Comparison of three isomers of butanol essay



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SCH 4UI Abstract

The Hydroxyl group on alcohols relates to their reactivity. This concept was explored by answering the question "Does each alcohol undergo halogenation and controlled oxidation?". Using three isomers of butanol; the primary 1-butanol, the secondary 2-butanol and the tertiary 2-methyl-2-propanol, also referred to as T-butanol, two experiments were performed to test the capabilities of the alcohols.

When mixed with hydrochloric acid in a glass test tube, the primary alcohol and secondary alcohols were expected to halogenate, however the secondary and tertiary ended up doing so. This may have been because of the orientation of the Hydroxyl group when butanol is in a different shape than 1-butanol. As hypothesised, when 1-butanol and 2-butanol samples were mixed with potassium permanganate in a test tube, signs of oxidation reactions resulted. Introduction It is often discussed that various functional groups bare ability to change the physical and chemical properties of an organic molecule.

There are many varieties of functional groups, for example; Hydroxyl (a simple group with oxygen and hydrogen bonded to one another resulting in high polarity) Carbonyl (with the presence of carbon double bonded to oxygen), Carboxyl (a group with carbon double bonded to oxygen and also to a hydroxyl group), and Amine (containing nitrogen bonded to what could be a variety of elements). Each of these groups provides specific properties that

are vary depending on the quantity and orientation of the groups in the molecule.

Alcohols in particular (organic compounds holding one or more hydroxyl groups) are known to be very reactive because of the presence of that group. Thus the purpose of this investigation was to verify the theories of how organic molecular structure affects the properties of the molecule in question. In this specific experiment, three different alcohols with the same molecular formula but varying structures were compared. Because of this relationship, these alcohols are isomers of each other. Specifically, Butanol, an alcohol with the molecular formula C4H9OH was used.

The three isomers of this alcohol used were: -butanol (1-butanol) – Produced industrially from hydroformylation of propylene and then subsequent hydrogenation of the resultant butanal. It is used industrially to produce various butyl esters. It can also be formed naturally as a minor product of the fermentation of sugars, and thus found in many foods and beverages. It is a primary alcohol meaning the carbon to which the hydroxyl is attached only makes one other bond to a carbon. 2-butanol – flammable, colourless liquid. It is mainly produced on the pathway to producing the very popular industrial solvent: methyl ethyl ketone.

It is a secondary alcohol meaning the carbon to which the hydroxyl is attached makes 2 other bonds to carbons. T-butanol (2-methyl-2-propanol) – A very unique alcohol, Tert-Butanol holds titles as the simplest tertiary alcohol (tertiary because the carbon to which the hydroxyl is attached makes bonds with three other carbon atoms). It is also special as an alcohol in that

it is usually a white crystalline solid at room temperature, with a melting point of 25°C. The three alcohols of varying degree were tested for their ability to undergo oxidation and halogenation.

It was hypothesized that the primary alcohol (n-Butanol) would be able to undergo oxidation, resulting in the aldehyde Butanal, the secondary alcohol would also do so, resulting in Butanone, but the tertiary alcohol lacking enough hydrogen atoms to produce water would not be able to undergo the reaction. As far as halogenation, the hypothesis was that the primary and secondary alcohols would be able to halogenate because of the abundance of hydrogen atoms to replace, and the tertiary alcohol conversely would not be able to produce the alkyl halide. Materials

Eye Protection 1-butanol 2-butanol T-butanol (2-methyl-2-propanol)

Concentrated HCl(aq) (12 mol/L) 3 test tubes Test-tube rack 4 eye droppers

KMnO4(aq) (Potassium Permanganate) (0. 01 mol/L) 10-mL graduated

cylinder

Procedure

- 1. Three test tubes were placed in a test tube rack...
- 2. Using a clean eye dropper, 2 drops of 1-butanol were placed in the first tube, 2 drops of 2-butanol were placed in the second tube, and 2 drops of T-butanol were placed in the third tube.
- 3. Under a fume hood, drops of concentrated HCl(aq) were added to each test tube.
- 4 . Each mixture was shaken gently and subsequently returned to the test tube rack.

- 5. The tubes were observed for approximately a minute, noting any evidence of cloudiness.
- 6. The mixtures were then correctly disposed of, and steps 1. and 2.
 were repeated.
- 7. To each fresh tube of alcohol, 2 mL of 0. 01 mol/L KMnO4 was added, and step 4. was repeated.
- 8. The Tubes were observed for a final 5 minutes, noting any color changes in the solutions.

Observations and Results

Table 1. 1 – Structural Diagrams of Isomers of Butanol.

2-butanol 1-butanol 2-methyl-2-propanol OH OH OH CH3
- C - CH3 CH3 - CH2 - CH -CH3 CH2 - CH2-CH2-CH3 CH3 Table
1. 2 Reaction Analyses Type of Alcohol Results when HCl is added Results
when KMnO4 is added 1-butanol There was no change in the solution,
The Solution was a dark purple color. after the full minute of observation.
Post-Shaking: The solution appeared slightly lighter (magenta).
When the solution coated the test tube surface, a residual film of
color remained where the solution had travelled. 2-butanol The solution
had a slightly yellow tinge, The Solution was a dark purple color. after
30 seconds of obervation. Post-Shaking: The solution appeared slightly
lighter (magenta). When the solution coated the test tube
surface, a residual film of color remained where the solution had
travelled. T-butanol The solution turned cloudy and yellowish, after 15
The Solution was a dark purple color. seconds of observation. The
color remained uniform throughout the duration of the experiment.

| | | | | When the solution was shaken, the liquid splashed around in | | | | droplets, and collected itself back to the pool of liquid | | | | at the bottom. |

Table 1. Demonstrates the results of the experiment. 2-butanol did not provide equal cloudiness to T-butanol. 1-butanol appeared clear throughout. 1-butanol and 2-butanol showed color change and change of physical properties, where T-butanol did not. Analysis 1-butanol: did not undergo halogenation. No cloudiness means that only a miniscule quantity of the relatively insoluble halides could be present. This alcohol underwent controlled oxidation, indicated by the slight color change in the KMnO4 + Alcohol solution. The solution also changed in its ability to leave a residual tinge on a surface of glass, indicating a reaction. 2-butanol: appeared to have underwent halogenation.

The yellow tinge exhibited in the solution may have been due to a small enough amount of halides present for all the solute to dissolve. The color change seemed to indicate a reaction. This alcohol underwent controlled oxidation, indicated by the slight color change in the KMnO4 + Alcohol solution. The solution also changed in its ability to leave a residual tinge on a surface of glass, indicating a reaction. T-butanol: underwent halogenation. The solution appeared cloudy at plain sight, characteristic of the halides that could not dissolve in it. This alcohol did not appear to undergo an oxidation reaction, and the solutions properties remained the same.

Conclusions

The Hypothetical predictions on 1-butanol's potential to oxidate were correct. The solution exhibited the change that indicates the presence of an

oxidation reaction. 1-butanol when reacted with Hydrochloric acid did not appear to undergo a halogenation reaction, meaning the hypothesis was null in that area. 2-butanol behaved as predicted, showing signs of both reactions, although the halogenation reaction did not rival that of T-butanol, the cloudiness of which clearly indicated halogenation. The hypothesis was proven wrong in regards to T-butanol's Halogenation ability, but correct in stating that T-butanol would not undergo the oxidation reaction.

Evaluation

As predicted, due to the abundance of Hydrogen atoms available for Halogenation, 1-butanol and 2-butanol readily oxidized into Butanone and Butanal. As expected, T-butanol did not. Unexpectedly T-butanol halogenated the most. This may be becuase halogenation of the alcohol replaced the hydrogen on the hydroxyl group instead of on a carbon's hydrogen. 2-butanol appeared to halogenate, but more evidence would have been ideal. 1-butanol showed no evidence of halogenation. The only difference between it and the other isomers is that its hydroxyl group bonds to a carbon with more carbon hydrogen bonds and less carbon carbon bonds. This may be the underlying reason for the reason of the results in regards to halogenation.