

Pyrolysis of aryl sulfonate esters in the absence of solvent: e1 or e2 - lab repo...

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Chemistry Lab Report 28 November High purity alkenes can be produced by pyrolysis of aryl sulfonate esters that contain a basic substituent (such as acetamido group). This experiment aimed at synthesizing an aryl sulfonate ester from a substituted aryl sulfonylchloride and an alcohol. It also intended to pyrolyze the aryl sulfonyl ester obtained and further determine whether the reaction mechanism for the pyrolysis of the aryl sulfonate ester was either E1 or E2 depending on the gas chromatographic evaluation of the pyrolysis products. Synthesis of methyl N-acetylsulfanilate, an aryl sulfonate, obtained in this experiment involved a reaction between N-acetylsulfanilyl chloride and menthol in the presence of pyridine. The produced methyl N-acetylsulfanilate was pyrolysed at a reduced pressure to produce an aryl sulfonic acid and an alkene. The pyrolysate was analyzed using gas chromatography to determine whether the pyrolysis reaction occurred via an E1 or E2 mechanism. The melting point of the methyl N-acetylsulfanilate synthesized was 105 oC while its mass was 1. 632 g, which translated to % yield of 73. 35 %. The pyrolysis products were an alkene and an aryl sulfonic acid, which occurred via E1 mechanism in the absence of a solvent.

Introduction

One way through which an alcohol can be activated for subsequent reactions such as conversion into alkenes is being converted into a sulfonate ester.

The esterification process involves a reaction between an alcohol and a sulfonyl chloride (Bruice 443). The formation of sulfonate ester is a

nucleophilic substitution reaction in which the alcohol displaces the chloride ion. The reaction is as shown

Thermal decomposition (pyrolysis) of sulfonate esters in the absence of solvent frequently leads to the generation of sulfonic acid and alkenes via E1 mechanism (Vollhardt and Schore 464). For high yield to be achieved in this elimination process, the carbon attached to the oxygen-bearing carbon must contain a hydrogen β to the oxygen (CHM 26500 93). For pyrolysis of an aryl sulfonate ester at relatively low temperature, the following reaction takes place

Questions

1. Moles of N-acetylsulfanyl chloride = $(233.67\text{g/mol})/1.6875\text{g} = 7.22 \times 10^{-3}$
= moles of methyl N-acetylsulfanilate

Mass of methyl N-acetylsulfanilate = $(309.39\text{ g/mol}) \times 7.22 \times 10^{-3}\text{ moles} =$

2.23g = theoretical yield

Actual yield = 1.632g

% yield = $(\text{actual yield} / \text{theoretical yield}) \times 100\%$

= $(1.632\text{g} / 2.23\text{g}) \times 100\% = 73.35\%$.

The high percentage yield (73.35%.) can be attributed to the presence of a hydrogen β to the oxygen.

2. The melting point of methyl N-acetylsulfanilate obtained in this experiment was 105°C indicating that the product obtained is pure since it had narrow temperature range of $1-2^\circ\text{C}$.

3. E1 mechanism

E2 mechanism

4. The chromatogram obtained can be used to determine whether pyrolysis reaction occurs via E1 or E2 depending on the number of peaks obtained. For this experiment, the number of peaks in the chromatogram is one indicating an E1 mechanism. The peak belongs to methyl N-acetylsulfanilate. For two peaks in the chromatogram, the mechanism will be E2 as the peaks will belong to the sulfonate ester and base used.

5. The basic nature of the aryl sulfonate ester due to the presence of the acetamido group and a hydrogen β to the oxygen allows the aryl sulfonate ester to produce a single alkene during pyrolysis. Therefore, the pyrolysis of any aryl sulfonate ester would produce a single alkene so long as there is hydrogen β to the oxygen.

Works Cited

Bruice, Y. Paula. Organic Chemistry. 4th ed. New York: Pearson Prentice Hall, 2004, Print.

CHM 26500- Handout 14: Experiment 14

Vollhardt, K. Peter and Schore, E. Neil. Organic Chemistry: Structure and functions. 6th ed. New York: W. H Freeman and Company, 2011. Print.