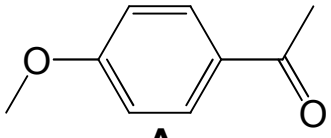
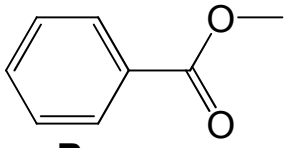
CHEM 266 - Homework 1 **Name**_____

(Due on Tuesday, September 12, 2016 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)

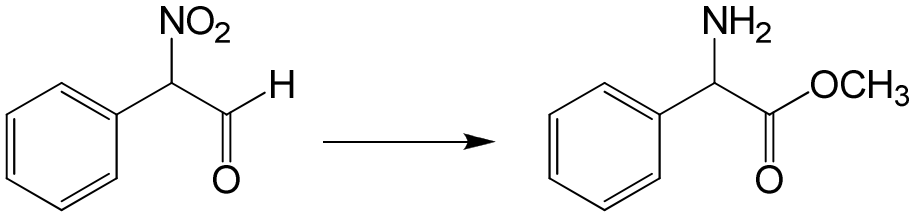


A



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.

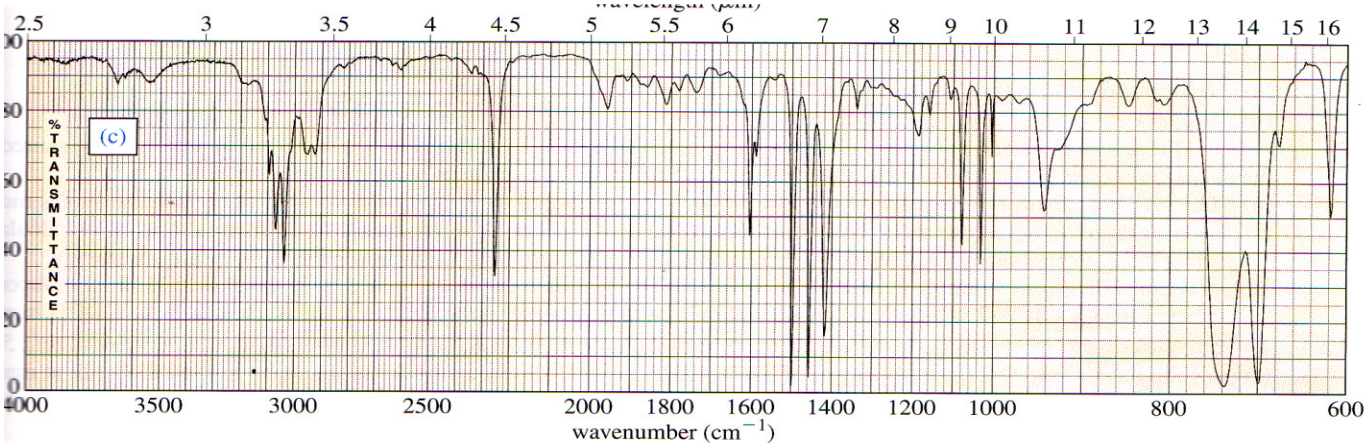


IR vibrational signals (5 pts)

Starting material **Products**

Explain (2 pts)

3. The compound with the IR spectrum below has a molecular formula of **$C_{12}H_{14}$**. Propose **two** structures consistent with the IR spectrum and explain your answer.

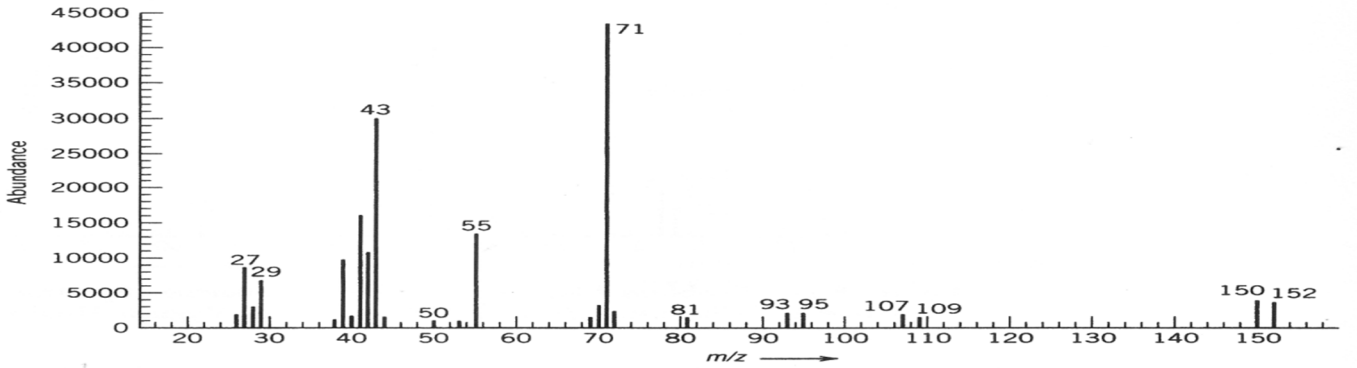


Structures (4 pts)

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)

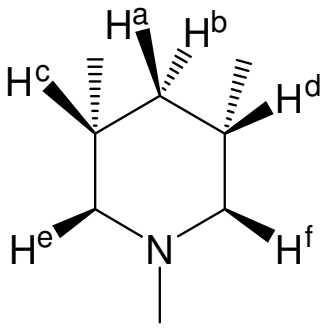
5. Propose **three (03)** possible structures that can produce the mass spectrum given below and explain your answer (**beside carbon and hydrogen, this molecule contains only one other atom**)



Structures (4.5 pts)

Explain (1.5 pts)

6. State the relationship between the labeled protons 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 ($C_7H_{14}O_2$) have the ^{1}H-NMR data shown below. Both compounds have strong band around 2950, 1750 and 1075 cm^{-1} in their IR spectrum. Elucidate the structure of these two compounds and explain your answer.

Compound A: ^{1}H NMR (δ): 0.90 (3H, triplet), 1.19 (3H, doublet), 1.29 (3H, triplet), 1.79 (2H, quintet), 2.49 (1H, multiplet), 4.21 (2H, quartet).

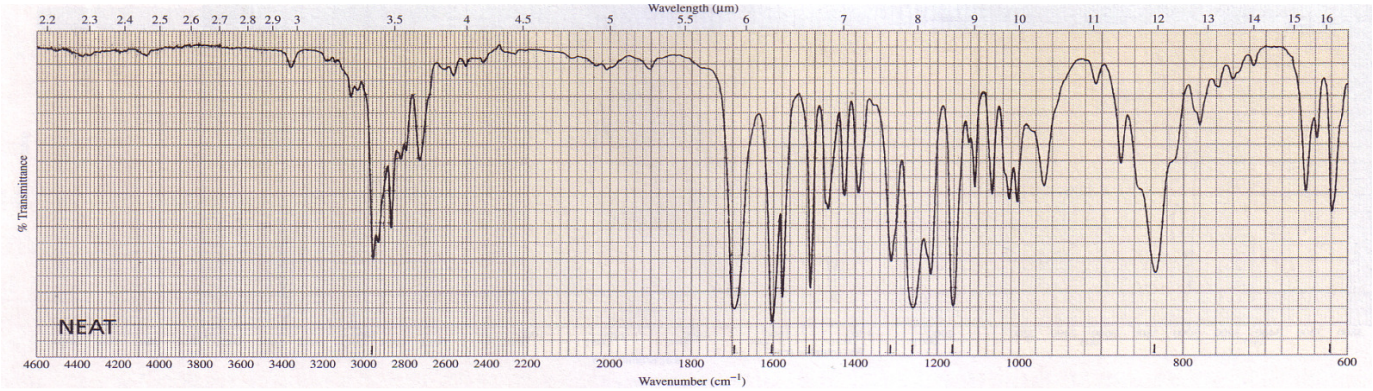
Compound B: ^{1}H NMR (δ): 0.90 (3H, triplet), 1.32 (6H, doublet), 1.79 (2H, multiplet), 2.32 (2H, triplet), 4.93 (1H, multiplet).

Structures (4 pts)

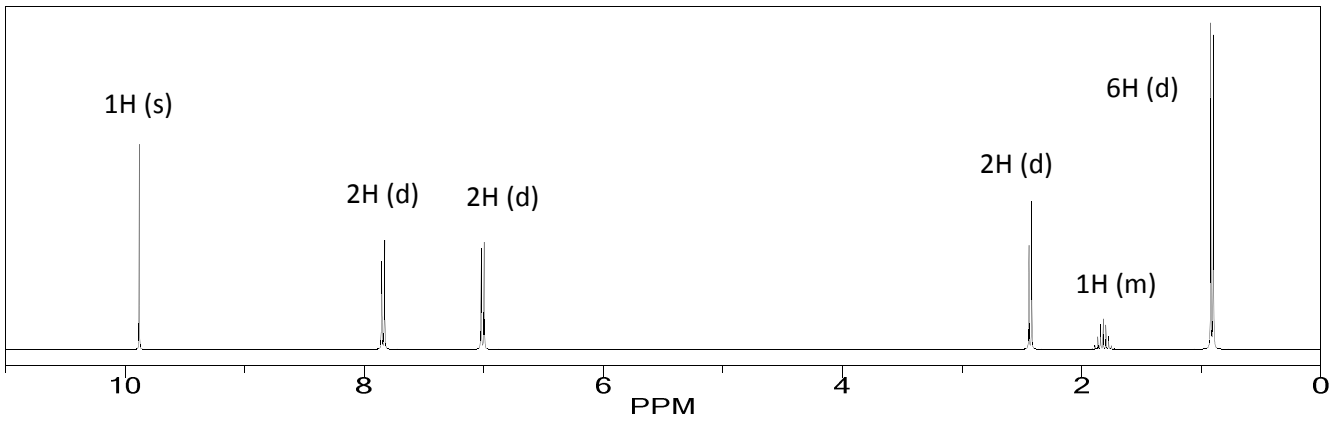
Compound A **Compound B**

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 **$C_{11}H_{14}O$** (3 pts)



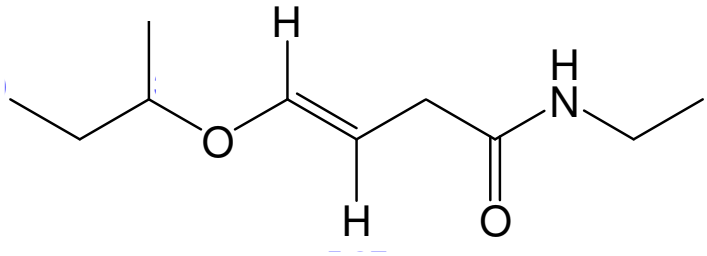
(b) The ^{1}H-NMR shown below is that of the same compound with the IR spectrum shown in (a). Determine its structure and explain your answer.



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 1-phenylhexan-2-one (see structure below). Provide a structure for each of the fragments corresponding to the peaks indicated by the *m/z* 176, 134, 119, 91, 85, 57, 41 and 29 (you must show the fragmentation pattern to receive full credit) (4 pts)