CHEM221 Section 01 Dr. C. Rogers **NAME:**

INTRODUCTORY ORGANIC CHEMISTRY I --- **PROBLEM SET #1**

INSTRUCTIONS: HAND IN STAPLED, COMPLETED ASSIGNMENT (no extra pages please) **AT THE BEGINNING OF CLASS on Thursday Sept.29.** LATE SUBMISSIONS WILL **NOT** BE ACCEPTED. YOU MUST ANSWER ALL QUESTIONS. NOT ALL THE MATERIAL HAS BEEN COVERED YET; IF NOT, IT WILL BE COVERED SOON IN CLASS.

 # 1. Consider the following condensed structural formula: $CH_3CHBrC(CH_3)_2OCH_3$

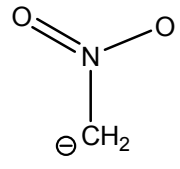
(a) Draw the molecule's complete Lewis structure.

(b) Draw a skeletal (line) structure of the molecule. Label the molecule (using δ^+ & δ^-) to show the polarity of the bonds; do not include bond dipoles that would cancel out on average.

(c) Sketch and label the orbitals (valence bond theory style) to show the overlap involved in the C-Br σ-bond, and another picture showing the corresponding antibonding (σ^*) orbital.

(d) What would happen to the C-Br σ-bond if another molecule collided with this molecule in a way that allowed a lone pair to enter the region of space defined by the σ^* orbital?

 # 2. Complete the Lewis structure of the following *closed-shell* species (*i.e.,* all atoms have full valence; you should add the lone pairs & any missing formal charges). Draw another closed-shell resonance contributor, and predict which species will contribute more to the character of the resonance hybrid.

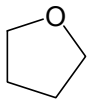


 # 3. Which species is more acidic: vinylamine (CH_2CHNH_2) or ethylamine ($CH_3CH_2NH_2$) ?
Your answer should include a brief written explanation, and:
(i) a structural diagram (Lewis or skeletal) of each acid & its conjugate base;
(ii) any additional structures that support your explanation.

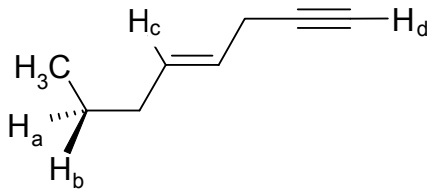
 # 4. You wish to do a chemical reaction involving the *tert*-butoxide anion, $(CH_3)_3CO^-$, so you plan to treat *tert*-butanol ($(CH_3)_3COH$) with sodium hydride (NaH).

(b) Will you need to take precautions to remove traces of water from your solvent before adding your reagents? Why or why not?

(b) Which solvent would be better to use, and <u>why</u>? Ethanol (CH_3CH_2OH) *or* tetrahydrofuran ?



 # 5. Consider the four "H_x" hydrogen atoms (labeled H_a, H_b, H_c, H_d) in the molecule shown at the right, and answer the following questions:



a) Are the double bond and triple bond in this molecule isolated or conjugated? Explain.

b) What is the approximate bond angle of H_a-C-H_b?

c) Which C-H_x bond should be the shortest?

d) Which C-H_x bond should have the highest bond dissociation energy?

e) What is the approximate pK_a of H_a?
H_b?
H_c?
H_d?

f) Which orbitals are involved in the σ-bond between C and H_d?

g) Why is the pK_a of H_b higher than that of H_c? In other words, explain what causes H_c to be more acidic than H_b.

 # 6. Imagine you add a small amount of pentanoic acid, $CH_3(CH_2)_3COOH$, to a separatory funnel that contains the organic solvent diethyl ether ($CH_3CH_2OCH_2CH_3$) and water at a pH of 7.0.

(a) What is the dominant form of the acid after you mix the phases? Draw the line structure of this compound, and explain why the majority of the molecules are present in this "protonation state".

(b) After the layers separate (water and diethyl ether are immiscible liquids), will the species identified in part (a) be found in the organic phase or in the aqueous phase? Why?

 # 7. Complete the following table about the structures of some common organic compounds.

Common name	**IUPAC name**	**Condensed formula**	**Lewis Structure (not Kékulé)**	**Line (skeletal) structure**
t-butyl methyl ether				
		$(CH_3)_2CHOH$		
sec-butyl bromide				