

Nucleophilic substitution essay sample

[Science](#), [Chemistry](#)



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Abstract

The synthesis of the alkyl halide n-Butyl Bromide from alcohol is the foundation for the experiment. During the isolation of the n-butyl bromide, the crude product is washed with sulfuric acid, water, and sodium bicarbonate to remove any remaining acid or n-butyl alcohol. The primary alkyl halide n-butyl bromide is prepared by allowing n-butyl alcohol to react with sodium bromide and sulfuric acid. The sodium bromide reacts with sulfuric acid to produce hydrobromic acid. Excess sulfuric acid acts to shift the equilibrium and speed up the reaction by producing a higher concentration of hydrobromic acid. The sulfuric acid protonates the hydroxyl group of n-butyl alcohol so that water is displaced instead of the hydroxide ion OH^- . The acid also protonates the water as it is produced in the reaction and deactivates it as a nucleophile. Deactivation of water keeps the alkyl halide from being transformed back to the alcohol by nucleophilic attack of water. The reaction of the primary substrate continues via an $\text{S}_{\text{N}}2$ mechanism.

Introduction

Halogenoalkanes, also known as haloalkanes or alkyl halides, are organic compounds in which one or more hydrogen atoms in an alkane have been replaced by halogen atoms, fluorine, chlorine, bromine or iodine. In carbon-halogen bond, halogens have significantly greater electronegativities than carbon except iodine. In result, this group is polarized so that the carbon is electrophilic and the halogen is nucleophilic. Halogenoalkanes can be classified depending on the halogen atom position on the chain of carbon

atoms. The carbon which is attached with the halogen atom is linked up with only one other alkyl group in primary halogenoalkanes, whereas directly linked up with two and three other alkyl groups in secondary halogenoalkanes and tertiary halogenoalkanes.

In some instances, primary halogenoalkanes are counted even though there are no alkyl groups attached to the carbon with the halogen on it. Three characteristics provide important influences on the chemical behavior of halogenoalkanes, these are electronegativity, covalent bond strength, and the relative stability of the corresponding halide anions. Haloalkanes are used in as refrigerants, solvents, blowing agents, aerosol propellants, fire extinguishing media , and in semiconductor device fabrication. One of big consumption of halogenoalkanes is as a raw material to prepare plastics such as PVC from chloroethene and polytetrafluoroethene from tetrafluoroethene.

Halogenoalkanes react with lots of compounds resulting in a wide range of different substances. They are useful intermediates in making other organic compounds. 1-Bromobutane, also known as n-butyl bromide is a primary alkyl halide, with the formula $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$. It is colorless liquid, insoluble in water, but soluble in ethanol and ether. Its melting point is 112 C and its boiling point is between 101 and 102 C. It is used as an alkylating agent to introduce the butyl groups to form carbon-carbon bonds in organic synthesis. They are also used as intermediate to form alkylated amines and alkylated metallic compounds. The end products include pharmaceuticals, insecticides, quaternary ammonium compounds, flavors and fragrances.

Materials and Methods

17.0 grams of sodium bromide was placed in a 100 mL round bottom flask and 17 mL of water and 10.0 mL of n-butyl alcohol was added. The mixture was cooled in an ice bath and 14 mL of concentrated sulfuric acid was slowly added making sure that there was continuous swirling in the ice bath.

Several boiling stones were added to the mixture and a reflux apparatus and trap were assembled according to the Pavia text. The mixture was heated to a gentle boil for 60-75 minutes via a heating mantle. For the extraction process the heat source was removed and the apparatus cooled so that the round bottom flask could be disconnected. The reaction mixture was carefully poured into a 125 mL separatory funnel. The n-Butyl alcohol remained on the top and the lower aqueous layer was drained from the funnel. 14 mL of 9 M H₂SO₄ was added to the separatory funnel and the mixture was shaken. The layers were given a small amount of time to separate.

The remaining n-butyl alcohol was extracted by the H₂SO₄ solution therefore, there was only one organic top layer. The lower aqueous layer was drained and discarded. 14 mL of H₂O was added to the separatory funnel. A stopper was placed on the separatory funnel and it was shaken while being vented occasionally. The layers separated and the lower layer which contained the n-butyl bromide was drained into a smaller beaker. The aqueous layer was then discarded after ensuring that the correct layer had been saved by completing the "water drop test" (adding a drop of water to the drained liquid and if the water dissolves, it confirms that it is an aqueous

layer). The alkyl halide was then returned to the separatory funnel. 14 mL of saturated aqueous sodium bicarbonate was added a little at a time while the separatory funnel was being swirled. A stopper was placed on the funnel and it was shaken for 1 minute while being vented frequently to relieve any pressure that was being produced.

The lower alkyl halide layer was drained into a dry Erlenmeyer flask and 1.0 g of anhydrous calcium chloride was added to dry the solution. A stopper was placed on the Erlenmeyer flask and the contents were swirled until the liquid was clear. For the distillation procedures, the clear liquid was transferred to a dry 25 mL round bottom flask using a Pasteur pipet. A boiling stone was added and the crude n-butyl bromide was distilled in a dry apparatus that was modeled after a figure in the Pavia text. The material that boiled between 94 and 102°C was collected. While the liquid distilled, close attention was paid to the apparatus to determine the range where most of the liquid distilled. The value for the boiling point of 1-bromobutane was noted. The product was weighed.

Results

The boiling point of 1-bromobutane was 98°C. The final weight of the product was 2.83 g and the calculated percentage yield was 16.65%.

Discussion and Conclusion

The reason that the percent yield might have been low may be due to experimental errors such as loss of product in any or all of the steps in the extraction and/or simple distillation

A Nucleophilic substitution is the reaction of an electron pair donor, the nucleophile, with an electron pair acceptor, the electrophile. An sp^3 -hybridized electrophile must have a leaving group in order for the reaction to take place.

Basic Theory of Gas Chromatography:

Gas Chromatography is a commonly used analytic technique in many research and industrial laboratories. A broad variety of samples can be analyzed as long as the compounds are sufficiently thermal stable and volatile enough. Like for all other chromatographic techniques, a mobile and a stationary phase are required. The mobile phase is made up of an inert gas e. g. helium, argon, nitrogen, etc. The stationary phase consists of a packed column where the packing or solid support itself acts as stationary phase, or is coated with the liquid stationary phase. Capillary columns are more commonly used in many instruments where the stationary phase coats the walls of a small diameter tube. The main reason why different compounds can be separated this way is the interaction of the compound with the stationary phase where the “like-dissolves-like” rule can be associated. The stronger the interaction is the longer the compound remains attached to the stationary phase, and the more time it takes to go through the column.

Polarity of the stationary phase is one thing that influences the separation. Polar compounds interact strongly with a polar stationary phase, so they have a longer retention time than non-polar columns. Chiral stationary phases based on amino acid derivatives, are capable to separate enantiomers, because one form is slightly stronger bonded than the other

one. This is often times due to steric effects. Temperature is another influence on the separation. The higher the temperature, the more of the compound is in the gas phase. It interacts less with the stationary phase so the retention time is shorter, but the quality of separation deteriorates.

Carrier gas flow is another influence on the separation. If the carrier gas flow is high, the molecules do not have a chance to interact with the stationary phase. Column length affects separation as well. The longer the column is the better the separation usually is. The trade-off is that the retention time increases proportionally to the column length. There is also a significant broadening of peaks observed, because of increased back diffusion inside the column. The Amount of material injected impacts the separation. If too much of the sample is injected, the peaks show a significant tailing, which causes a poorer separation. Most detectors are relatively sensitive and do not need a lot of material. High temperatures and high flow rates decrease the retention time, but also deteriorate the quality of the separation.

References

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