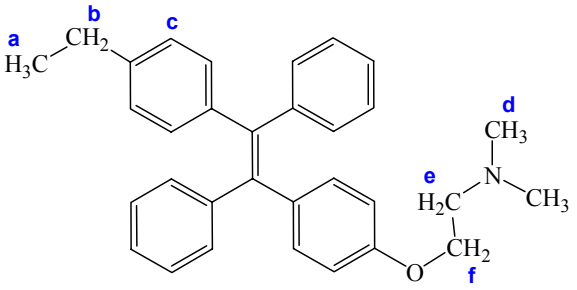
Chem 221 W08 Sect 52 Dr. C. Rogers **NAME:**

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

INSTRUCTIONS: ANSWER ALL QUESTIONS ON THESE PAGES. HAND IN (stapled, with no extra pages please) **AT THE BEGINNING OF CLASS on Thursday Feb.14.** LATE SUBMISSIONS WILL **NOT** BE ACCEPTED (EARLY IS FINE). ALL MATERIAL CAN ALL BE FOUND IN THE CLASS NOTES AND IN BRUICE CHAPTERS 1, 2, 3 & 7.

 # 1. Tamoxifen is a compound with activity against some breast cancer tumours (see Bruice Ch.3 #40). Answer the following questions:



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

b) Which orbitals are involved in the σ-bond between C and H_c?

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

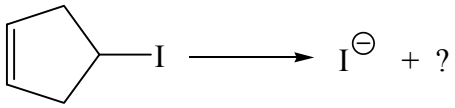
d) What is the approximate pK_a of H_b?
H_c?
H_e?
H_f?

e) Which is the most acidic H in this molecule?

f) Briefly explain <u>what causes</u> H_b to be more acidic than H_c.

g) If you wanted to prepare a solution of this substance, would you have the best "luck" with water, ethanol or hexane as the solvent? Explain very briefly.

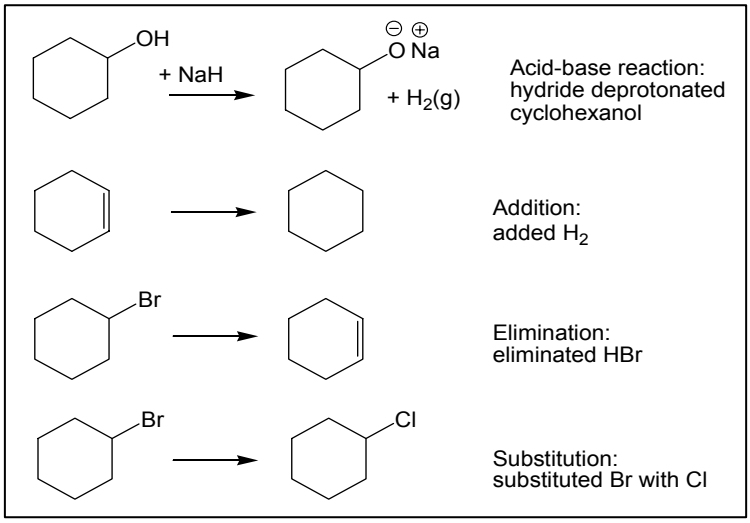
 # 2. Carbocations are highly reactive, open-shell species. They exist briefly as *reactive intermediates* during the course of some common reactions of alkenes and alkyl halides. Consider the two alkyl iodides below: if the iodine atom leaves as I^-, what reactive intermediate forms? **Draw the structure of each reactive intermediate. Which is more stable, and why?**



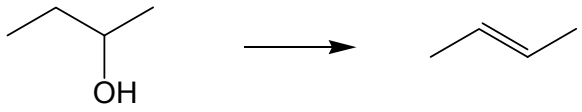
 # 3. Shown at the right are examples of the four reaction types we will see in this course: *acid-base, addition, elimination & substitution.* We will learn how they happen in Ch.4, 8 & 9.

For reactions a-d shown below, identify the reaction type and net change that occurred during the reaction (as shown for examples).

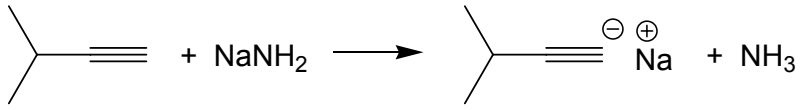
Hint: drawing the implied H-atoms & lone pairs will help.



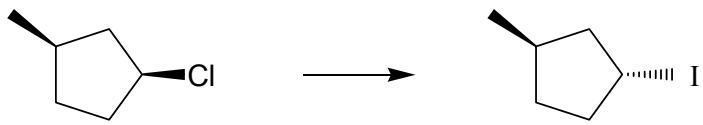
a)



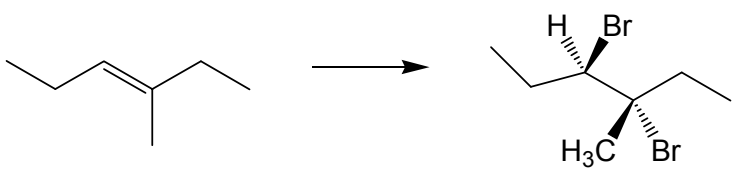
b)



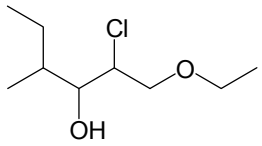
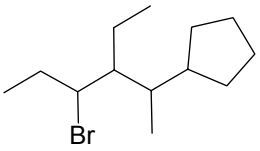
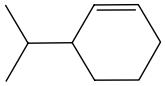
c)



d)



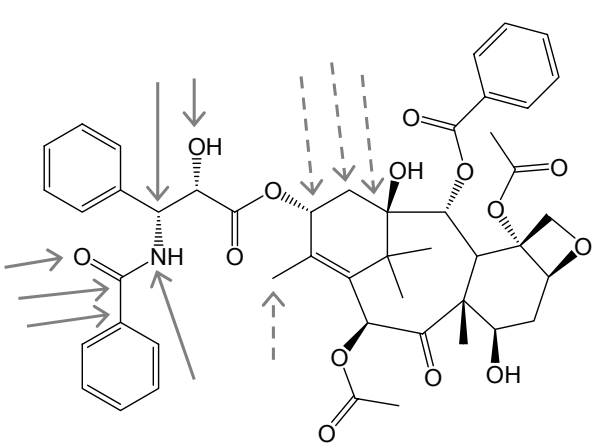
 # 4. Complete the following table.

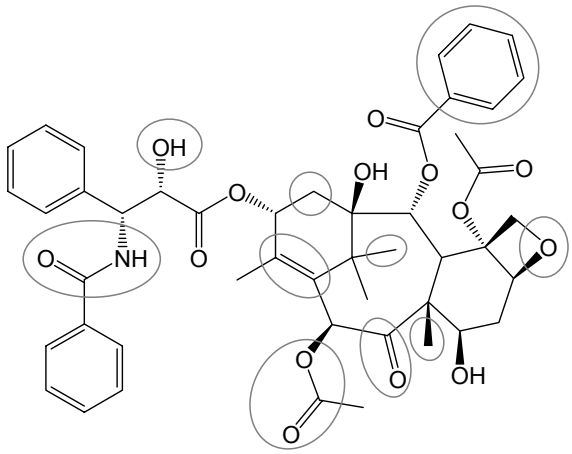
Systematic (IUPAC) name	**Line (skeletal) structure**
	
cis -1-iodo-3-methoxycyclohexane	
	
E -4-ethyl-5-phenyl-3-heptene	
	

 # 5. Which is more soluble in water: ethyl propyl amine *OR* ethyl dimethyl amine (common names)? Your explanation should include structural diagrams showing which regions of the molecules would be involved in each type of intermolecular force.

 # 6. Paclitaxel, known as Taxol® (shown below – both same), is a very potent anti-cancer drug. It is a naturally occurring substance discovered in extracts of the bark of the Pacific Yew tree. The extremely low yields of Taxol from yew bark, and the resulting decline of the yew population, quickly made the synthesis of Taxol the target of many research laboratories. It took over a decade for chemists to devise even a very low yielding total synthesis of Taxol. Currently, the large-scale semi-synthesis of Taxol starts from a more easily extracted compound in the yew tree's needles.
[Facts from Wikipedia] To see a 3D view of Taxol, go to: *http://www.3dchem.com/molecules.asp?ID=34#*

Your tasks here: **(i) 6 solid arrows: give the hybridization of the non-H atom indicated**
(ii) 4 dashed arrows: label the indicated C atom as 1°, 2°, 3° or 4°
(iii) 7 circled groups: name the alkyl group or functional group indicated





 # 7. Consider the conformations of *cis* -1,3-dimethylcyclohexane. *Note: see Bruice Ch2#36 & Table 2.9*

a) Draw the two chair conformations for this molecule, and label all the axial and equatorial positions.

b) Which conformer would predominate in an equilibrium sample of this substance? Why?

c) The energy difference between these conformations is about 23 kJ (5.4 kcal) per mole.
Which conformer is lower in energy?

How much of the energy difference is due to the torsional energy of gauche relationships?

How much of this energy difference is due to the steric strain of the 1,3-diaxial interaction?