

Worksheet #3: September 10, 2021. Complete the following worksheet by collaborating with a group of 3-4 students. You can use a text book or your lecture video notes. You must work together, with the names of all students included on **ONE** sheet and turned in for a group grade.

$$HD = (2n+2) - 12$$

$$= 16 - 12$$

$$HD = 4$$

(1) **Structure Identification and IR.** An unknown organic compound has a formula of C_7H_{12} .

(a) Calculate the Hydrogen Deficiency for this unknown: 4

(b) Based on the HD and Formula, what type(s) of functional groups might be present? CIRCLE all possibilities from the list below:

alkene
(C=C double bond)

carbonyl
(C=O double bond)

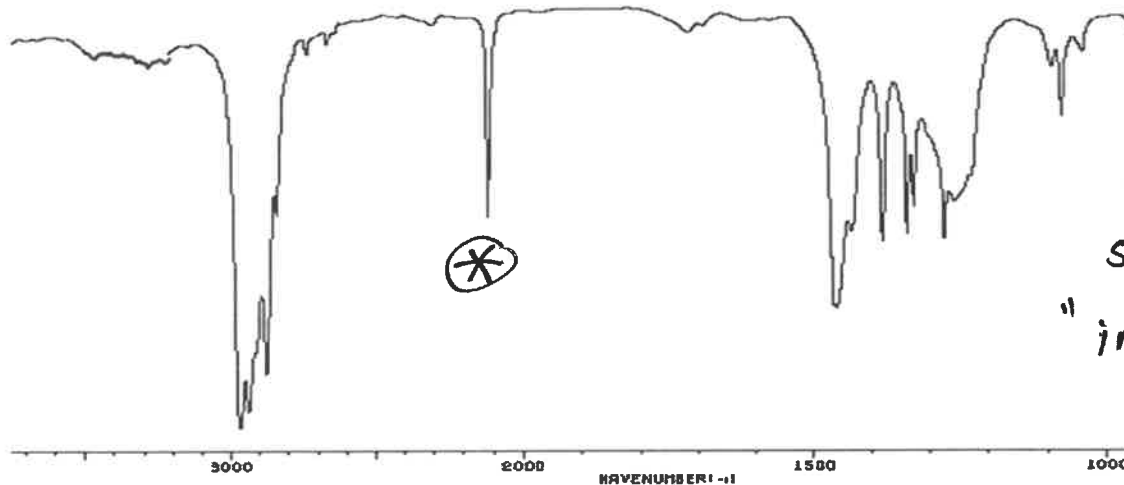
alkyne
(C≡C triple bond)

alcohol
(R-OH)

ether
(R-O-R)

cycloalkyl
(C atoms form a ring)

(c) The IR spectrum for this unknown is given below. What does the IR spectrum suggest about this unknown?



Answer:

The sharp band at ~2100-2200 suggests an "internal" alkyne.



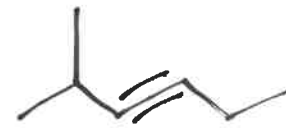
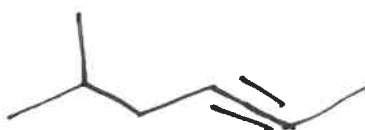
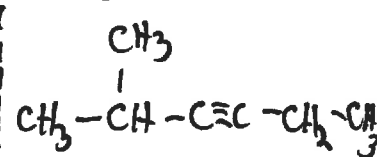
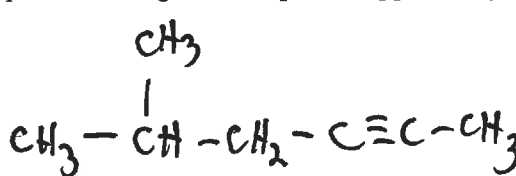
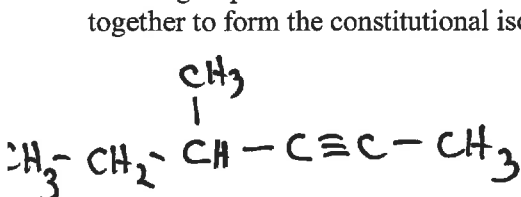
(d) In addition to all the data given in parts a, b and c above, the unknown also has:

three 1° carbons
-CH₃ -CH₃ -CH₃

one 2° carbon
-CH₂-

one 3° carbon -C- + -C≡C-

In the space below, draw three constitutional isomers for this unknown that are consistent with all the data given to you. HINT: Using all data, first make a list of the simplest C group for 1°, 2°, and 3° carbons. For example, the simplest 2° carbon group is a -CH₂-. Then take these "puzzle pieces", along with the piece suggested by the IR, and put them together to form the constitutional isomers.



(2) Practice Calculations. For the compound in problem #1 (C₇H₁₂):

(a) Determine the molecular mass of this molecule (4 significant figures):

96.17 g/mole

(b) If you had 0.03101 moles of this compound, how many grams would you have?

2.982 g

(c) You accidentally spilled this compound on the lab bench. You used a glass pipette to recover as much as possible. After re-weighing, you now have 2.233 g.

Calculate your % Recovery

74.88 %

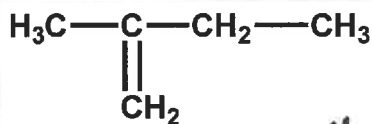
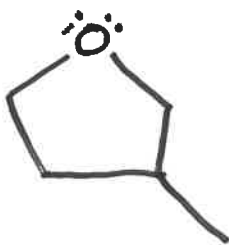
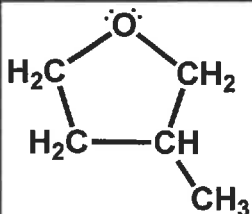
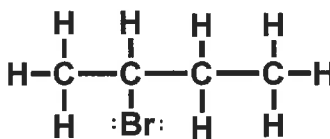
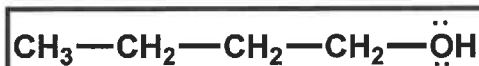
Show your work below and use correct significant figures and units:

$$\begin{array}{r} (a) \quad 7 \times 12.01 \text{ g/mole} \\ + \quad 12 \times 1.008 \text{ g/mole} \\ \hline = 96.17 \text{ g/mole} \end{array}$$

$$\begin{array}{r} (b) \\ 0.03101 \text{ mole} \times 96.17 \frac{\text{g}}{\text{mole}} \\ = 2.982 \text{ g} \end{array}$$

$$\begin{array}{r} (c) \\ \% \text{ Recovery} = \\ \frac{\text{Recovered}}{\text{Original}} \times 100 \\ = \frac{2.233 \text{ g}}{2.982 \text{ g}} \times 100 \\ = 74.88 \% \end{array}$$

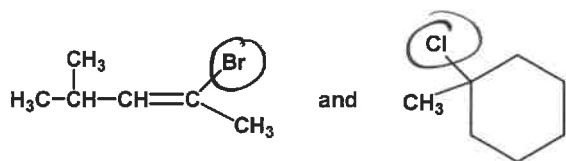
(3) "Zig-Zag" structures. Re-draw each of the following four compounds as "zig-zag" structures.



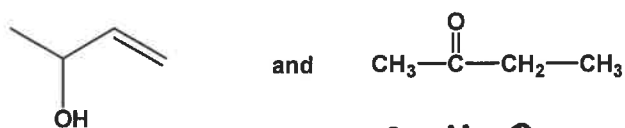
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(4) Comparing Organic Structures. Are the following pairs of compounds:

Identical or Different or Constitutional Isomers?



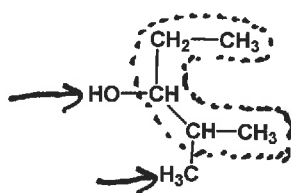
Different



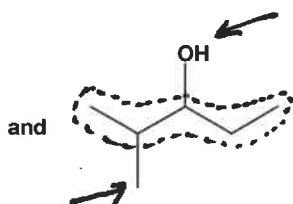
Constitutional

C_4H_8O

C_4H_8O



$C_6H_{14}O$



$C_6H_{14}O$

Identical