SN1 Reaction: Synthesis of 2-chloro-2-methylbutane

This is the first synthesis that you will carry out. Amyl alcohol (2-methyl-2-butanol) will be reacted with hydrochloric acid and 2-chloro-2-methylbutane will be formed. This proceeds via a SN1 mechanism. The product will separate due to decreased water solubility. The product will be analyzed by a silver nitrate test. The percent yield of the reaction will be calculated.

PRE-EXPERIMENT ASSIGNMENT

Study this chapter of the manual and the lecture notes on the Chemistry Department web site. Read sections 7.3, 7.4, 7.5, 7.6 of Klein. Do the first parts of your notebook writeup.

A student who has prepared for the SN1 Reaction experiment should be able to:

1. Give a balanced equation for the synthesis of 2-chloro-2-methylbutane from hydrochloric acid and amyl alcohol.
2. Write the mechanism of the reaction.
3. Give the name if given the structure, and write the structure if given the name of all chemicals involved in this reaction.
4. Explain why the product separates from the starting material.
5. Explain why the product floats on top of the aqueous layer instead of settling to the bottom.
6. Explain the proper use and all the components of a separatory funnel.
7. Identify and explain safety considerations for this experiment.
8. Perform the day's experiments safely and successfully.

Quizzes given after the experiment has been performed may also include:

9. Calculate the theoretical maximum amount of product that may form if given a reaction and all starting amounts.
10. Calculate the percent yield of a reaction if given amount of product produced and theoretical maximum amounts.
11. Give the balanced equation for the reaction of silver nitrate with alkyl halides.
12. Be able to predict the results of silver nitrate analyses with various compounds.

Safety Concerns

Wear goggles and gloves the entire time. Hydrochloric acid is very corrosive and will burn skin and eyes upon contact. In case of accidental contact wash affected area with copious amount of soap and water. Neutralize any acid spills with sodium bicarbonate (baking soda).

Gasses will be released when sodium bicarbonate is added to your separatory funnel. Do not stopper funnel after the addition of sodium bicarbonate solution. Vent separatory funnel frequently while shaking. Do not vent sep funnel toward another person or yourself. Liquids may spray out while venting.

Chlorinated hydrocarbons tend to be toxic materials. The target organs are the liver and kidneys. Be careful not to breathe product or get on skin.

A student who has prepared for the SN1 experiment should be able to:

PROCEDURE

Measure approximately 2 mL of 2-methyl-2-butanol using your 10 mL graduated cylinder and place it in your 10 mL Erlenmeyer flask. (Remember it is not necessary to obtain exactly 2.00 mL but it is necessary to read the graduated cylinder to 2 decimal places and write this value directly in your lab notebook). In the hood, with constant swirling, slowly add 5 mL of concentrated hydrochloric acid. Be careful when handling concentrated acid. Swirl the flask constantly for 5 minutes. Observe and note the changes which occur. Write these in your notebook.

Transfer the reaction mixture to your separatory funnel. Drain off the aqueous layer. (If you are unsure which layer this is, perform a check.) Then add approximately 2 mL saturated sodium bicarbonate solution. CAUTION! Gas will be released during this step. Swirl the funnel to mix well. Do not stopper.

Allow the layers to separate. Drain off the aqueous layer. Add 2 mL of saturated sodium chloride solution (brine). Stopper, shake and vent the separatory funnel to mix well. Allow the layers to separate, drain off the aqueous layer. Again add 2 mL of brine. Stopper, shake, vent. Allow the layers to separate, drain off the aqueous layer.

Drain the organic layer into a clean 10 mL Erlenmeyer flask. Add anhydrous sodium sulfate until some material remains free flowing like sand. Let material sit and dry for approximately 5 minutes. This time can be used to start cleaning up.

Using a pipette, transfer the dry organic material to a pre-weighed clean glass vial. Be sure to leave the sodium sulfate behind. Weigh the vial. Calculate the mass of product synthesized. Calculate the percent yield.

Product Analysis

Add approximately one milliliter of 0.1M aqueous silver nitrate to two test tubes. It is not necessary to measure out exactly 1.0 mL of the reagent. Simply put liquid into the test tube to the approximate depth of a pinky finger width. (The diameter of a test tube is approximately 1 cm. The width of a pinky finger is approximately 1 cm. If these distances were exact, the volume contained would be the volume of a column which is height times pi radius^2 ($V = h\pi r^2$ or $h \times \pi(d/2)^2$. In our case this is 1 cm x $\pi(1cm/2)^2$ or $0.8cm^3$ which is equal to 0.8 mL. This is close enough.) Add four drops of 2-methyl-2-butanol material to one test tube. Using a clean pipette add four drops of product to the other test tube. Note observations.

CLEANUP

Discard used pipettes in broken glass container. Dispose of all aqueous solutions and any surplus 2-methyl-2-butanol down sink. Place organic product in the HALOGENATED organic liquid waste container. Wipe up work area with damp sponge.

POST-EXPERIMENT

Fill in blanks and answer all questions on the datasheet provided.

REFERENCES

Gilbert, J. C., Martin, S. F., *Experimental Organic Chemistry*, 2nd Edition, Saunders College Publishing, 1998, p387-393.

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