

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 $1650-1660\text{ cm}^{-1}$. The 1H NMR spectra of **A** and **C** are tabulated below.

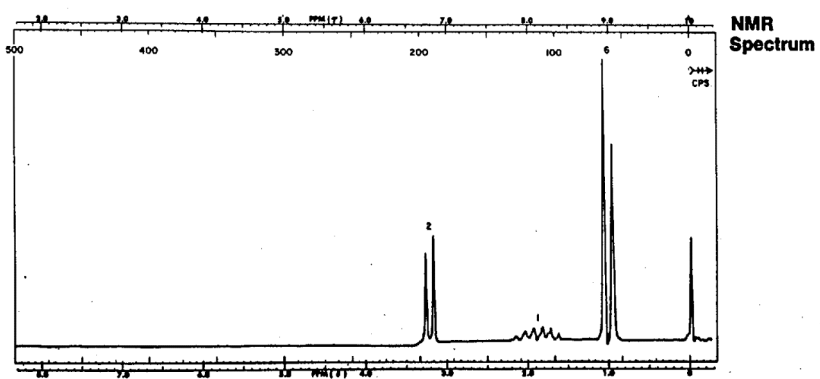
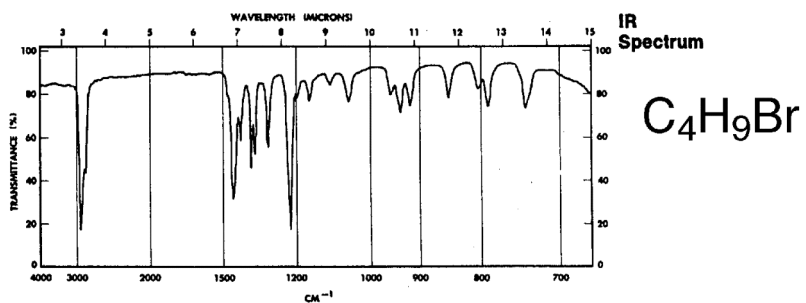
Propose structures for **A–D** that are consistent with the experimental observations. Assign each of the 1H NMR resonances to sets of equivalent protons in **A** and **C**.

1H NMR (A)			1H NMR (C)		
δ (ppm)	Area	Multiplicity	δ (ppm)	Area	Multiplicity
1.01	3H	triplet	1.57	3H	doublet
1.51	6H	singlet	1.60	3H	singlet
1.73	2H	quartet	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, $J = 7.1\text{ Hz}$, rel. area 3), 1.93 (q, $J = 7.1\text{ Hz}$, 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)



b)

