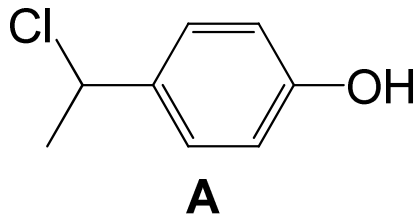
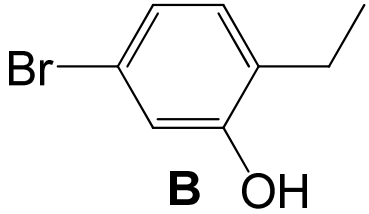
CHEM 266 - Homework 1 **Name_____Keys_____**

(Due on Thursday, September 14, 2017 at the beginning of the class, no late return, no exam under my office's door will be accepted)

1. Can IR be used to distinguish between the following compounds? Explain your answer (2 pts)

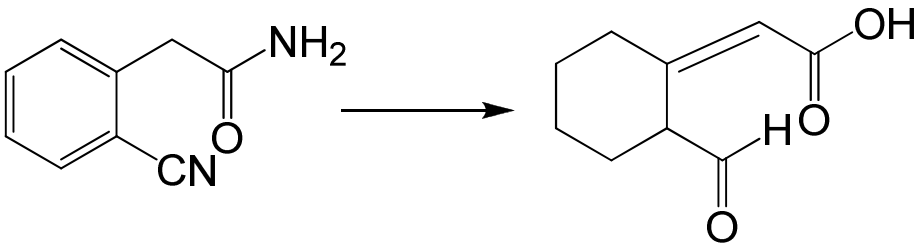


A



B

2. You have performed the reaction below in the lab. List all the signals observed in the IR spectrum of the starting material and in the IR spectrum of the product. Explain how IR can be used to tell whether the reaction took place or not.



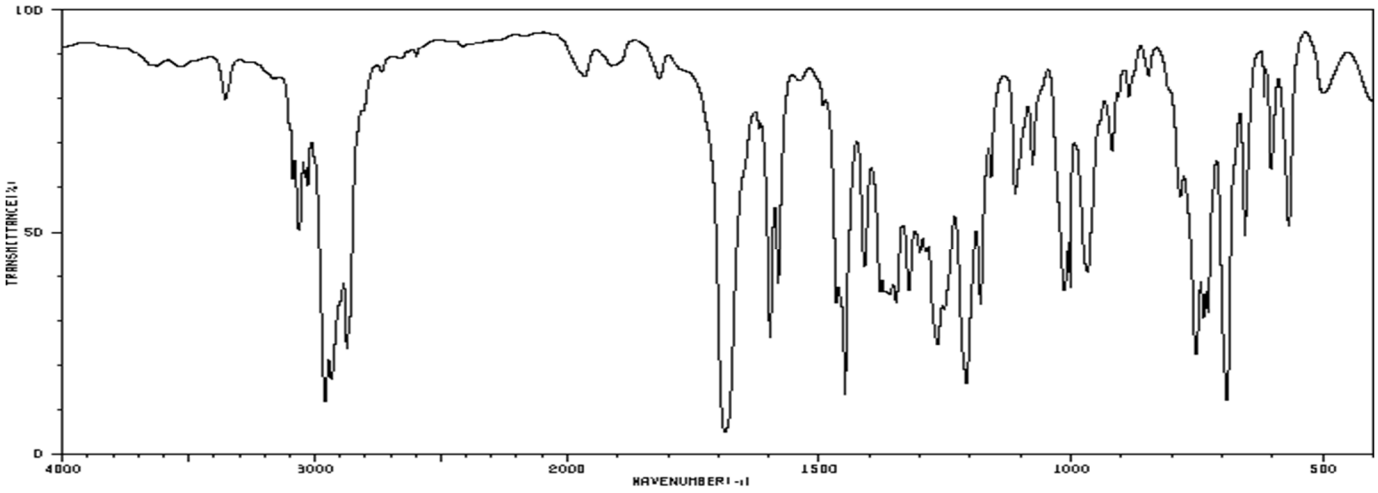
IR vibrational signals (5 pts)

Starting material

Product

Explain (2 pts)

3. The compound with the IR spectrum below has a molecular formula of $C_{11}H_{14}O$. Propose **two** structures consistent with the IR spectrum and explain your answer

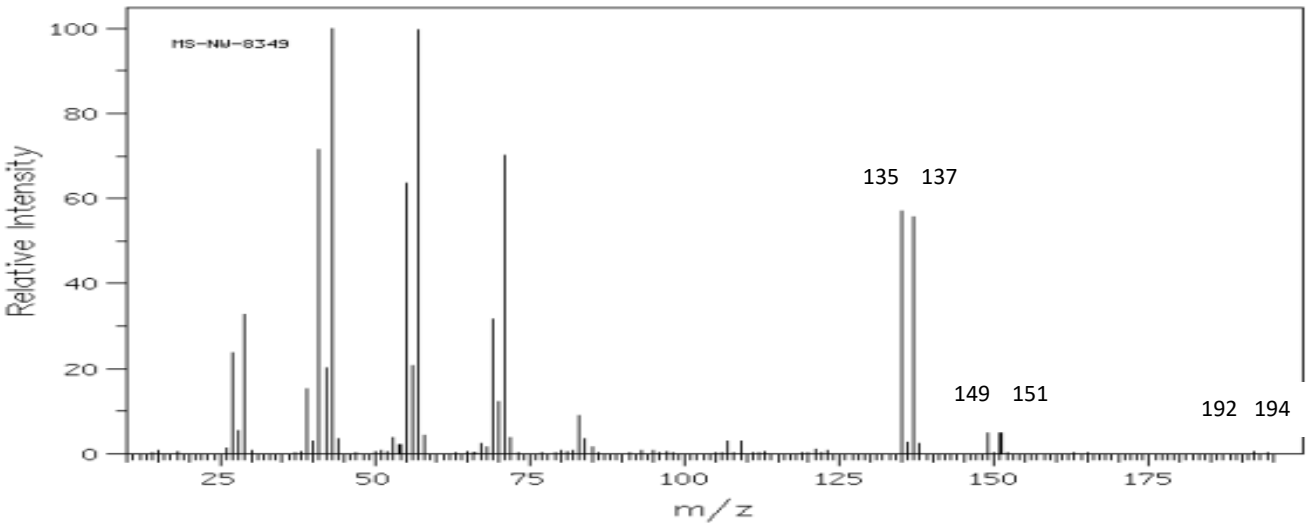


Structures (4 pts) – **Any two of the structures below will do.**

Explain (2 pts)

4. Both C_6H_9N and C_5H_5NO have the same nominal mass, namely 95. Show how these compounds can be distinguished by the *m/z* ratio of their molecular ions in high-resolution mass spectrometry (C 12.0107; O 15.9994; H 1. 00794; N 14.0067) (3 pts)

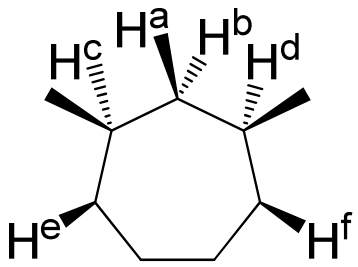
5. Propose **three (03)** possible structures that can produce the mass spectrum given below and explain your answer (**beside carbon and hydrogen, this molecule contains only one other atom**)



Structures (3 pts)

Explain (3 pts)

6. State the relationship between the protons indicated in the structure below (as: equivalent, enantiotopic, diastereotopic, or unrelated). (1 x 5 = 5 pts)



H^a and H^b are_____ _____

H^b and H^c are _____ _____

H^c and H^d are _____ _____

H^c and H^f are_____ _____

H^f and H^e are _____ _____

7. Two compounds A and B with the same molecular formula ($C_6H_{12}O_2$) have the ^{1}H-NMR data shown below. Both compounds have strong band around 2950 and 1710 cm^{-1} in their IR spectrum. Elucidate the structure of these two compounds and explain your answer.

Compound A: ^{1}H NMR (δ): 1.14 (6H, doublet), 1.29 (3H, triplet), 2.67 (1H, multiplet), 4.13 (2H, quartet)

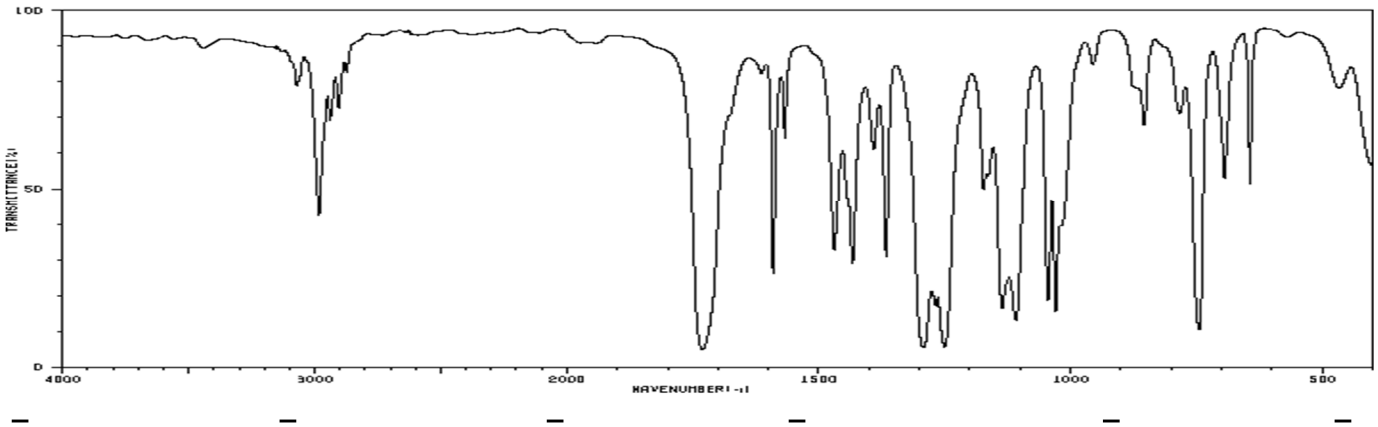
Compound B: ^{1}H NMR (δ): 0.91 (6H, doublet), 2.21 (2H, doublet), 2.39 (1H, multiplet), 3.68 (3H, singlet)

Structures (4 pts)

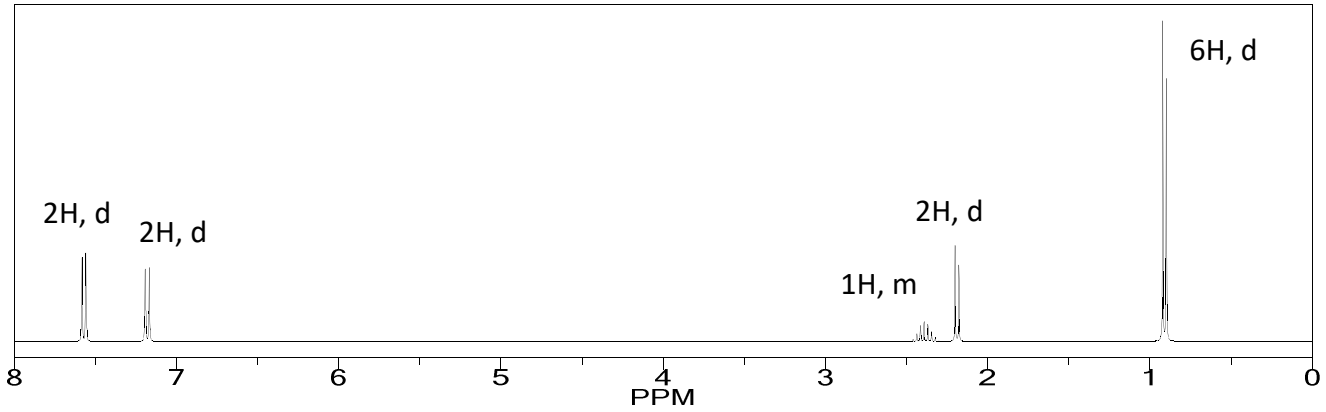
Compound A **Compound B**

Explain (2 pts)

8. (a) Identify the major signals and the corresponding bond types present in the compound having the following IR spectrum; Molecular formula **$C_{11}H_{13}BrO_2$** (3 pts)



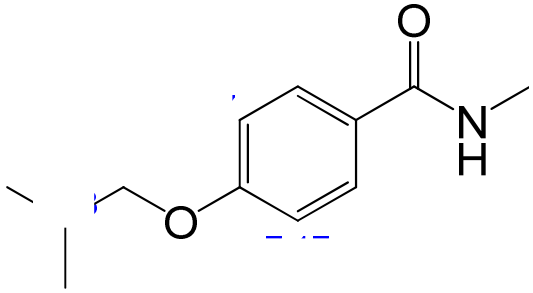
(b) The ^{1}H-NMR shown below is that of the same compound with the IR spectrum shown in (a). Determine its structure and explain your answer.



Structure (3 pts)

Explain (2 pts)

9. Predict the number of signals expected, their chemical shifts, their multiplicity, and the number of protons under each signal in the ^{1}H NMR spectrum of the following compound (3 pts)



10. The mass spectrum below is that of benzyl 3-methylbutanoate (see structure below). Provide a structure for the fragments at m/z 192, 150, 107, 101, 91, 85, 57 and 41 (**You must show the fragmentation pattern**) (0. 5 x 8 = 4 pts)