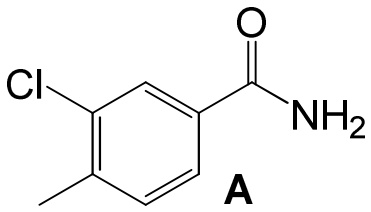
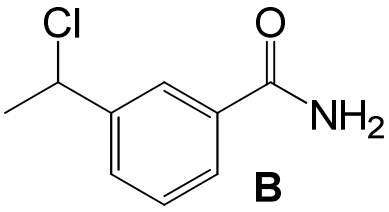
CHEM 266 - Homework 1 **Name**_____

(Due on Wednesday, February 21, 2018 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)



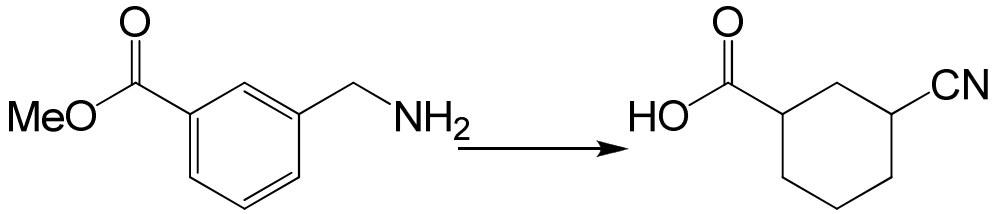
A



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

_____
_____
_____
_____
_____
_____
_____
_____
_____

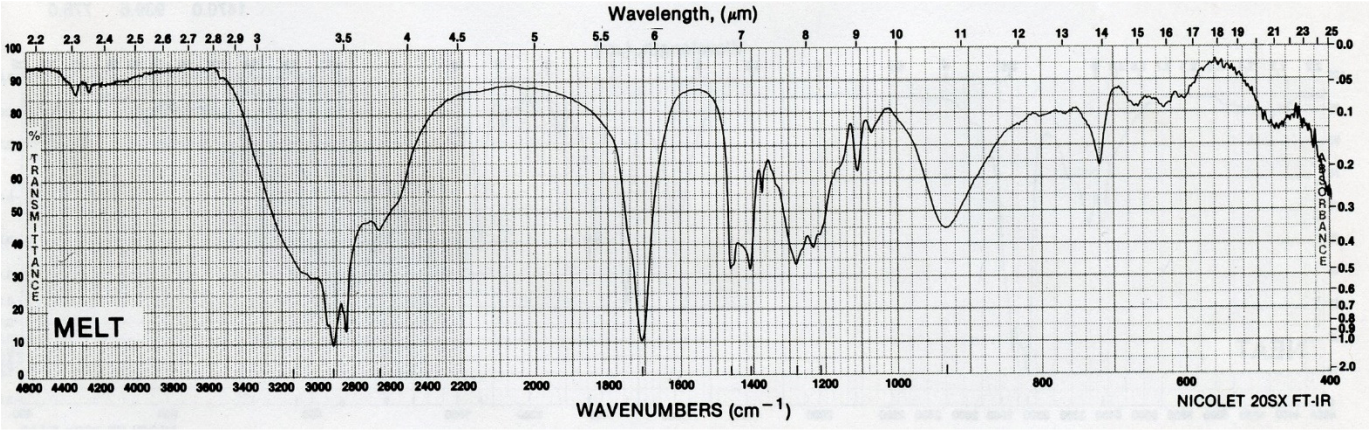
Product

_____
_____
_____
_____
_____
_____
_____
_____
_____

Explain (2 pts)

_____
_____
_____
_____
_____
_____
_____

3. The compound with the IR spectrum below has a molecular formula of **$C_5H_{10}O_2$**. Propose **two** structures consistent with the IR spectrum and explain your answer.



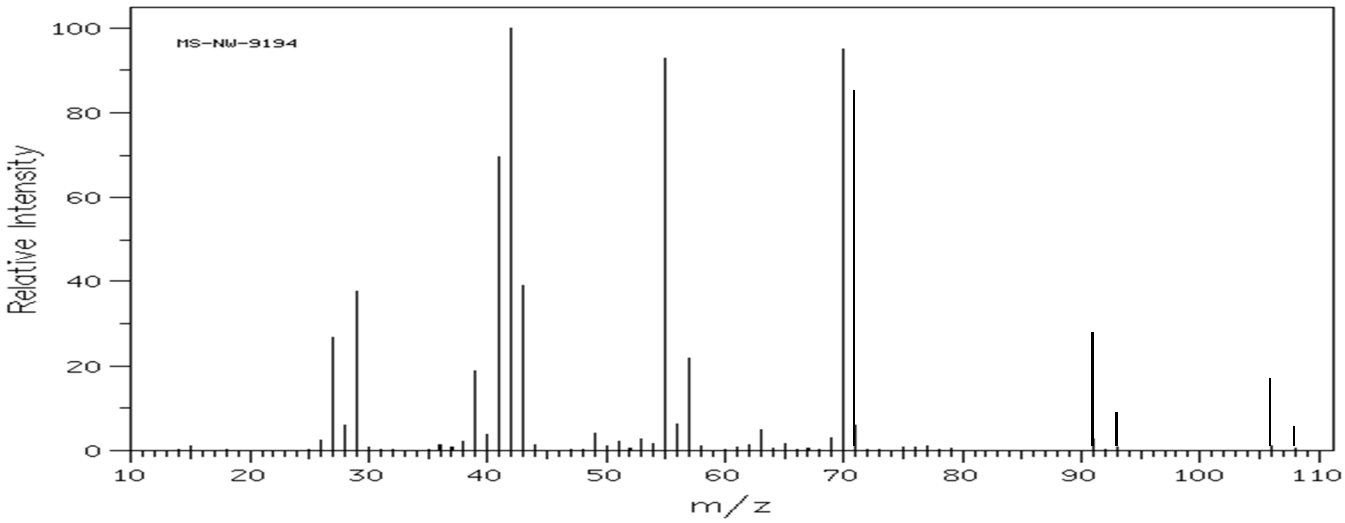
Structures (4 pts)

Explain (2 pts)

_____
_____
_____
_____
_____
_____
_____
_____

4. Both **$C_6H_{13}NO_2$** and **$C_5H_9NO_3$** have the same nominal mass of 131. 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 kind of atom**)

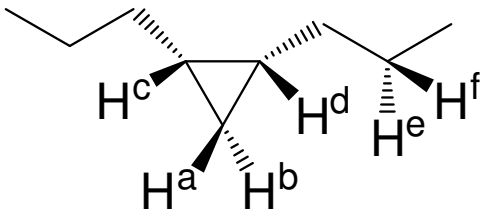


Structures (3 pts)

Explain (3 pts)

_____
_____
_____
_____
_____
_____

6. State the relationship between the **protons labelled** in the structure below (as: homotopic, 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^d and H^e are_____

H^f and H^e are _____

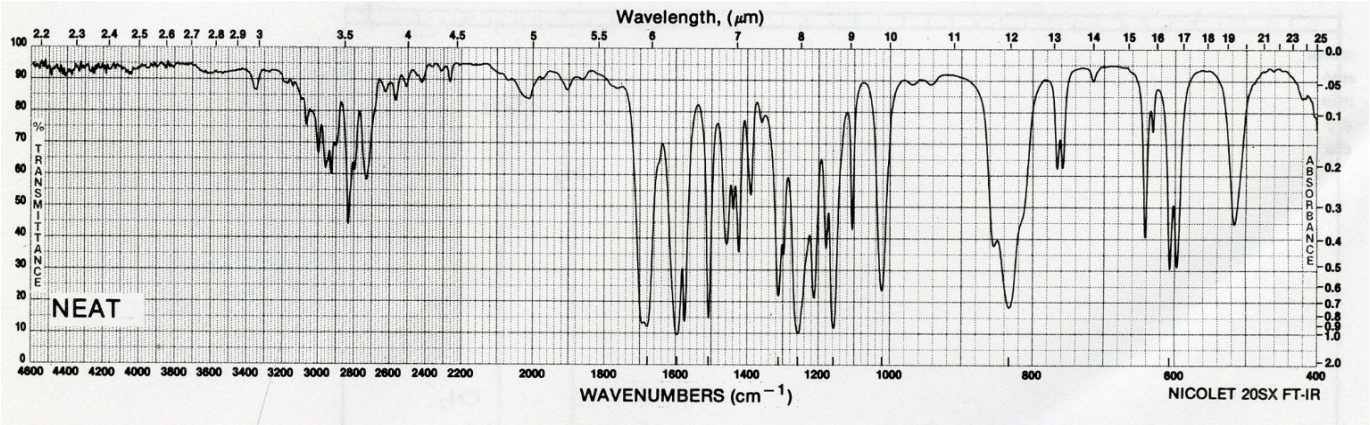
7. A compound with a molecular formula **$C_8H_{17}NO$** has the ^{1}H-NMR data listed below. The compound displays characteristic bands around 3454, 2950 and 1685 cm^{-1} in its IR spectrum. Elucidate the structure of this compound and explain your answer.

^{1}H NMR (δ): 0.90 (3H, triplet), 1.00 (6H, doublet), 1.19 (3H, doublet), 1.68 (2H, quintet), 2.60 (1H, multiplet), 3.81 (1H, multiplet), 8.03 (1H, broad singlet).

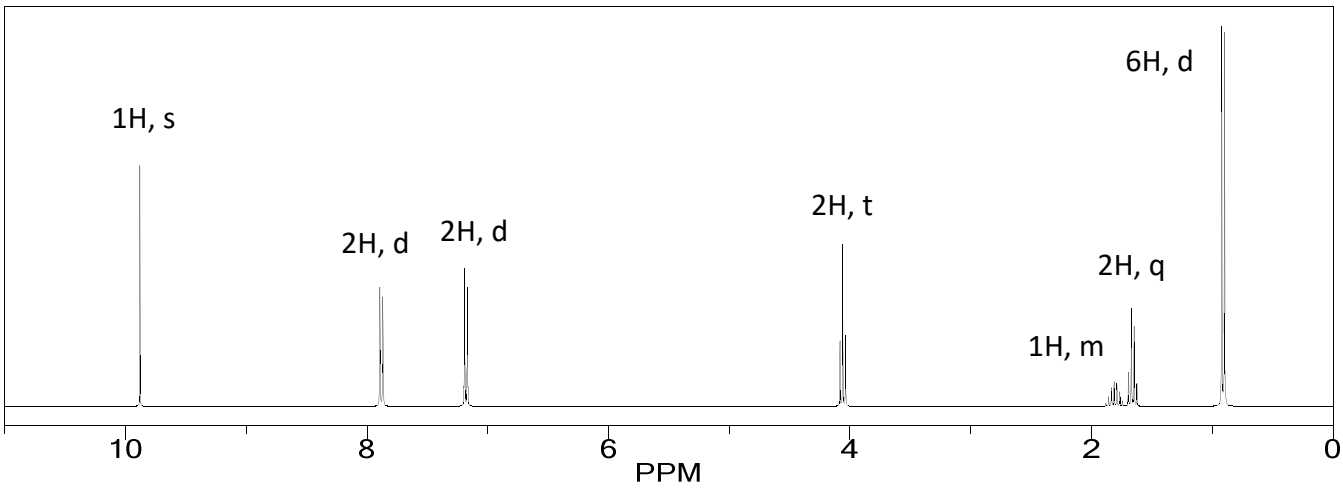
Structures (4 pts)

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 **$C_{12}H_{16}O_2$** (3 pts)



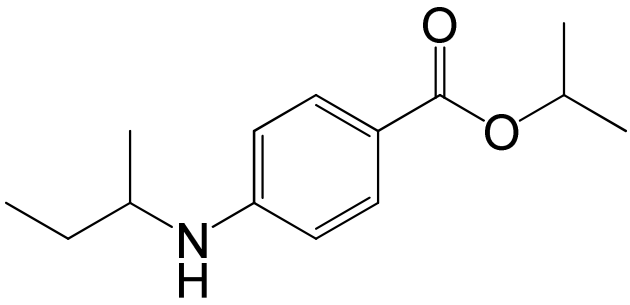
(b) The ^{1}H-NMR shown below is that of the same compound with the IR spectrum shown in (a). Determine its structure and explain your answer.



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 1-phenylhexan-2-one (see structure below). Provide a structure for the fragments at m/z 176, 134, 120, 91, 85, 57, 41 and29 (**You must show the fragmentation pattern**) (0. 5 x 8 = 4 pts)