ORGANIC CHEMISTRY **CH 385, Winter 2010**

Structure Determination Workshop

1. Compounds **A** and **B** have the formula $C_5H_{11}Cl$. Neither **A** nor **B** react with NaI in acetone or with $NaSCH_3$ in dimethylsulfoxide with any appreciable rate. **B** also does not react with $NaOCH_2CH_3$ in dimethylsulfoxide at an appreciable rate. In contrast, **A** reacts with $NaOCH_2CH_3$ in dimethylsulfoxide to give compounds **C** and **D**, which both have formula C_5H_{10} and IR bands between 1650-1660 cm^{-1}. The ^1H NMR spectra of **A** and **C** are tabulated below.

   Propose structures for **A–D** that are consistent with the experimental observations. Assign each of the ^1H NMR resonances to sets of equivalent protons in **A** and **C**.

^1H NMR (**A**)

δ (ppm)	Area	Multiplicity
1.01	3H	triplet
1.51	6H	singlet
1.73	2H	quartet

^1H NMR (**C**)

δ(ppm)	Area	Multiplicity
1.57	3H	doublet
1.60	3H	singlet
1.68	3H	singlet
5.17	1H	quartet

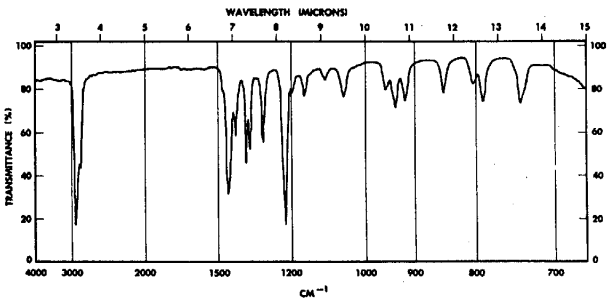
2a. Compound **E**, C_5H_9N, exhibits strong absorption in the infrared spectrum at 2252 cm^{-1} and gives the following ^{13}C NMR spectrum: 13.2 (q), 16.8 (t), 21.8 (t), 27.4 (t), 119.8 (s).

2b. Compound **F**, $C_9H_{16}O_4$, exhibits strong absorption in the infrared spectrum at 1735 cm^{-1} and gives the following ^1H NMR spectrum: 0.80 (t, J = 7.1 Hz, rel. area 3), 1.93 (q, J = 7.1 Hz, rel. area 2), 3.71 (s, rel. area 3).

3. An optically active compound **G**, C_6H_{10}, was hydrogenated over a platinum catalyst to give an optically inactive hydrocarbon, C_6H_{12}, which was identical to methylcyclopentane. Give the structure of the optically active C_6H_{10} compound and explain why this structure is uniquely consistent with the data.

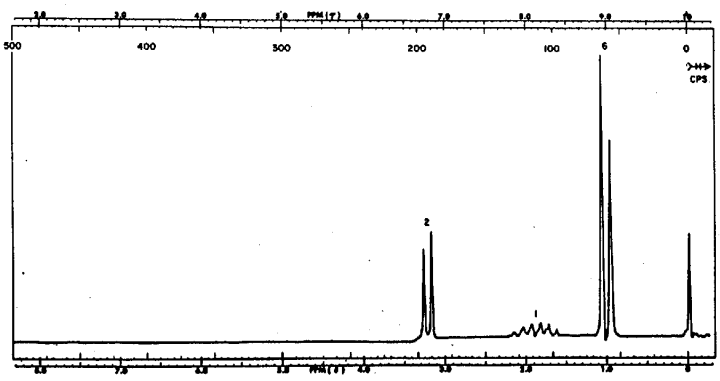
4. Deduce structures for the unknown compounds based on the spectroscopic data provided below.

a)



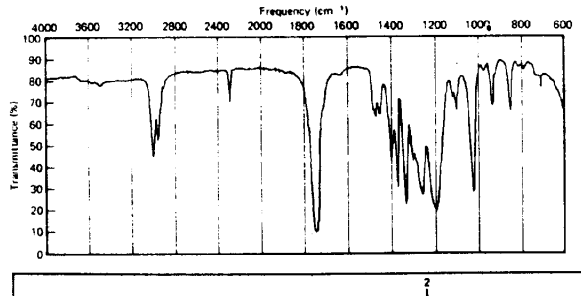
IR Spectrum

C_4H_9Br



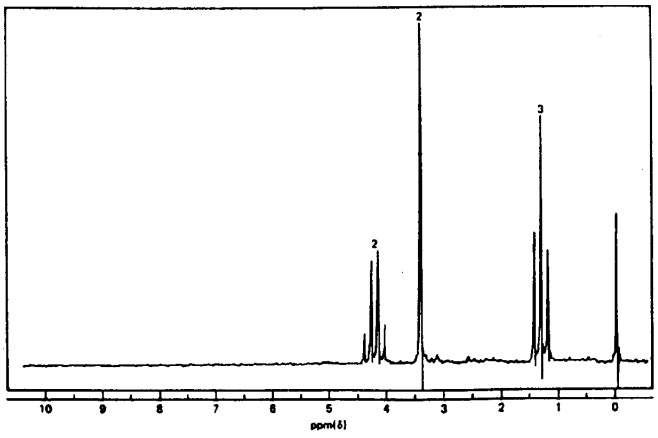
NMR Spectrum

b)



IR Spectrum

$C_5H_7NO_2$



NMR Spectrum