MCMP 205L Name:……..

Post – Laboratory Exercise

Borohydride Reduction of Estrone Section (Day & Time):……...

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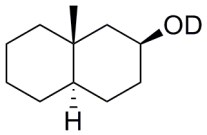
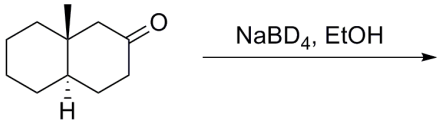
1. A summer undergraduate student was assigned the task to synthesize the compound given below.



He started off the synthesis by reacting the (5*S*,10*R*)-10-methyl-2-decalone with $NaBD_4$ in ethanol followed by quenching the reaction with water. On analyzing the NMR spectrum, the student was surprised to see a broad singlet at δ 3.58. He was also expecting a peak at δ 3.17 which was absent in the NMR spectrum. *(He had used $CDCl_3$ as a solvent for the NMR.)*



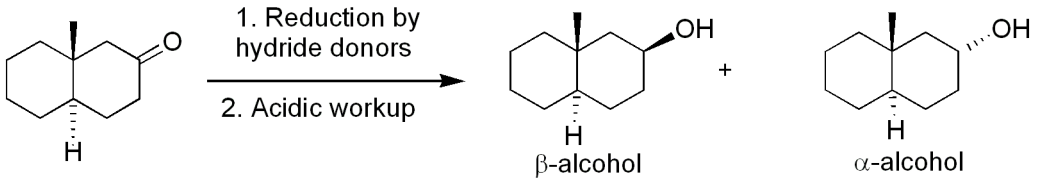
(5*S*,10*R*)-10-methyl-2-decalone

a. **(1 Point)**Write the structure of the compound (the major diastereomer) the student obtained in the box above.

b. **(2 Points)** Explain how the NMR spectrum of the desired product (the major diastereomer) would differ from the one he obtained. *(Think of the differences in peaks only above δ 2.5ppm. Base your answer on chemical shifts involved and consider a simpler splitting pattern to answer the question.)*

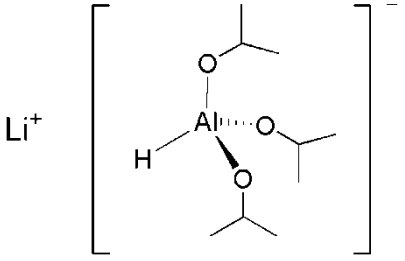
c. **(2 Points)** Design a synthetic scheme the student could use to get to the desired product. Demonstrate mechanistically how this new synthesis would yield the desired product. (*Use chair structures while writing the mechanism). You may continue at the back of this page.*

2. Answer the following questions based on the relative amounts of alcohols produced on reduction of (5*S*,10*R*)-10-methyl-2-decalone with different reducing agents as given below:



Reducing agent	*β*-alcohol (%)	*α*-alcohol (%)
$NaBH_4$ (in isopropanol)	70	30
$LiAlH_4$ (in diethyl ether)	60	40
$LiAlH(O\ ^{i}Pr)_3$ (in diisopropyl ether)	95	5

Where $LiAlH(O\ ^{i}Pr)_3$ ≡



A. **(2 Points)** What reducing agent (out of the three given above) would you use to achieve the fastest reduction of 10-methyldecalone? *(Assume you do not need a stereochemically pure compound.)* Explain why you chose a particular reducing agent and compare its reactivity with the other two in the list.

B. **(1 Point)** Explain why a significantly higher amount *β*-alcohol is formed on reduction of (5*S*,10*R*)-10-methyl-2-decalone with lithium triisopropoxyaluminumhydride as compared to sodium borohydride.