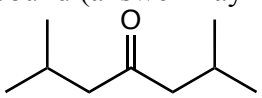
Organic Chemistry for Life Sciences: CHM 223 Section A

Problem Set Chapter 15/16

Name_____

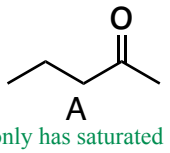
DUE: Wednesday Oct 18 @ 8am

1. Which answer contains stretches that are expected in the IR spectrum of the following compound (answer may not have ALL of the expected stretches)?

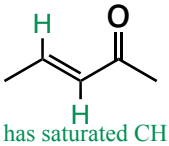


A. 1710, 1080 cm^{-1} C=O, C–O
B. 3520, 1705 cm^{-1} OH, C=O
C. 3010, 1730 cm^{-1} unsat CH, C=O
D. 2950, 1720 cm^{-1} sat CH, C=O

2. Which region in the IR spectrum could be used to differentiate the following two compounds?



A
• only has saturated CH @ ~ 2950



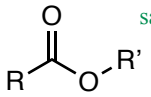
H
• has saturated CH @ 2950 AND unsaturated CH > 3000

A. 3010 cm^{-1} region would be present in A but not B
B. 2950 cm^{-1} region would be present in A but not B
C. 3010 cm^{-1} region would be present in B but not A
D. 2950 cm^{-1} region would be present in B but not A

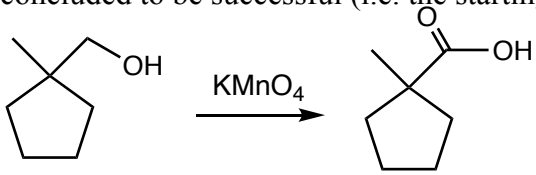
3. An IR spectrum contains stretches at 2950, 1720 and 1169 cm^{-1}. Most likely, what class (type) of organic compound is it?

sat CH C=O C–O

an ester



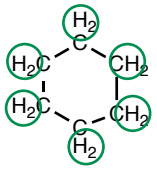
4. The following reaction is run. An IR spectrum is collected on the ***product.*** The reaction can be concluded to be successful (i.e. the starting material has been converted to product) if:



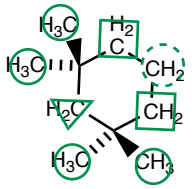
starting material **product**

A. There is an at 1220 cm^{-1} C–O present in both
B. There is an absorption at 2940 cm^{-1} sat CH present in both
C. There is an absorption at 1045 cm^{-1} C–O present in both
D. There is an absorption at 1702 cm^{-1} C=O only present in product!

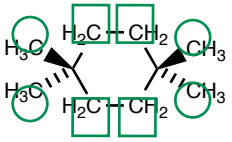
5. How many different chemical environments are present for the following molecules?



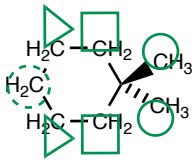
1 chemical environment



4 chemical environments



2 chemical environments

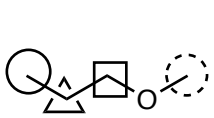


4 chemical environments

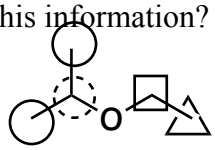
sat CH C–O

6. A molecule with molecular formula has important IR absorptions at 2960 and 1100 cm -1 only. From the NMR spectrum there are 3 chemical environments. Which one of the following is consistent with this information?

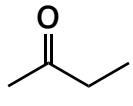
• data suggests an ether!



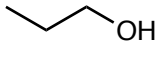
• an ether!
• 4 chemical environments
• NOT consistent



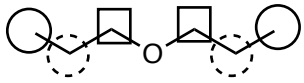
• an ether!
• 4 chemical environments
• NOT consistent



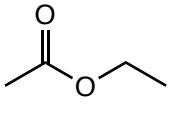
• a ketone!
• NOT consistent



• an alcohol!
• NOT consistent

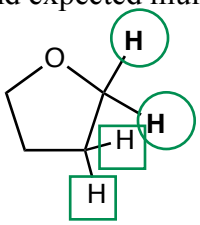


• an ether!
• 3 chemical environments
• **YES consistent**

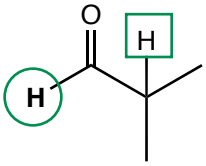


• an ester!
• NOT consistent

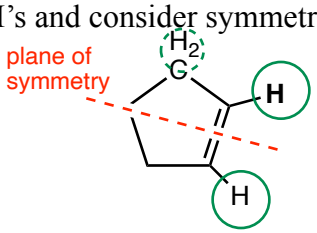
7. For the bold proton(s) located in each of the following molecules, provide the expected chemical shift range and expected multiplicity (HINT: draw in missing H's and consider symmetry where appropriate):



2.5-4.5 ppm
triplet



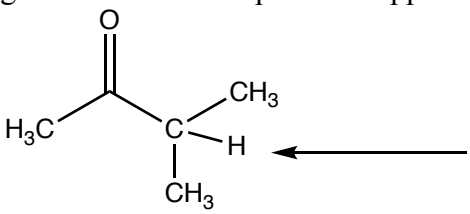
9–10 ppm
doublet



4.5–6.5 ppm
triplet

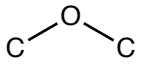
- will only couple to chemically inequivalent CH_2 protons

8. A ketone containing 5 carbons has a septet at 2.5 ppm. What is its structure?



will be a septet beween 1.5-2.5 ppm

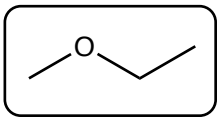
9. The IR of a compound shows it to be an ether. The mass spectrum shows an M+ peak = 60. What is the structure of the compound?



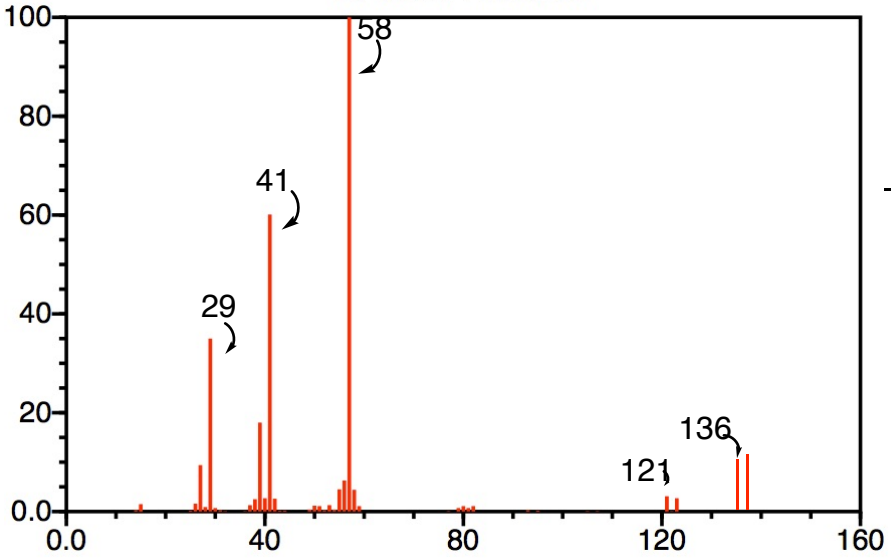
- generic ether structure
- 3 heavy atoms accounted for

 # heavy atoms:
60/14 ~ 4 heavy atoms

- need to add one additional carbon atom to the generic structure
- addition to either side is identical



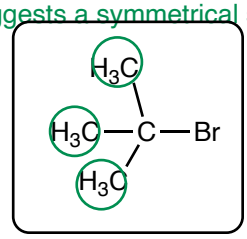
10. A compound is analyzed by 1H NMR and found to exhibit *only* a singlet at 1.2 ppm. The IR spectrum only shows saturated C-H stretches. The mass spectrum is provided below. What is the structure of the compound?



- IR suggests alkane or alkyl halide (RX)
- MS suggests the presence of a Br (so compound is likely an alkyl bromide (RBr)

$\frac{136-79}{14}$ ~ 4 carbons + Br

- the fact that a 4 carbon alkyl halide has all of the hydrogens in a single enviroment suggests a symmetrical structure



- predict singlet at 0–1.5 ppm consistent with data provided

double check MW:
4C x 12 = 48
9H x 1 = 9
1Br x 79 = 79

MW = 136 which is equivalent to M+ peak in MS