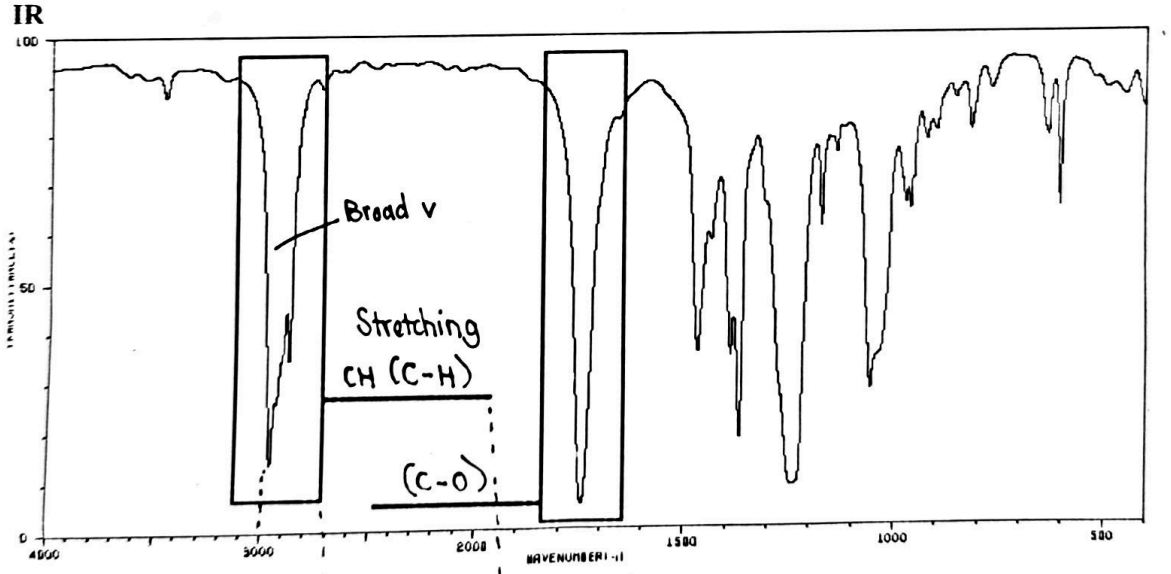
Your Name: LILY·R·OTIENO

Synthesis and Spectroscopy

Part I

1. Provided below is the IR and ^{1}H NMR for a compound having the molecular formula of $C_7H_{14}O_2$. Using this information, determine the degrees of unsaturation for this structure and solve and draw the structure responsible for these spectral data. To validate your answer, you need to assign the type of bond (ie. stretch) responsible for each peak highlighted by a box in the IR. You must also assign each ^{1}H NMR peak **(a)-(e)** to the correct set of protons in your proposed structure. The integration for each peak has been provided for you. You must label the multiplicity observed for each peak. Is your structure consistent with all of this data? If not, chances are you do not have the correct structure, or the peaks have been assigned incorrectly. In your peer review, offer feedback concerning the accuracy of the submitted structures and spectral assignments. If you believe the answers are incorrect, then you need to provided explanation. In the end, you should all be getting the same correct structure. Please draw the final structure in the box provided underneath the NMR.

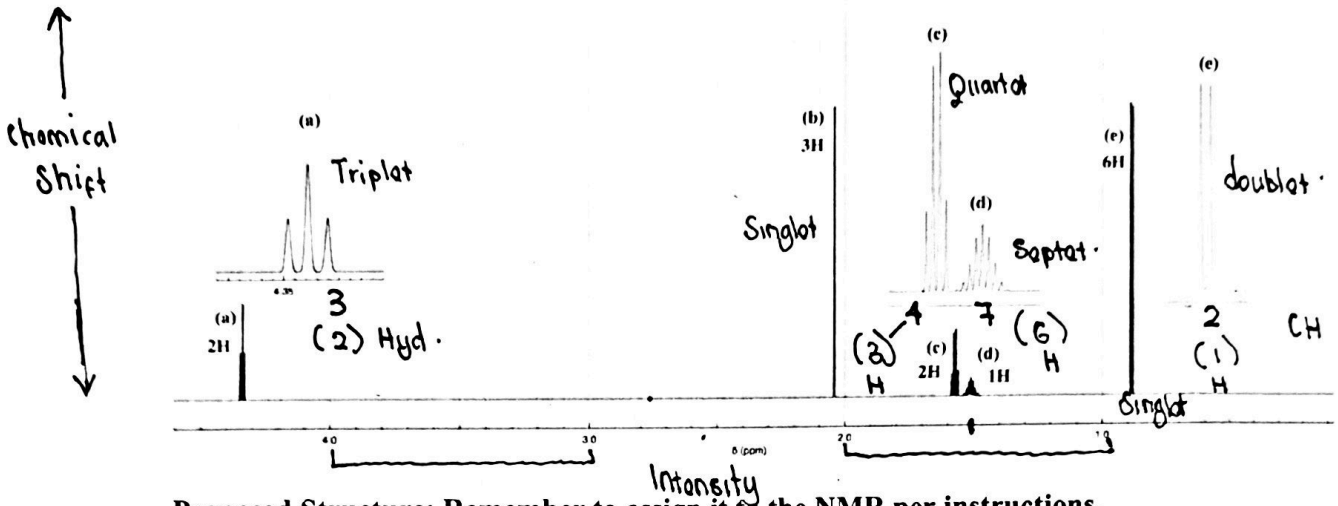
IR



Peak duo duo to CH stretch. (3000cm) Intensity

peak due to ester group (1730-1750) Intensity

1H NMR – for clarity, expansions have been provided for peaks that are not a singlets.



Proposed Structure: Remember to assign it to the NMR per instructions.

NMR - 6H = doublet thus attached to CH
Multiplicity rule = $2nI+1$ (2 =
n = # of protons
I = nuclear spin of proton = $\frac{1}{2}$)

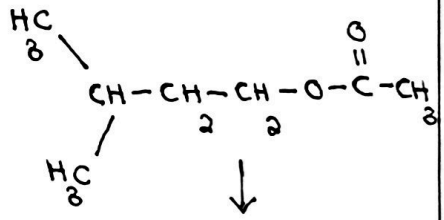
e) ∴ Splitting = $(2*1*\frac{1}{2}) = 2$ (Doublet) CH

d) Septet CH attached to 6H = $(2*6*\frac{1}{2}) = 7$ CH attached to

c) Quartet - Methylene attached to methylene

b) Singlet -No coupling CH_3 attached to Carbonyl = CH_3-COO

a) 2H at 4.2 = COO-CH_2 Triplet = methylene to Oxygen

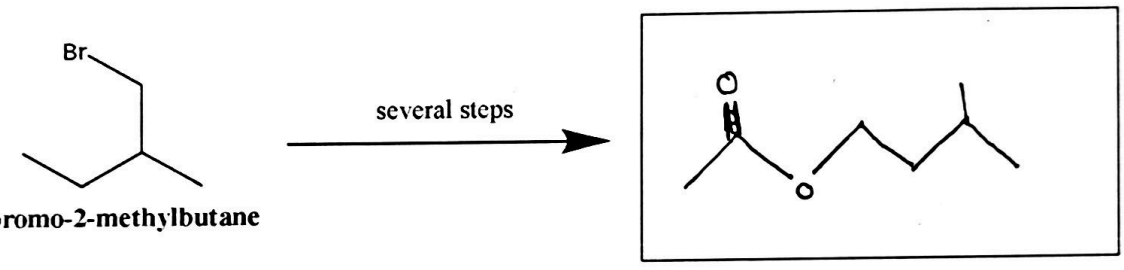


Isoamyl acetate

2. Below is a synthetic scheme that is missing the structure of the desired product. This product is the same structure that you solved for in prompt 1 using the molecular formula, IR and NMR data. Draw the structure of the desired product (hint, it has one degree of unsaturation but is not an alkene or a ring). Starting from 1-bromo-2-methylbutane, design a multi-step synthesis for this desired product. **Your synthetic plan may not use any SN1 or E1 reactions. You may only use SN2 reactions, reactions that involve the use of PBr_3, $SOCl_2$, or TsCl, E2 reactions, and any necessary alkene addition reaction from chapter 8 (including the reaction discussed in chapter 10.5).**

Separate each individual reaction in your proposal with a reaction arrow. For each step, write in the reagents necessary to carry out each step either above or below the reaction arrow. Also draw the expected product for each step after each reaction arrow. For reactions types where more than one regioisomer product is possible, you must use reagents that are regiospecific. For example, in E2 reactions, the choice of bulky base or non-bulky base can dictate which alkene is formed preferentially. Also, several (but not all) of the alkene addition reactions learned in chapter 8 and 10.5 are regiospecific and are either Markovnikov or Anti-Markovnikov addition reactions. Please indicate which steps this was important to consider. Your reagent choices should address these concerns appropriately. Discuss with your peers alternative approaches that would be better should you feel that a step is incorrect. Furthermore, discuss with your peers any other synthetic routes that would have led to the same product.

Synthetic Transformation Desired



1-bromo-2-methylbutane

Desired Product: $C_7H_{14}O_2$
(as determined by 1R and 1H NMR)

Proposed Synthesis: