

*<sup>13</sup>C NMR Spectroscopy: Interpretation & Prediction; Reactions*

Names: \_\_\_\_\_  
Chem 227/ Dr. Rusay

Consult the IR/MS data and your predicted functions from **Activity 1**.  
See **Activity 2** for <sup>13</sup>C NMR spectra and weight percent/molar mass data :  
<http://chemconnections.llnl.gov/organic/Chem227/227assign-06.html>

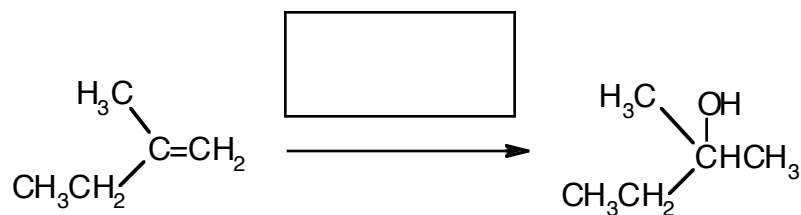
Provide structures and NMR data supporting your respective structures.

<i>Unknown's Structure and labeled carbon atoms</i>	<i>Provide chemical shifts (δ ppm), and respective splitting patterns: singlet (s), doublet (d), triplet (t), quartet (q) for each <sup>13</sup>C signal.</i>
<i>EXAMPLE:</i>  <i>a</i> <i>b</i> CH <sub>3</sub> CH <sub>2</sub> OH	  <i>a</i> δ = 18.13 (q) <i>b</i> δ = 57.79 (t)
<i>UNKNOWN A</i>	
<i>UNKNOWN B</i>	
<i>UNKNOWN C</i>	

<i>UNKNOWN D</i>	
<i>UNKNOWN E</i>	
<i>UNKNOWN F</i>	
<i>UNKNOWN G</i>	
<i>UNKNOWN H</i>	

CC(C)C(=O)CCOC(=O)CC>>CC(C)C(O)CCO[illegible]
$$\begin{array}{ccc} & \text{CH}_3 & \\ & | & \\ \text{CH}_3\text{CH}_2\text{CH}_2\text{CCH}_2\text{OH} & \xrightarrow{\quad\quad\quad} & \text{CH}_3\text{CH}_2\text{CH}_2\text{CCO}_2\text{H} \\ & & | \\ & & \text{CH}_3 \end{array}$$
[illegible]

3) Provide appropriate reagent(s):



Identify the respective carbons in the reactant that have identical chemical shifts, label them as **a**, **b**, **c**, etc.; complete the table with their respective estimated chemical shifts and splitting patterns: singlet (s), doublet (d), triplet (t), quartet (q) or multiplet (m). Repeat for the product.

[illegible]

4) A Chem 298 summer research student attempted to reduce 2-octanone with lithium aluminum hydride. The following  $^{13}\text{C}$  NMR data was obtained.

14.10 (q)
23.45 (t)
25.88 (t)
29.48 (t)
31.98 (t)
39.49 (t)
68.03 (d)

Draw the structure of the expected product and explain whether the reduction was successful based on the  $^{13}\text{C}$  NMR data.

<i>Structure:</i>	<i>Explanation:</i>

5) Run the  $^{13}\text{C}$  NMRs of both partner's unknown, draw their respective structures below, identify the equivalent carbon atoms that have identical chemical shifts, label them as **a**, **b**, **c**, etc.; complete the table with their respective chemical shifts and splitting patterns from the spectra.

Unknown #: \_\_\_\_\_

Unknown#: \_\_\_\_\_

--	--

[illegible]