^1H NMR Spectrosopy: Interpretation & Prediction; Reactions

Names: _____
Chem 227/ Dr. Rusay

For spectra and weight percent/molar mass data refer to **Activity 2**:
http://chemconnections.llnl.gov/organic/Chem227/227assign-06.html

Provide structures and NMR data supporting your respective structures.

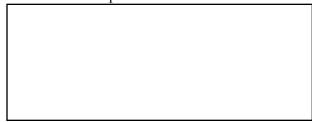| *Unknown's Structure and labeled Hs*	*Provide chemical shifts (δ ppm), and respective splitting patterns: singlet (s), doublet (d), trriplet (t), quartet (q) or multiplet (m) for each signal and the signal's integration relative to the number of Hs.*
EXAMPLE: $\quad a \quad\quad b \quad\quad c$ CH_3CH_2OH	$a \quad δ = 1.23$ (t, 3H) $b \quad δ = 2.61$ (q, 2H) $c \quad δ = 3.90$ (s, 1H)
UNKNOWN A	
UNKNOWN B	
UNKNOWN C	

UNKNOWN D	
UNKNOWN E	
UNKNOWN F	
UNKNOWN G	
UNKNOWN H	

1) Consider the following reduction: (Sodium borohydride reduces ketones but not esters.)

$$H_3C\!\!-\!\!\underset{H_3C}{\overset{}{CH}}\!\!-\!\!\overset{\overset{O}{\|}}{C}\!\!-\!\!CHCCH_2CO_2CH_2CH_3 \qquad \xrightarrow{\;NaBH_4\;}$$

a) Provide the expected number of ¹H nmr **signals** for the reactant: _____

b) Label the respective protons in the reactant's structure that produce the same signal as: *a, b, c*, etc.; complete the table, identifying the type for each of them as being equivalent (**Eq**), enantiotopic (**En**), or diastereotopic (**D**).

Proton(s)	Type

c) Draw the structure for the product.

d) For the product, provide the expected number of ¹H nmr **signals**: _____

e) Label the respective protons in the product's structure that produce the same signal as: *a, b, c*, etc.; complete the table, identifying the type for each of them as being equivalent (**Eq**), enantiotopic (**En**), or diastereotopic (**D**).

Proton(s)	Type

2) Consider the following oxidation: (PCC is an oxidizing reagent with limited reactivity; it will oxidize 1° alcohols to the next highest oxidation level and will not go to higher levels, i.e. it does not produce carboxylic acids.

$$CH_3CH_2CH_2CCH_2OH \quad \xrightarrow{\text{PCC}}$$

(with CH_3 above and CH_3 below the central carbon)

For the reactant, provide the number of ^1H nmr signals: _____

Label the respective protons in the reactant's structure that produce the same signal as: **a**, **b**, **c**, etc.; complete the table with their respective estimated chemical shifts and splitting patterns: singlet (s), doublet (d), trriplet (t), quartet (q) or multiplet (m).

Proton(s)	δ ppm	Splitting

Provide a structure for the product in the box above. In the box below, briefly explain which proton signals in the reactant will change and what changes in the product's spectrum would be tell tale that it had formed.

3) Provide appropriate reagent(s):

$$\underset{CH_3CH_2}{\overset{H_3C}{>}}C=CH_2 \quad \longrightarrow \quad \underset{CH_3CH_2}{\overset{H_3C}{>}}CHCH_2OH$$

Label the respective protons in the reactant's structure that produce the same signal as: **a**, **b**, **c**, etc.; complete the table below 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		
Proton(s)	δ ppm	Splitting	Proton(s)	δ ppm	Splitting

4) Run the ^1H NMR of each of the unknown samples that was provided for FT-IR analysis, draw a proposed structure for each unknown below. For each structure, identify the respective protons that produce the same signal as: *a*, *b*, *c*, etc..; complete the table by correlating the protons with the observed chemical shifts and splitting patterns from the actual spectrum.

Unknown #: _____   *Unknown#:* _____

Proton(s)	δ ppm	Splitting	Proton(s)	δ ppm	Splitting