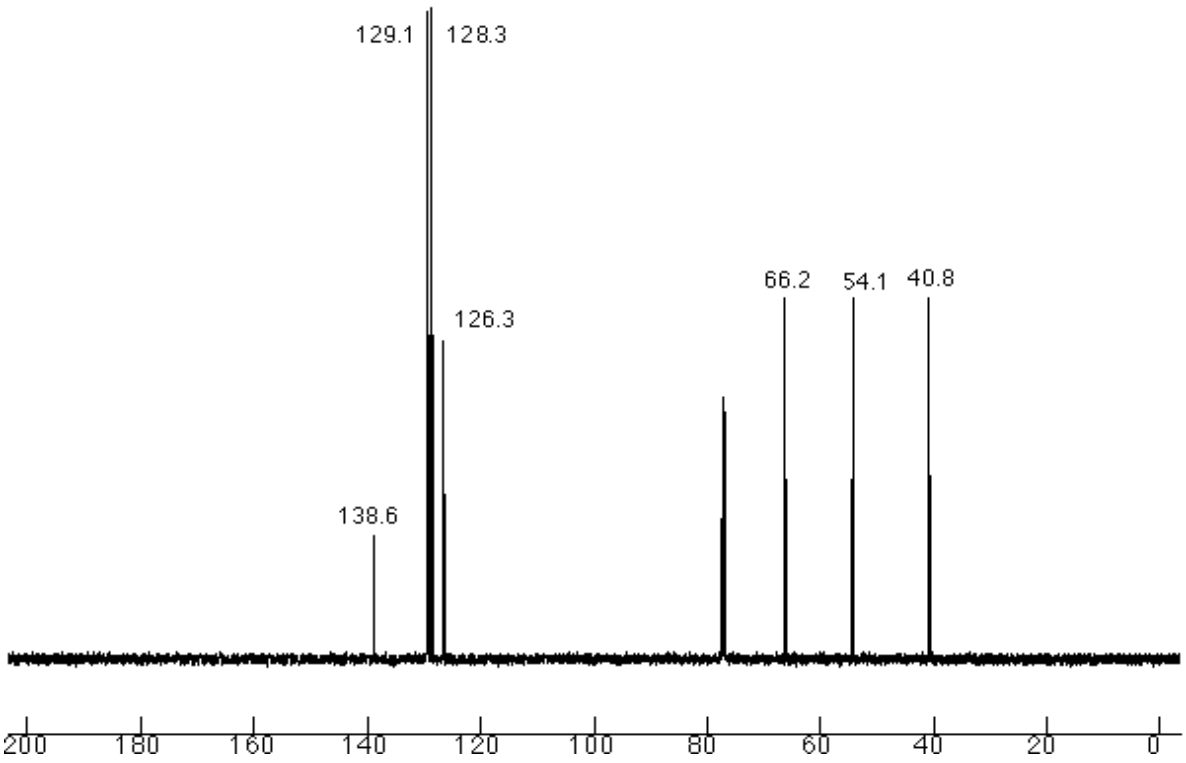






[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#15 $C_9H_{13}NO$ back to problems



[^{1}H NMR spectrum] [^{13}C NMR spectrum] [IR spectrum]

#15 $C_9H_{13}NO$ back to problems