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UNIMOLECULAR SUBSTITUTION AND ELIMINATION REACTIONS COMPLETIONS

Abstract.

Substitution reactions are an essential element in Organic chemistry. Substitution reactions occur whenever a single functional atom or a group is removed and replaced with another functional atom or a group. These reactions, which are initiated through heating are essential in deciding which conditions should proceed until completion and which ones should be terminated.

Through unimolecular substitution (SN1) 2-methyl-2-butanol molecule is used in obtaining 2-chloro-2-methyl-butane molecule. HCL was used as a catalyst agent of the nucleophile and protonating during this process. Reaction is then purified using a separatory funnel resulting in 2.507g (69.73 mmol, 76.26%) of 2-chloro-2-methylbutane recovery through the unimolecular elimination, E1. From cyclohexanol, molecule cyclohexene was obtained. Sulphuric acid was utilized as the protonating substance and water as a base which results in obtaining 0.342g(3.33mmol,19.4%) of cyclohexene as a way of determining whether the process of E1 reaction and unimolecular substitution have been completed. ¹H NMR is then utilized to check the structure of the molecules of both elimination and substitution reactions.

Introduction

A reaction activity that nucleophilic atom is included is a substantial reaction. Nucleophilic atom has more electron density while attacking an electrophile, atom, specifically an atom comprising an area of a lower density reaction. The two kinds of substitution reaction that involve unimolecular SN1 that occurs in 2 stages; first on carbocation is obtained, an intermediate through the group that could be removed. The second one is whereby a nucleophile produces 2 electrons to the carbocation as a result of establishing the final substance. Because the SN1 reaction is a nucleophilic substitution, it is observed that determining the rate of stage is the procedure of creating carbocation intermediate which is not dependent of the rate of concentration of electrophile. The resulting product is a racemic mixture as the SN1 proceeds with high intensity in protic solvents. At any stage, the group that is leaving must be stable for them to leave or first protonated. If not the reaction will not proceed.

Elimination reaction occurs when a functional nucleophilic atom which acting as a base so as to attack an electrophile by deprotonating it, thus the formation of a double bond. E1 are of two kinds; unimolecular elimination E1, similar to SN1 reactions which occur in two steps the first one involves carbocation formation which is an intermediary through the leaving group. At the second step involves nucleophile getting rid of the proton from the carbon neighboring the carbocation producing the product. Since it's an elimination reaction, the rate of carbocation in the identification stage and is also independent on the concentration of the electrophile. Carbocation occurs in similar ways in both E1 and SN1. Therefore demonstrating that the utilization of heat is the only factor that would aid in distinguishing the two reactions.

Results and Discussion.

SN12 Chloro- 2- methyl butane. After completion of SN1 reaction and through using a separatory funnel, 2.507g (69.73 mmol, 76.26%) of 2-chloromethyl butane was obtained. Resulting in 76.26% of 2 chloro-2- methylbutane being obtained, which neighbors the theoretical figure 3.329 g, where 2-methyl-2- butanol as the restrictive reagent. This demonstrates that the leaving functional group which is the alcohol group was replaced with the nucleophile chlorine in the 2-methyl -2-butanol. H_b was discovered more downfield and this demonstrates that the proton embedded to the carbon is the one responsible for the allotment of chlorine and the proton is thus exposed. H_a was discovered up-field indicating that the proton is detected far from the atom which is the most chlorine, electromagnet and least exposed or more protected. As a result, the 3 signals and the breaking patterns along the amount of the proton which had formed the signs demonstrate that the reaction of 2-methyl-2-butanol occurred up to completion into 2-chloro 2-methyl butane.

E1 Cyclohexene.

After the elimination process where heat was used is completed, 0.342g (3.33mmol, 19.4%) of cyclohexene was gained. In this reaction, the restrictive reagent was sulphuric acid, as 19.4% of cyclohexene was gained from the theoretical figure of 1.54g. Even though 19.4% is not a large figure, the reaction can still be termed as completed. This means that alcohol, which is the leaving group was removed and the carbocation process became stabilized through nucleophile, H₂O, the deprotonating next to the hydrogen and production of an alkene. Spectra interpreted are in Appendix 1, the wave values are in cm⁻¹ in which the value ranges lacked cm⁻¹, For instance, C-H sp³-sp³ a hybridized stretch got detected at 2933.84 cm⁻¹ -2837.54 cm⁻¹ which is midst the range of 2830 cm⁻¹ -2695 cm⁻¹.

C-H stretch detection demonstrates that the E1 reaction continued to its completion and some of the carbons were not sp² hybridized. Also, a hybridized CH sp² -sp³ stretch was detected around 3022.84 cm⁻¹, which is a near range of 3100 cm⁻¹ -3000 cm⁻¹. Therefore, C-H sp² -sp³ stretch presence shows that an alkene was existent and the deprotonating of the E1 reaction occurred. Additionally, the detection of the C=C sp² -sp² stretch at 1652 cm⁻¹ confirms the alkene existence, as well as the deprotonating, didn't take place. Henceforth, the results of not having ν usually occur around 3500 cm⁻¹-3200 cm⁻¹ showing that the reaction of cyclohexanol to cyclohexene was completed successfully.

H_a was detected more downfield demonstrating that it is a positive ion being held onto the carbon which is tangled in the alkene. H_b was discovered further up-field than H_a, which means that is far from the alkene and is less exposed from the alkene. This insinuates the detection of H_c up-field which means it is far from the alkene and is also more protected from it. The 3 signs presence together with the breaking patterns and the number of protons that generate the signal means the reaction of cyclohexanol to cyclohexene was set-up successfully.

Conclusion

The products that resulted from both E1 and SN1, reaction transmission were successful and FTIR utilization clearly indicates the lack of the obtainability of the O-H $\text{sp}^3\text{-sp}^3$ stretch and the respective ions in their corresponding niches confirmed the required properties cyclohexane and 2-cholor-2-methyl butane. Although both E1 and SN1 happen through analogous steps, heat presence distinguishes the competition between these two, favoring E1..

Experimental

The reactants were reagent grade and every of them were provided by the university of Colorado Denver Chemistry department, FTIR spectra were acquired with a Nicoleti IS5 FTIR spectrometer and the measurements were in cm^{-1} . The ^1H NMR spectra were acquired using a broker 400MHz spectrometer using CDCl_3 as the solvent. Every measurement was in ppm and the short forms used are as follows; s (singlet), d (doublet), q (quartet) and m (multiplet).

Synthesis of Cyclohexene

A 25 mL round bottomed flask was charged with 2mL of (9.46 mmol) and 1 mL of sulfuric acid, H_2SO_4 (18.8 mmol) with a magnetic bar. The round bottomed flask was attached to a reflux condenser and placed on bird's nest heater to initiate the reaction. The process was heated for around 15 minutes. the reflux condenser was placed with a three way adapter to complete simple distillation and a the zoetrope, 0.606g (18.8mmol, 39.3%), was collected in a scintillation vial. the product was then dried through anhydrous magnesium sulfate and the product and the product collected in a scintillation vial. as a result, 0.283 g (3.43 mmol, 18.3%) of cyclohexene was recovered from cyclohexanol. FTIR was obtained and produced a 2933.84 cm^{-1} - 2837.54 cm^{-1} , C-H $\text{sp}^3\text{-sp}^3$ hybridized stretch; 3022.84 cm^{-1} , C-H hybridized $\text{sp}^2\text{-sp}^3$ stretch; 1652 cm^{-1} , C=C $\text{sp}^2\text{-sp}^2$ stretch. ^1H NMR was obtained and produced three signals, Ha at 5.67 ppm, t, 2H; Hb at 2.00 ppm, q, 4H; Hc at 1.63 ppm, t, 4H.

Synthesis of 2-chloro-2-methylbutane A separatory funnel of capacity 12mL was added 10mL of 2-methyl-2-butanol (91.3 mmol) and 25 mL of concentrated 12 M HCl (697mmol). The separating funnel was then shaken inverted and vented to make an organic layer, the hydrochloric acid layer which is denser. The organic layer of the product was washed with deionized water (10mL*3) and 5% NaHCO_3 (10mL*2). The product was dried using anhydrous magnesium sulfate and was gravity filtered into a tarred 50mL beaker. As a result, 2.506g (68.73mmol, 75.26%) of 2 chloro-2 -methylbutanol. FTIR was obtained and produced an 801.91 cm^{-1} , C-Cl $\text{sp}^3\text{-sp}^3$ hybridized stretch; 2990.04 cm^{-1} - 2941.04 cm^{-1} , C-H hybridized $\text{sp}^3\text{-sp}^3$ stretch. ^1H NMR was obtained and produced three signals—Hb at 1.7962 ppm, q, 2H; Ha at 1.5609 ppm, s, 6H; Hc at 1.033 ppm, t, 3H.

References

Sarda, V., Farooqi, J. A., & Malhotra, S. (2017). Unit-16 Alkyl Halides: Substitution and Elimination Reactions.