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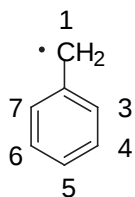
Chem 131(231)A; exam 2

1. The NBMO that is “home” to the odd electron of the benzyl radical is shown below as its LCAO-MO expansion, Ψ .

[a; 4 pts] Use it to determine the hyperfine coupling constant a_H at C_3 . Assume that $Q = 21$ Gauss. Show your work.

[b; 2 pts] How does this value compare with a_H at C_7 ?

[c; 4 pts] Indicate how one could prepare the radical in one step from PhCH_2X (you determine “X”).



$$\Psi = (7)^{-1/2} (2\chi_1 + \chi_3 + \chi_5 + \chi_7)$$

2. Use the information provided to respond to the following query.

[a; 2/4 pts] Which is easier to oxidize, propene or methyl vinyl ether? Indicate how you used the information to arrive at your conclusion.

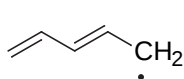
[b; 2/2 pts] In each case, illustrate the product of a one electron oxidation.

Compound	E(HOMO)	E(LUMO)
$\text{CH}_2=\text{CHCH}_3$	$-1 \beta $	$+1 \beta $
$\text{CH}_2=\text{CHOCH}_3$	$0 \beta $	$+1.414 \beta $

Problem 3 [(a) 2 pts; (b) 2/4 pts]

(a) Which of the following molecules is not an alternate hydrocarbon?

(b) Determine which **one** has a NBMO. How does the pairing theorem allow you to make your assessment? Please be **brief**.



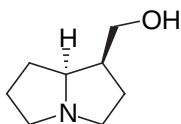
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problem 4 [4/4 pts]

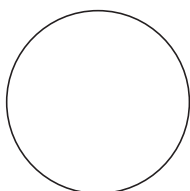
What would you expect to be the site of selective (a) protonation, and (b) deprotonation when the compound shown is treated with TsOH? with NaH? Illustrate the product in each instance.



problem 5 [(a) 4 pts; (b) 4 pts]

[a] Use the circle mnemonic to determine the relative energies of the pi MO's of the cyclopentadienyl anion.

[b] If the pKa of CpH is 15 and that of MeOH is 15, determine the equilibrium constant for the reaction of CpH with NaOMe. Show your work (be brief).

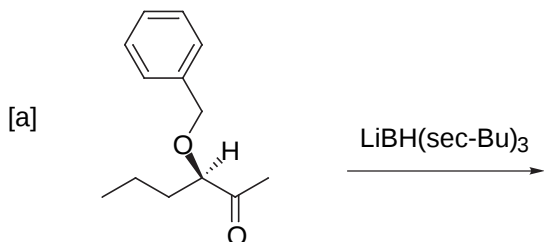


Problem 6.[4/product + 4/analysis + 2 descriptor. That is, 10 pts each]

Part I: In each instance, determine the product. Assume that an appropriate workup has been conducted. Of course, the stereochemical outcome of these reactions is of the utmost importance.

Part II: Provide a detailed analysis in each case. When appropriate, state which of the descriptors is appropriate. Choose from amongst these: Felkin-Anh, chelation control, Zimmerman-Traxler model, Houk model, Henbest epoxidation.

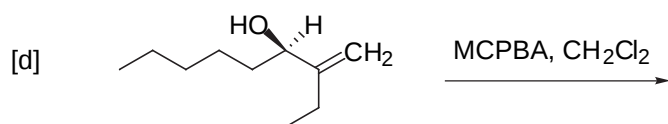
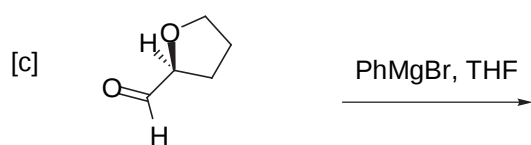
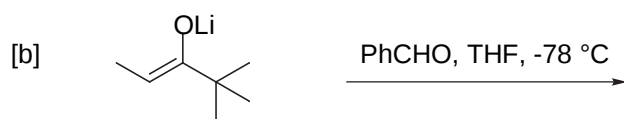
NOTE: You may use molecular models if you wish.



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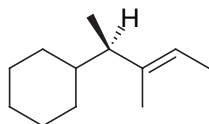


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[e]



(a) $\text{BH}_3\text{-THF}$

(b) $\text{NaOH, H}_2\text{O}_2$

Problem 7 [2 pts]

Has the reaction illustrated occurred via a 're' or a 'si' face attack?



problem 8 [4 pts]

Diastereomers **A** and **B** are produced with a de of 65%. How much of each diastereomer is present? Show your work.

Problem 9 [4 pts]

Given that $\log A = 15$ and $k = 10^6 \text{ s}^{-1}$, determine E_a . Merely set up the equation, don't solve it.