Methylcyclohexene case study essay sample

Food & Diet, Alcohol

Abstract: We treated 4-methylcyclohexanol with phosphoric acid, and after purification we produced the end product 4-methylcyclohexene. We determined we had a pure product based on the results of the tests with Br2 and KMnO4, as well as the IR absorbtion spectrum of the final product.

Purpose:

The purpose of this experiment is to obtain pure 4-methylcyclohexene by reacting 4-methylcyclohexanol and phosphoric acid. Through distillation, extraction, and drying, the crude product is isolated. The crude product is then distilled and collected to produce a product which was determined to be pure after testing it with Br2 and KMnO4 as well as completing an IR spectrum.

Reactions:

1. Main Reaction

2. Competing side reactions:

Separation Scheme:

Procedure: The experiment followed the experimental procedure given by E. Kluger in Introduction to Organic Lab Techniques pages 39-41 (Reference at end)

Calculations

Limiting Reagent Calculations:

Theoretical Yield:

Actual Yield:

Percent Yield:

Observed Properties and Analytical Data:

After the final distillation on the product was complete, it was tested for purity. A few drops of the product were combined with a few drops of Br2/CCl4 to test for unsaturation. The mixture turned colorless, a positive sign for the presence of a double bond that 4-methylcyclohexene contains. The second test mixed a few drops of the product with KMnO4 to test for the presence of alcohol. The color changed to brown, indicating the presence of the desired product. A drop of the product was also tested with IR spectroscopy. There were peaks at both 1600cm-1 and 3300cm-1 which are indicative of an alkene. 1600cm-1 correlates with the C= C stretch, while the 3300cm-1 signal correlates with the C-H stretch. The IR did not show a clear indication of the presence of alcohol, suggesting the product is pure since alcohol should not have been present. The IR reading confirms the previous tests performed.

Unsaturation Tests run on 4-methylcyclohexene and the starting 4-methylcyclohexanol

Br2 test:

Cyclohexanol = Yellow-orange

Cyclohexene = Colorless

Compounds containing double bonds are characterized through a red-colored bromine solution that turns colorless when it contacts an alkene

compound. The Br2 adds to the double bond and results in a positive test for an alkene.

KMnO4 test:

Cyclohexanol = Purple

Cyclohexene = Brown

The purple potassium permanganate solution will lose some of its color and form a brown precipitate of MnO2 when it reacts with an alkene and serves as a positive test for an alkene

Boiling Point of 4-Methylcyclohexene: 102 C

Melting Point of 4-Methylcyclohexene: -126 C

Questions:

1. Outline a mechanism for the dehydration of 4-methylcyclohexanol catalyzed by phosphoric acid.

2. What major alkene product is produced by the dehydration of the following alcohols?

a. Cyclohexanol = Cyclohexene

b. 1-Methylcyclohexanol = 1-Methylcyclohexene

c. 2-Methylcyclohexanol = 1-Methylcyclohexene

d. 2, 2-dimethylcyclohexanol = 1, 2-dimethylcyclohexene

3. Compare and interpret the infrared spectra of 4-methylcyclohexene and 4-methylcyclohexanol.

There is an O-H stretch at 3300 cm-1 on 4-methylcyclohexanol and 4-methylcyclohexene has a C= C stretch at 1650 cm-1.

4. Identify the C-H out-of-plane bending vibrations in the IR spectrum of 4-methylcyclohexene. What structural information can be obtained from these bands? The C-H bending is shown at 1444 cm-1 and 1368 cm-1. These bands portray the two different types of C-H bends present in the molecule, which are an alkene and alkanes.

Literature Assignment:

1. Flash point: 70°C

2. OSCA recommended personal exposure level (PEL): None

3. DOT classification: 3- flammable liquid, hazard

References:

Kluger, E. Introduction to Organic Laboratory Techniques: CHM 2211L Course Pack, Spring 2014. XanEdu Publishing, Inc.: Ann Arbor, MI, USA, 2014. p. 39-41