ORGANIC CHEMISTRY

CH 385, Winter 2012

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 NaSCH₃ in dimethylsulfoxide with any appreciable rate. **B** also does not react with NaOCH₂CH₃ in dimethylsulfoxide at an appreciable rate. In contrast, **A** reacts with NaOCH₂CH₃ 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.

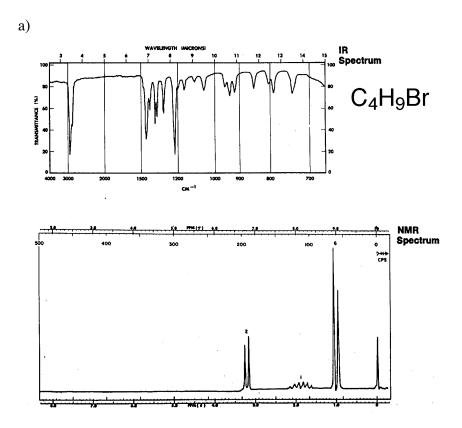
^{1}H NMR (A)

¹H NMR (\mathbf{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, C₅H₉N, exhibits strong absorption in the infrared spectrum at 2252 cm⁻¹ and gives the following ¹³C NMR spectrum: 13.2 (q), 16.8 (t), 21.8 (t), 27.4 (t), 119.8 (s).
- 2b. Compound **F**, C₉H₁₆O₄, 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.



b)

