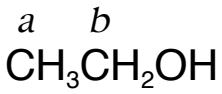
Names: _____ Sec. _____
Chem 227 / Dr. Rusay

^{13}C NMR Spectrosopy: Interpretation / Prediction & Reactions Lab Worksheet

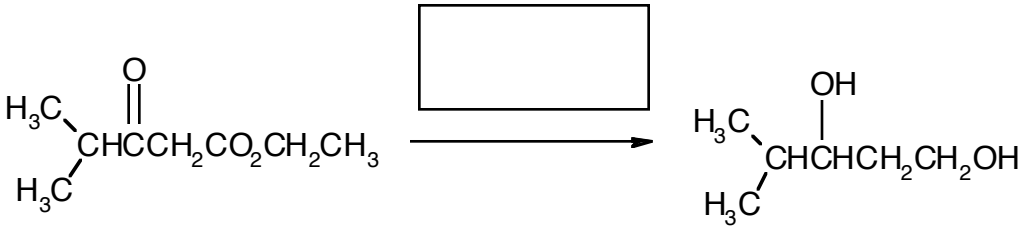
Refer to: *http://chemconnections.org/organic/chem227/IR-NMR/IR-MS-NMR-09.html* (Part IV)

Provide structures and ^{13}C NMR data supporting each respective structure with peak assignments.

Unknown's Structure and labeled carbon atoms	*Provide chemical shifts (δ ppm), and respective splitting patterns: singlet (s), doublet (d), triplet (t), quartet (q) for each ^{13}C signal.*
EXAMPLE: 	*a* δ = 18.13 (*q*) *b* δ = 57.79 (*t*)
UNKNOWN A	
UNKNOWN B	
UNKNOWN C	

UNKNOWN D	
UNKNOWN E	
UNKNOWN F	
UNKNOWN G	
UNKNOWN H	
UNKNOWN I	

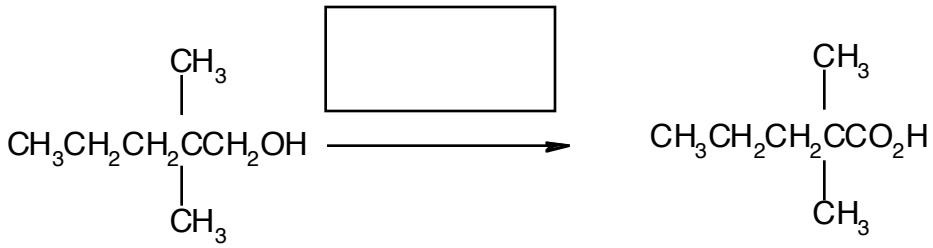
1) Provide reagents for the following reduction:



Identify the carbons in the reactant that are equivalent, 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) or quartet (q) that are determined from decoupling experiments. Repeat the process for the product.

REACTANT			*PRODUCT*		
Carbon(s)	δ ppm	Splitting	Carbon(s)	δ ppm	Splitting

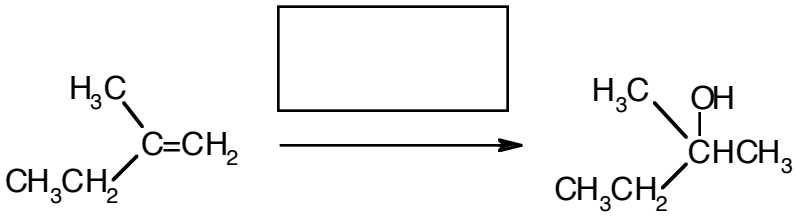
2) Provide reagents for the following oxidation:



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

REACTANT			*PRODUCT*		
Carbon(s)	δ ppm	Splitting	Carbon(s)	δ ppm	Splitting

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.

REACTANT			*PRODUCT*		
Carbon(s)	δ ppm	Splitting	Carbon(s)	δ ppm	Splitting

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

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

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

Structure:	*Explanation:*

5) Run the ^{13}C NMR of your individual unknown sample that was used in Part III. Using all of the previous spectroscopic and molecular data, draw a proposed structure for the unknown. Identify the respective carbon atoms in the structure that produce the same signal: ***a***, ***b***, ***c***, etc.. as in the example for ethanol on the first page. Complete the table by correlating the carbon atoms with the observed chemical shift.

Student Name: *Unknown #:*	*Student Name:* *Unknown #:*
Structure:	*Structure:*

Carbon(s)	δ ppm	Carbon(s)	δ ppm

Student Name: *Unknown #:*	*Student Name:* *Unknown #:*

Structure:	*Structure:*

Carbon(s)	δ ppm	Carbon(s)	δ ppm