Ketone reduction

Introduction

Ketone reduction is one of the fundamental reactions in organic synthesis and this results to the formation of the corresponding alcohol as the final product. In synthetic organic chemistry carbonyl reduction is an important process leading to a wide variety of reducing being realized. Several of these reducing agents can be used to reduce all carbonyl groups, but one class of compounds only react with hydride donors. Taking for example lithium aluminum hydride reduces in most occasion’s ketone, esters and aldehydes.

Experiment 5B:

The experiment was performed using the right procedures that was provided and the instructions followed to the latter and in this case sodiumborohydride was used as the reducing agent, the protocol followed came from a laboratory manual or primary literature. It is said in theory that the four hydrides in sodium borohydride are always in place to reduce a molecule of ketone, this suggests that one mole of sodium borohydride reduces four moles of ketone. Sodium borohydride in this experiment was used to reduce 4-t-butylcyclohexanone which has a large sized t-butyl group making it to exist in an almost exclusive chair conformation one of its kind.

Post-Lab assignment

1. a) The Lewis structure of a hydride ion is as shown;

H- (hydride) Lewis structure and the (electron dot diagram) [H]+ or H+

b) This is because the carbonyl carbon has two delocalized electrons thus tends to display high affinity for the four hydride ions (H-) off the Sodium borohydride which is highly neucleophilic

2) The mechanism involved the highly nucleophilic borohydride attacking at both the endo and the exo sides leading to the formation of both cis and trans isomers.

4. This was possible since the addition of dilute hydrochloric acid led to the formation of water molecule leading to neutralization of the excess reducing agent.

5. Percentage Yield = ratio of products to reactants multiplied by 100 percent

6. a) The melting point of the major product was rather low than the literature value melting point range.

b) This is so inorder to accommodate any experimental mistakes that might have occurred during the performance of the experiment also we can say that the presence and positioning of the t-butyl group contributed a great deal to the melting range of the product.

7. a) There is absorbtion in IR at wave number 1710 cm-1

8. The reaction forms two products since there is nucleophilic attack at both endo and exo sides of the main reactant 4-t-butylcyclohexanone, and the product structures are below, t.-Bu OH cis-4-t-butylcyclohexanol Or OH t-Bu trans-4-butylcyclohexanol the main product.

a) The Newman projection for the cis-isomer

b) The Newman projection for the trans-isomer

c) Using the integrated values the ratio of cis/trans being the products can be calculated using the complex signals, one centered at 4. 05 and the other

near 3. 5 thus the areas under these complex signals are 0. 85: 3. 66 or 1: 4. 3.

References

1. University of West Florida, NMR Analysis of 4-t-Butylcyclohexanols