NMR problems - Fall 2002

Sheet with grid and no page numbers

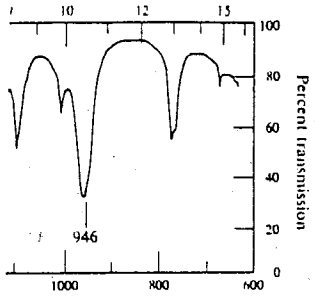
Formula	Relative Areas of Peaks (Low PPM to High PPM)
$C_3H_6Cl_2$	1: 2
$C_4H_8O_2$	3:3:2
C_4H_8O	3:3:2
$C_9H_{10}O_2$	3:2:5
C_9H_{12}	3:1
C_7H_8S	1:2:5

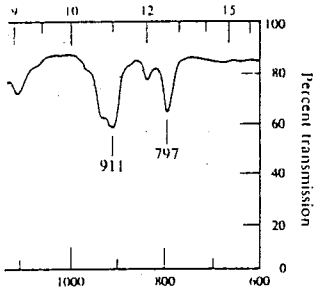
Sheets starting with page 482

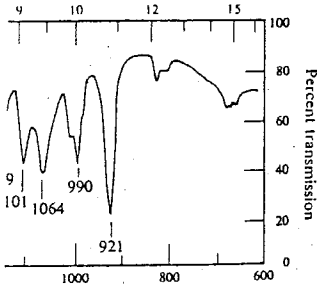
Formula	Relative Areas of Peaks (Low PPM to High PPM)
$C_3H_6Br_2$	1:2
$C_4H_7O_2Cl$	3:4
C_4H_9Br	6:1:2
C_8H_9Br	3:2:2:2
$C_4H_{10}O_2$	3:6:1

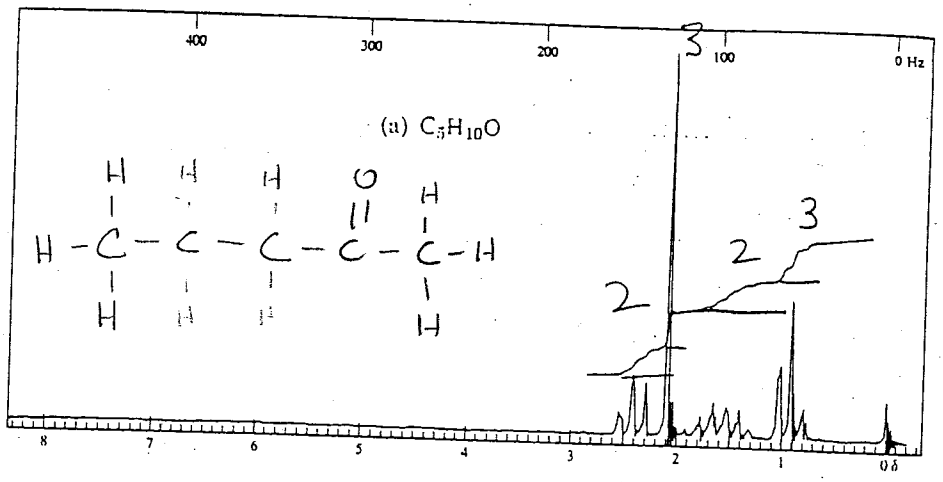
Sheets starting with page 436

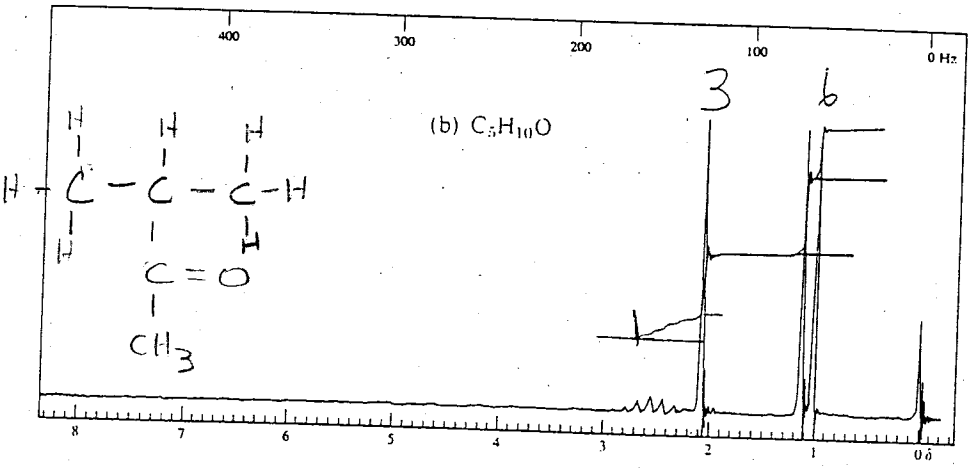
Formula	Relative Areas of Peaks (Low PPM to High PPM)
C_8H_{10}	3:2:5
C_3H_6Br	1:2
C_3H_7Br	3:2:2
$C_4H_{10}O$	6:1:2:1
$C_4H_{10}O$	3:2
$C_8H_{10}O$	3:1:1:5
$C_8H_{10}O$	2:3:5
$C_8H_{10}O$	3:2:5











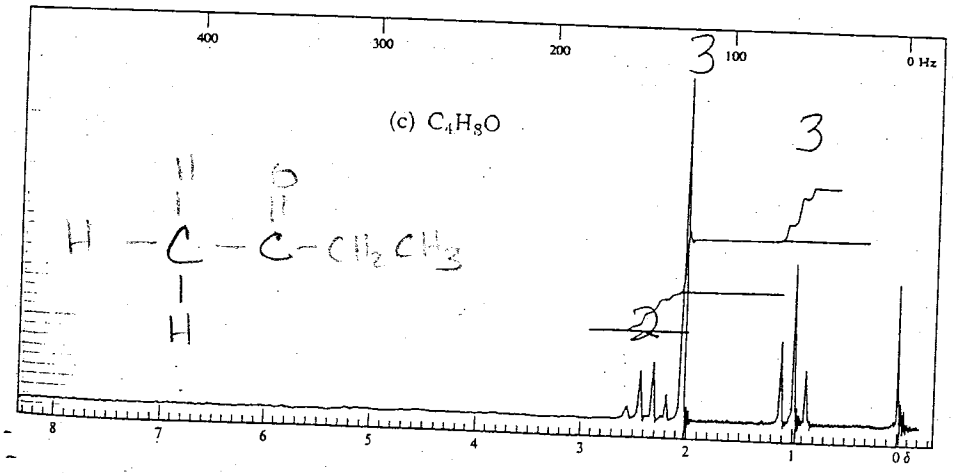
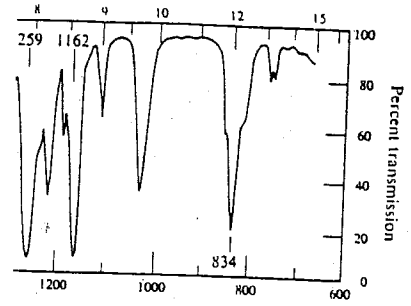
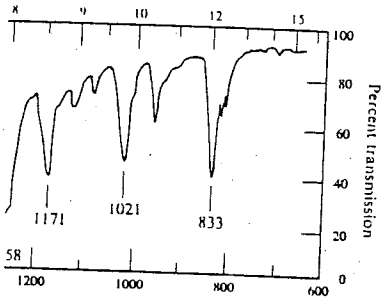
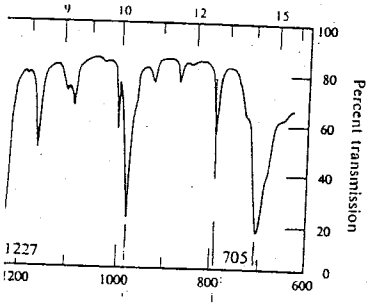


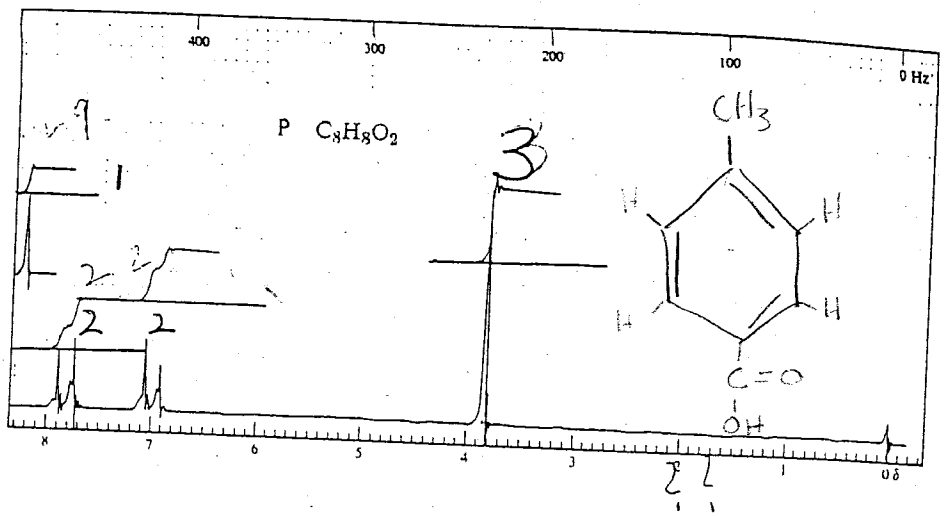
Figure 19.3. Nmr spectra for Problem 29, p. 653.

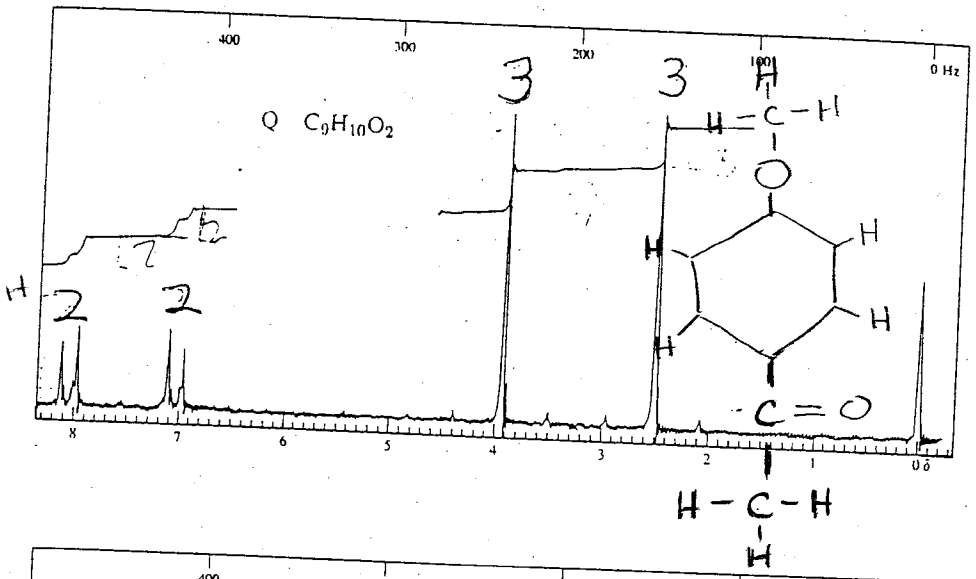






30, p. 653.





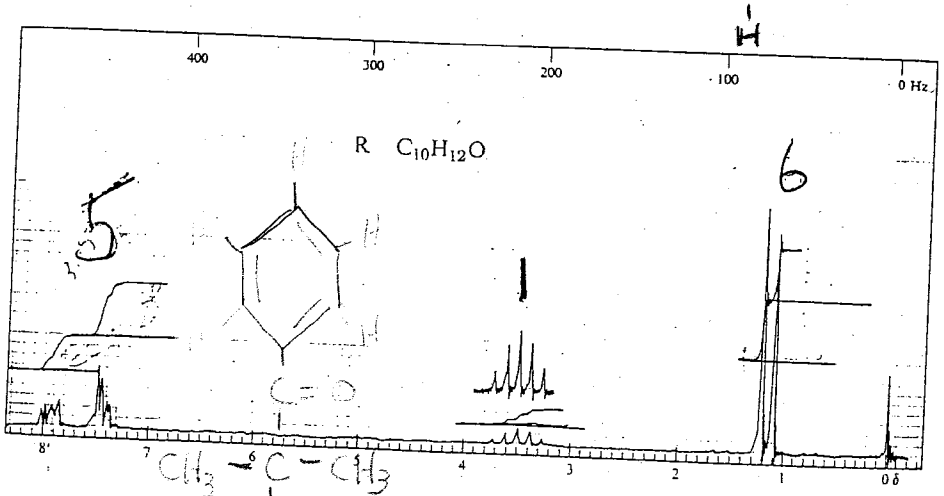


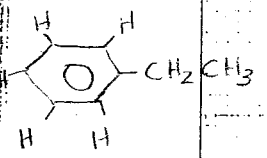
Figure 19.5. Nmr spectra for Problem 30, p. 653.

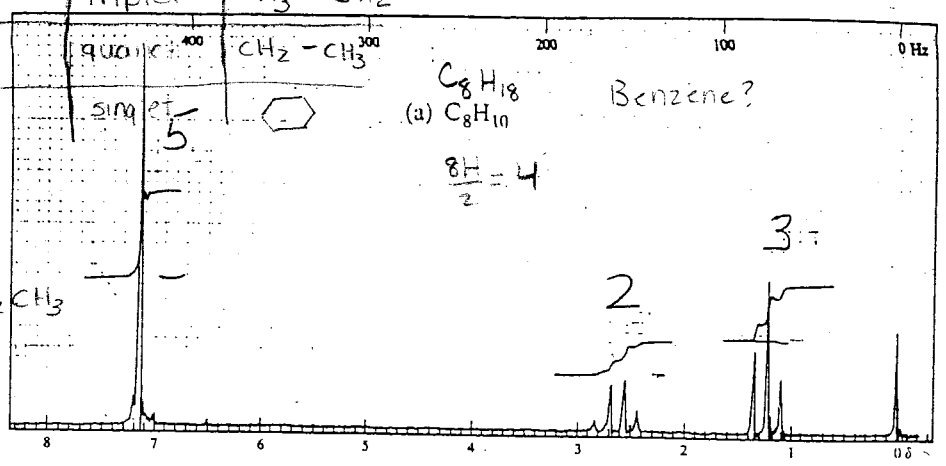
position	area	splitting	conclusion
1.1	3	triplet	CH_3-CH_2
2.6	2	quartet	CH_2-CH_3
7	5	singlet	

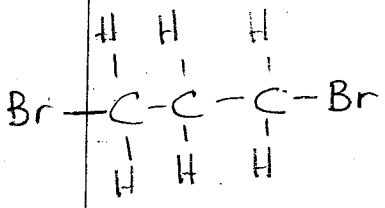
C_8H_{18} Benzene?

(a) C_8H_{10}

$\frac{8H}{2} = 4$







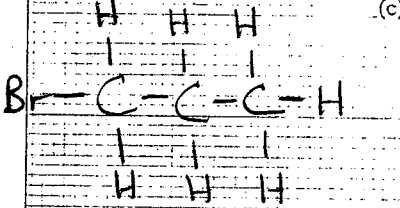
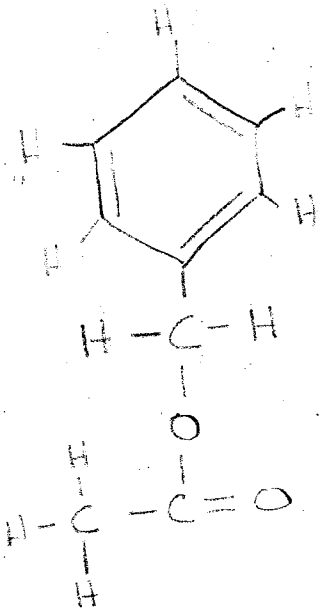
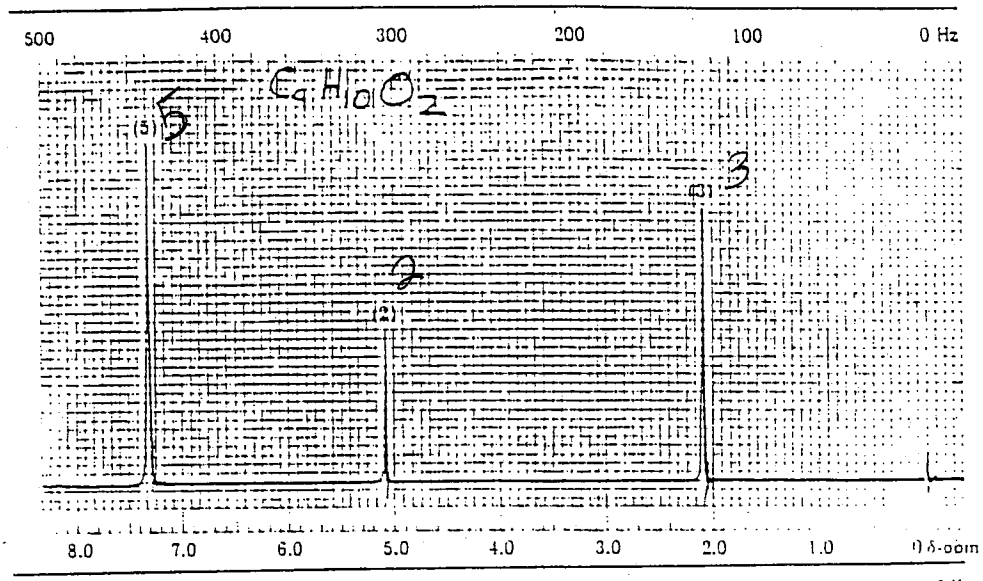
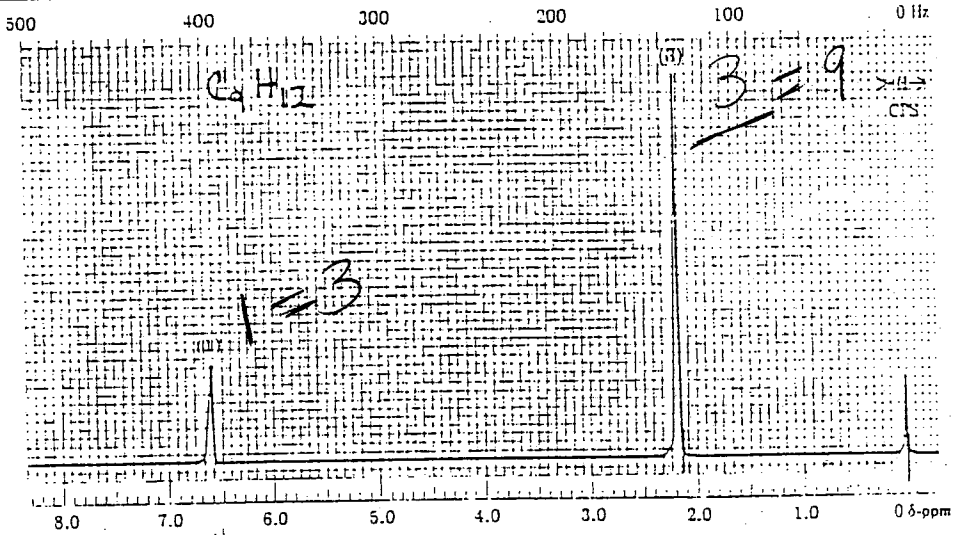
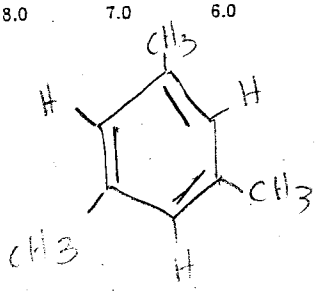


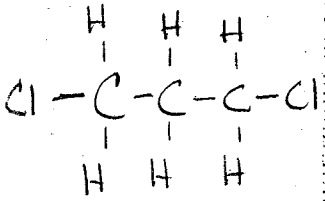
Figure 13.16. Nmr spectra for Problem 13.12, p. 435.

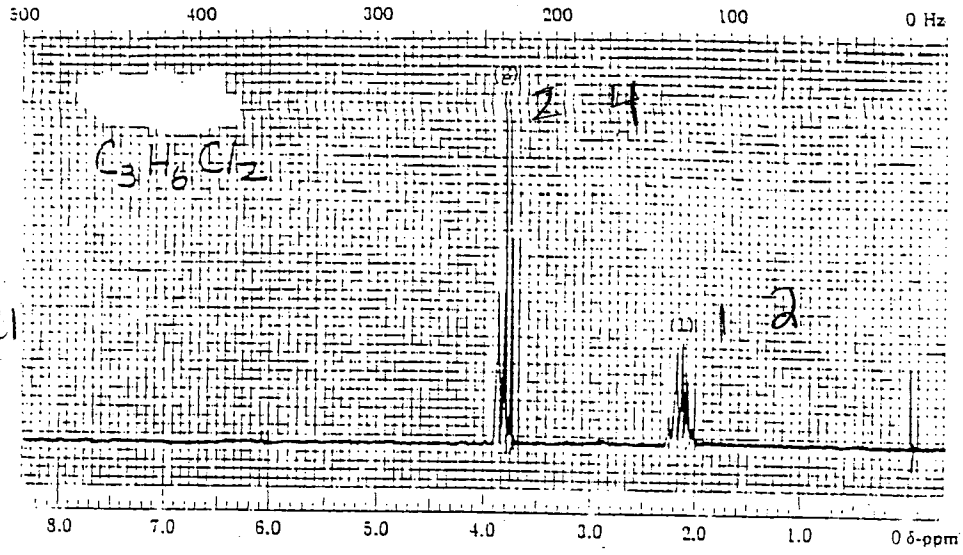


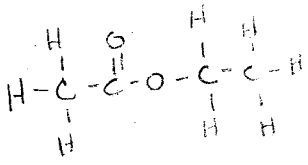

500
400
300
200
100
0 Hz
$C_9H_{10}O_2$
5
2
3
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0 δ-ppm

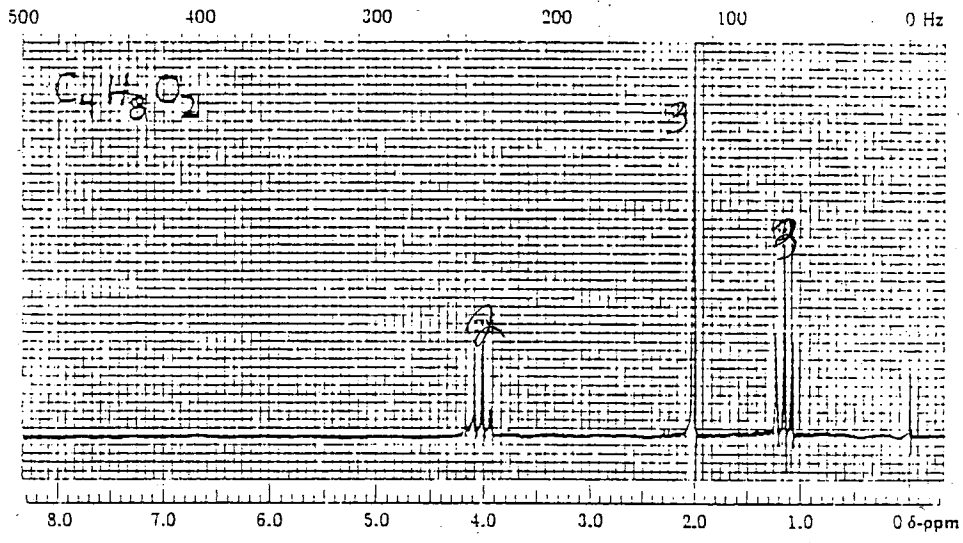

500
400
300
200
100
0 Hz
C_9H_{12}
3:2:9
1:2:3
CPS
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0 δ-ppm

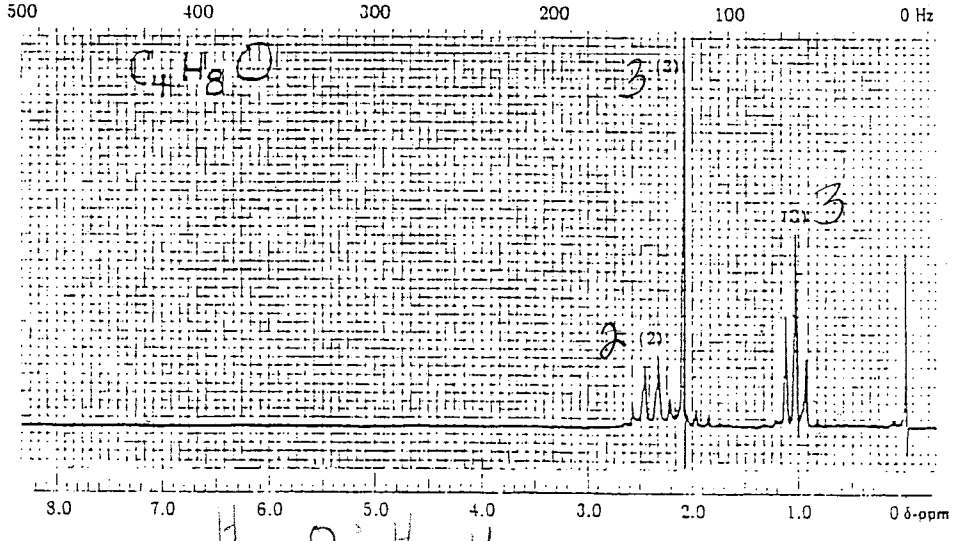


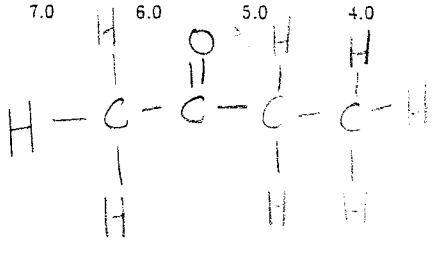



500
400
300
200
100
0 Hz
$C_3H_6Cl_2$
2
1
1
2
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0 δ-ppm




500
400
300
200
100
0 Hz
$C_4H_8O_2$
3
3
2
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0 δ-ppm

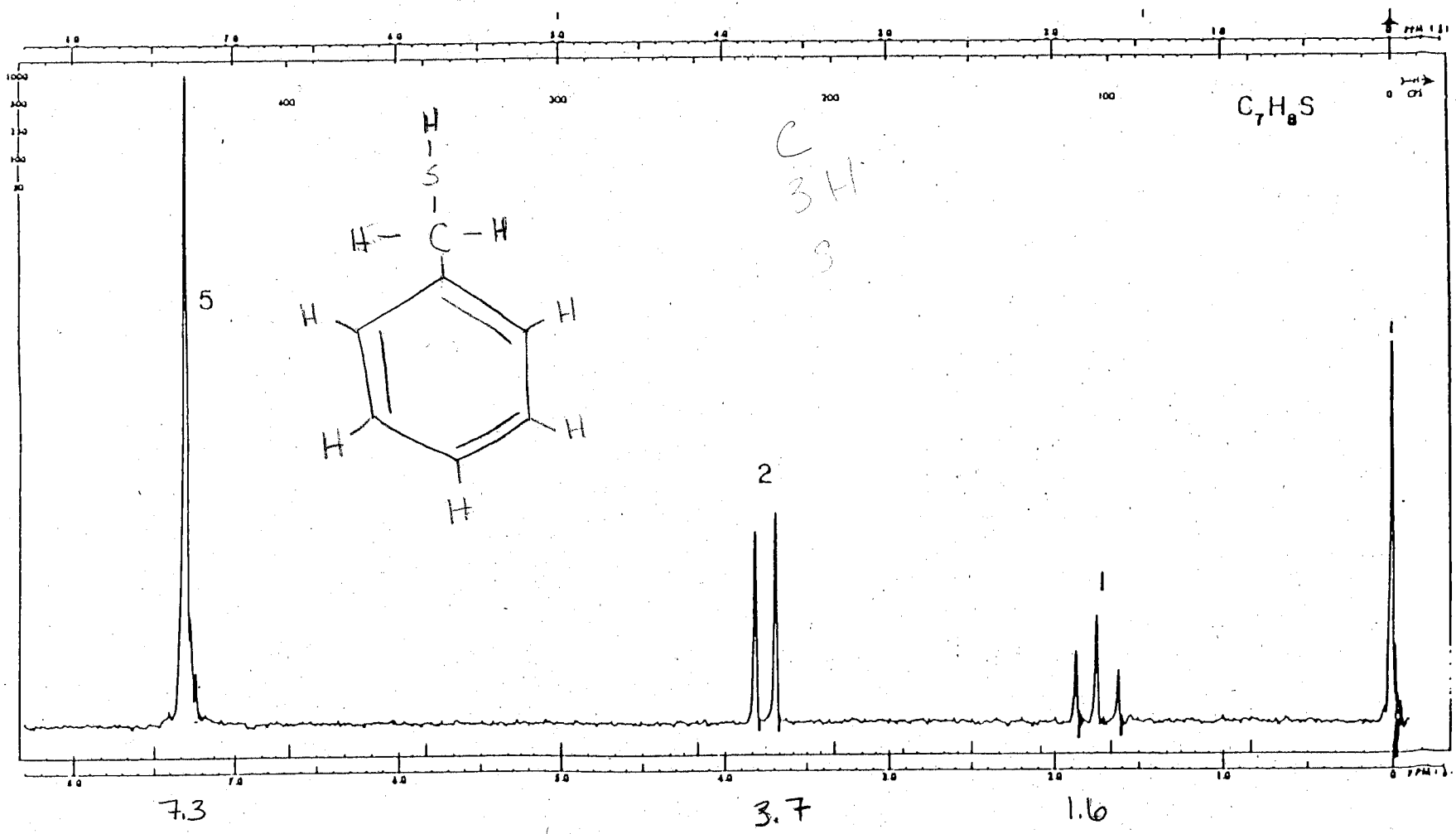

500
400
300
200
100
0 Hz
C_4H_8O
3
3
2
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0 δ-ppm



P	A	S	C
1.6	1	trip	$SH-CH_2$
3.7	2	doub	CH_2-SH
7.3	5	singl	⬡

what's left?

CH_2
CH
S



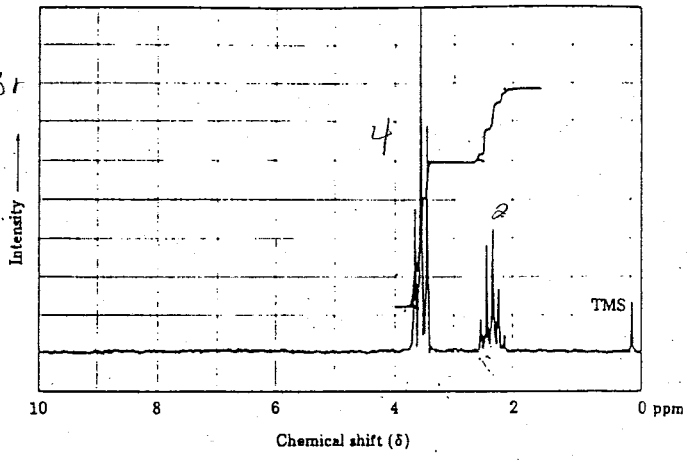
C
3H
S

$C_7H_{16}S$
C_7H_8S

$\frac{H8}{2} = 4$

13.39 How could you use IR spectroscopy to help you distinguish between the two compounds shown in Problem 13.38?

13.40 The compound whose ^1H NMR spectrum is shown here has the molecular formula $C_3H_6Br_2$. Propose a plausible structure.

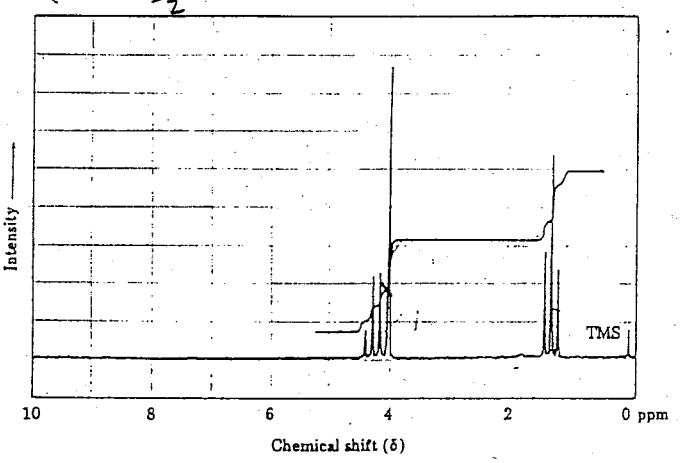


13.41 Propose structures for compounds that fit the following ^1H NMR data:

(a) $C_5H_{10}O$
- 6 H doublet at 0.95 δ, J = 7 Hz
- 3 H singlet at 2.10 δ
- 1 H multiplet at 2.43 δ

(b) C_3H_5Br
- 3 H singlet at 2.32 δ
- 1 H broad singlet at 5.35 δ
- 1 H broad singlet at 5.54 δ

13.42 The compound whose ^1H NMR spectrum is shown has the molecular formula $C_4H_7O_2Cl$ and shows an infrared absorption peak at 1740 cm^{-1}. Propose a plausible structure.



13.43 Propose structures for compounds that fit the following ^1H NMR data:

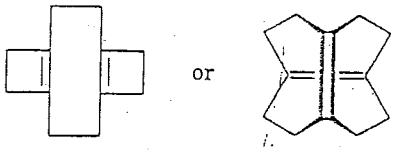
(a) $C_4H_6Cl_2$
- 3 H singlet at 2.18 δ
- 2 H doublet at 4.16 δ, J = 7 Hz
- 1 H triplet at 5.71 δ, J = 7 Hz

(b) $C_{10}H_{14}$
- 9 H singlet at 1.30 δ
- 5 H singlet at 7.30 δ

(c) C_4H_7BrO
3 H singlet at 2.11 δ
2 H triplet at 3.52 δ, J = 6 Hz
2 H triplet at 4.40 δ, J = 6 Hz

(d) $C_9H_{11}Br$
2 H quintet at 2.15 δ, J = 7 Hz
2 H triplet at 2.75 δ, J = 7 Hz
2 H triplet at 3.38 δ, J = 7 Hz
5 H singlet at 7.22 δ

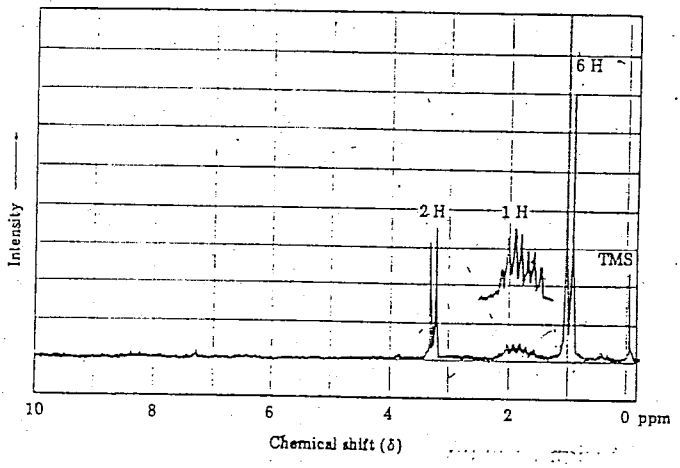
13.44 How might you use NMR (either ^1H or ^{13}C) to differentiate between the following two isomeric structures?



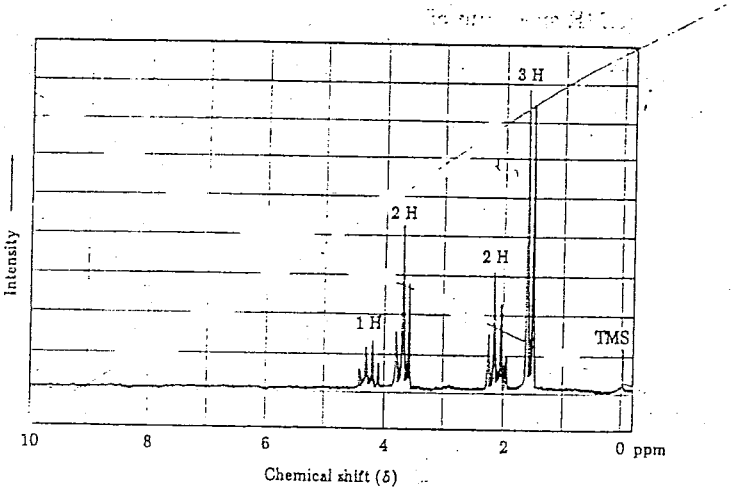
(You might want to build molecular models to help you examine the two structures more closely.)

13.45 Propose plausible structures for the two compounds whose ^1H NMR spectra are shown.

(a) C_4H_9Br

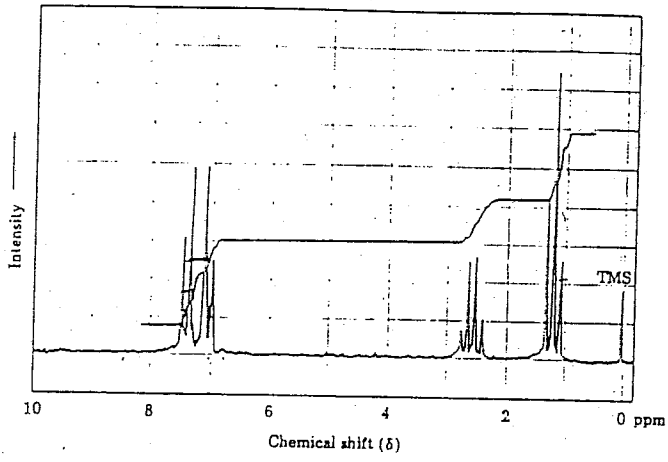


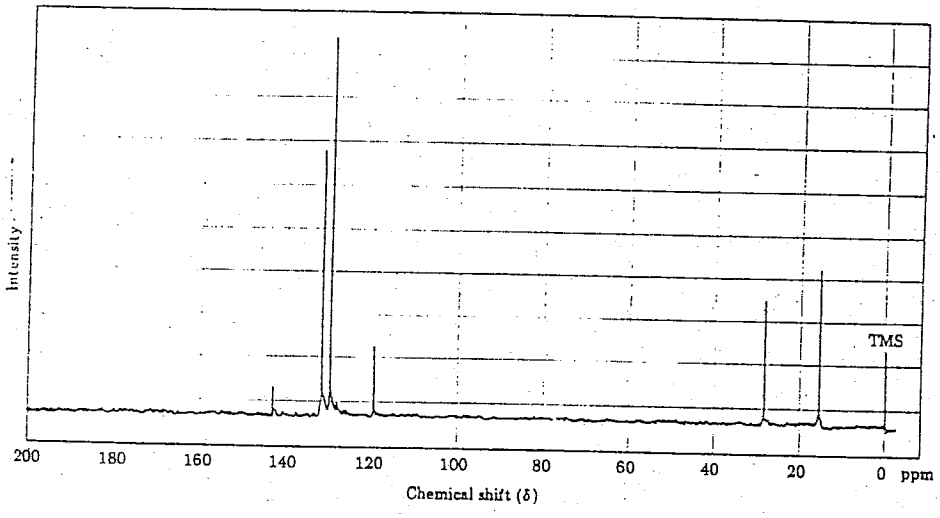
(b) $C_4H_8Cl_2$



13.46 We saw earlier that long-range coupling between protons more than two carbon atoms apart is sometimes observed when pi bonds intervene. One example of long-

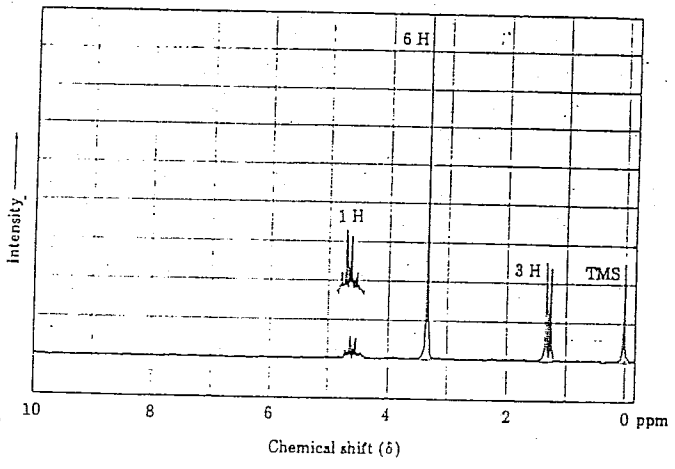
13.48 The ^1H and ^{13}C NMR spectra of compound A, C_8H_9Br, are shown. Propose a possible structure for A, and assign peaks in the spectra to your structure.



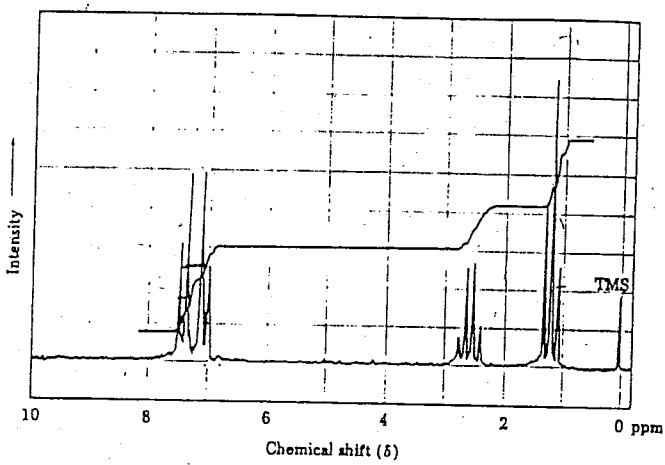


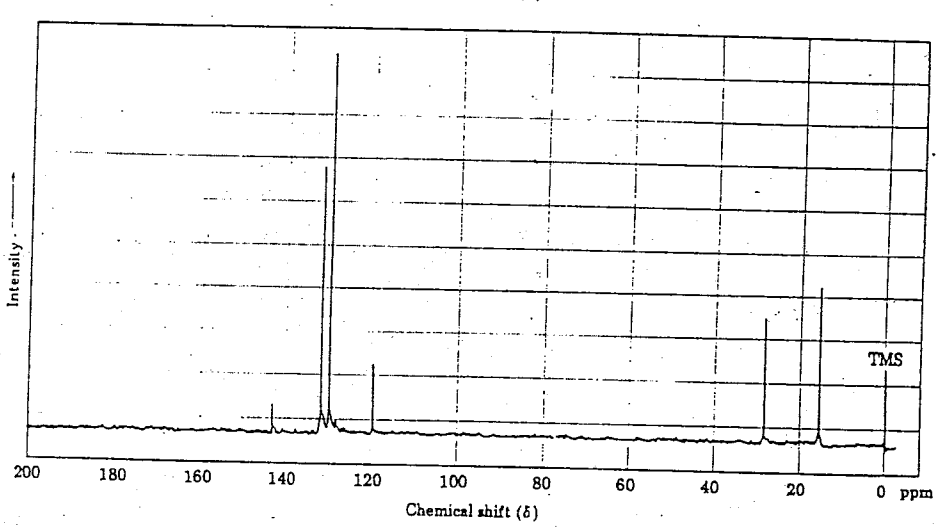
13.49 Propose plausible structures for the three compounds whose ^1H NMR spectra are shown.

(a) $C_4H_{10}O_2$



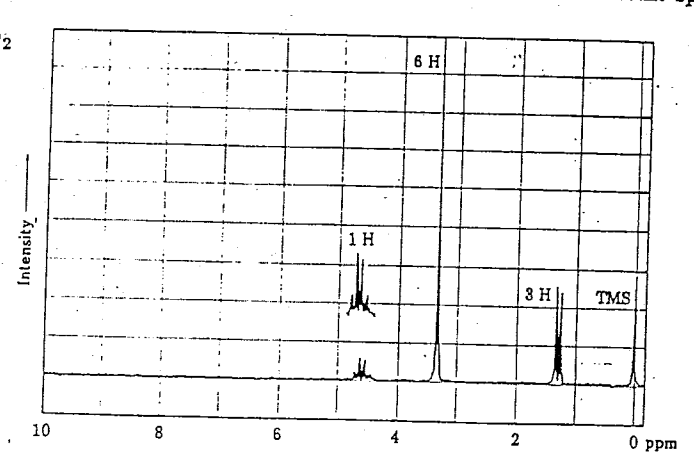
13.48 The ^1H and ^{13}C NMR spectra of compound A, C_8H_9Br, are shown. Propose a possible structure for A, and assign peaks in the spectra to your structure.





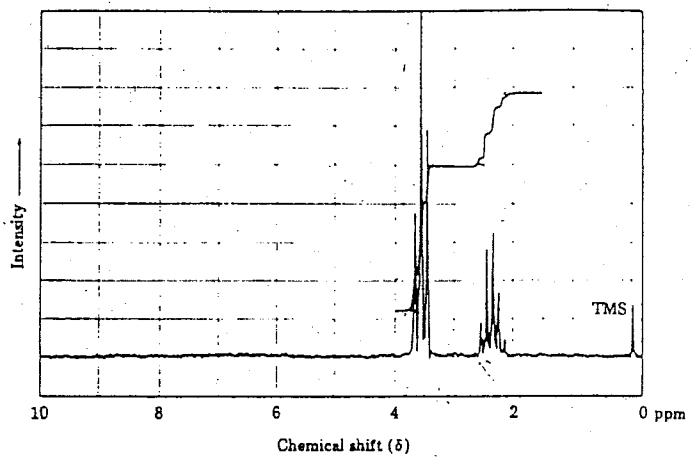
13.49 Propose plausible structures for the three compounds whose ^1H NMR spectra are shown.

(a) $C_4H_{10}O_2$



13.39 How could you use IR spectroscopy to help you distinguish between the two compounds shown in Problem 13.38?

13.40 The compound whose ^1H NMR spectrum is shown here has the molecular formula $C_3H_6Br_2$. Propose a plausible structure.

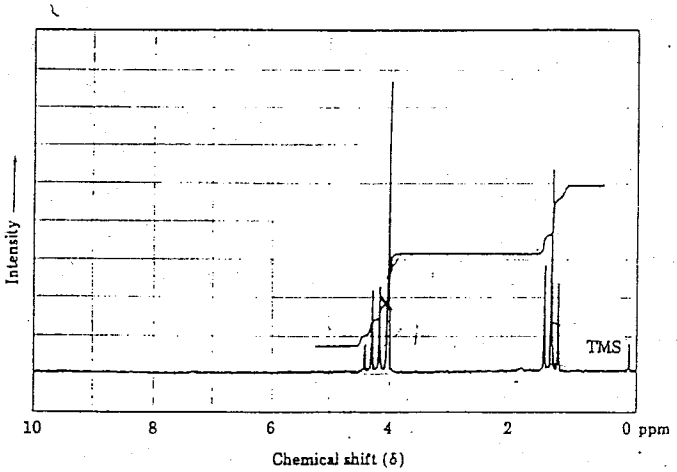


13.41 Propose structures for compounds that fit the following ^1H NMR data:

(a) $C_6H_{10}O$
6 H doublet at 0.95 δ, J = 7 Hz
3 H singlet at 2.10 δ
1 H multiplet at 2.43 δ

(b) C_3H_5Br
3 H singlet at 2.32 δ
1 H broad singlet at 5.35 δ
1 H broad singlet at 5.54 δ

13.42 The compound whose ^1H NMR spectrum is shown has the molecular formula $C_4H_7O_2Cl$ and shows an infrared absorption peak at 1740 cm^{-1}. Propose a plausible structure.



13.43 Propose structures for compounds that fit the following ^1H NMR data:

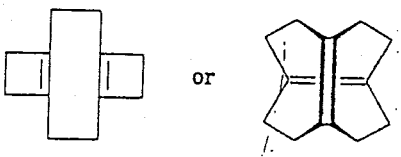
(a) $C_4H_6Cl_2$
3 H singlet at 2.18 δ
2 H doublet at 4.16 δ, J = 7 Hz
1 H triplet at 5.71 δ, J = 7 Hz

(b) $C_{10}H_{14}$
9 H singlet at 1.30 δ
5 H singlet at 7.30 δ

(c) C_4H_7BrO
3 H singlet at 2.11 δ
2 H triplet at 3.52 δ, J = 6 Hz
2 H triplet at 4.40 δ, J = 6 Hz

(d) $C_9H_{11}Br$
2 H quintet at 2.15 δ, J = 7 Hz
2 H triplet at 2.75 δ, J = 7 Hz
2 H triplet at 3.38 δ, J = 7 Hz
5 H singlet at 7.22 δ

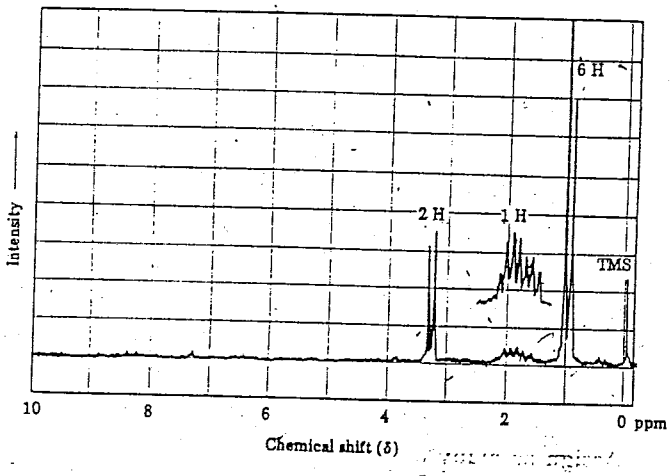
13.44 How might you use NMR (either ^1H or ^{13}C) to differentiate between the following two isomeric structures?



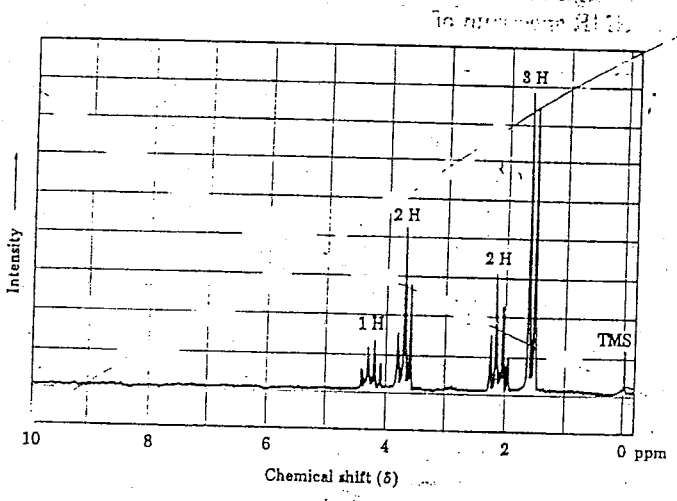
(You might want to build molecular models to help you examine the two structures more closely.)

13.45 Propose plausible structures for the two compounds whose ^1H NMR spectra are shown.

(a) C_4H_9Br



(b) $C_4H_8Cl_2$



46 We saw earlier that long-range coupling between protons more than two carbon atoms apart is sometimes observed when pi bonds intervene. One example of long-