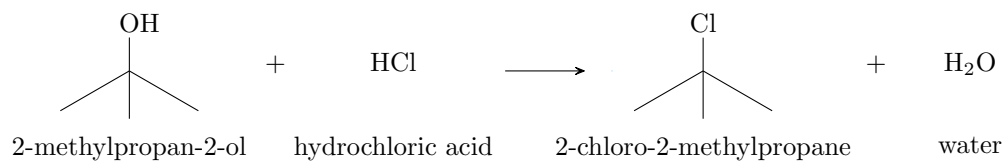
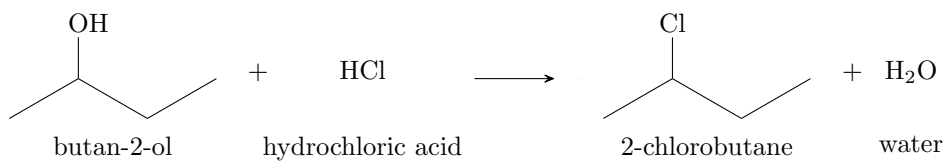
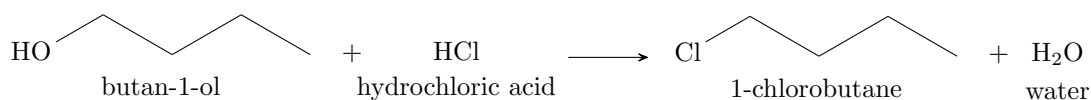


Comparison of Isomers of Butanol

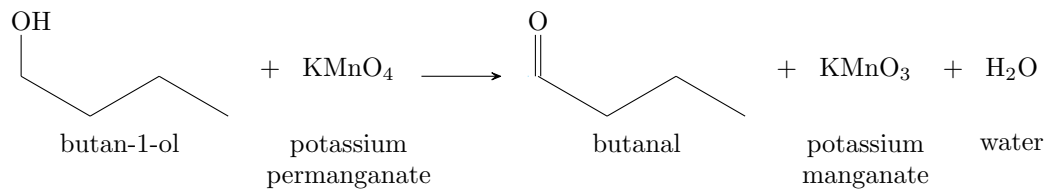
Benjamin Cheng

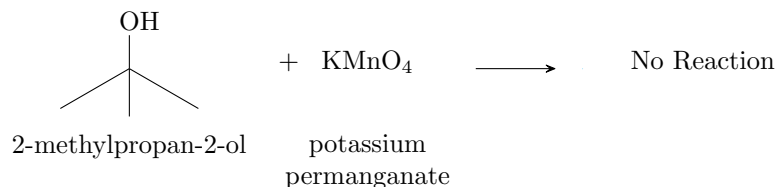
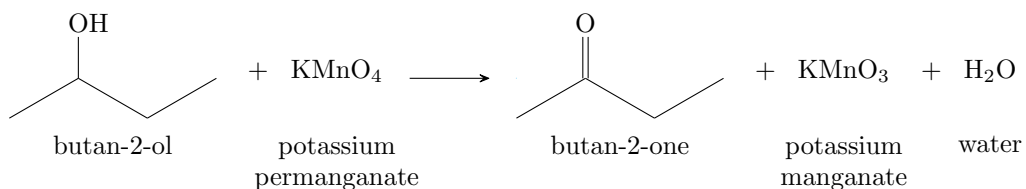
October 3, 2017

Part A - Halogenation



Part B - Oxidation





Part C - Unknown

Identification

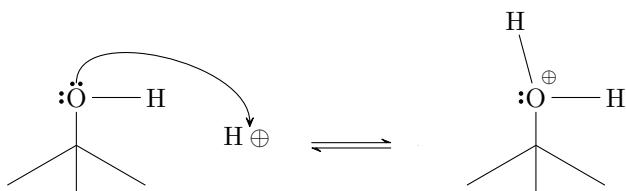
Based on lab results, the unknown alcohol was butan-2-ol. The halogenation reaction of the unknown was similar to the reactions of both butan-2-ol and butan-1-ol as it did not react nearly as vigorously as 2-methylpropan-2-ol. In the oxidation reaction, the unknown reacted similarly to the butan-2-ol, as it cleared slower than butan-1-ol, but much faster than 2-methylpropan-2-ol. Although, the colours were slightly different, this is most likely due to experimental error, such as contamination. When looking at the coil, the colours of the coil and the smell were nearly identical to that of butan-2-ol. The coil's colours were purple-redish, unlike the green of 2-methylpropan-2-ol, or the dull black of propan-1-ol. With all the reactions matching that of butan-2-ol, it is very likely that butan-2-ol is the unknown alcohol.

Reaction Speed

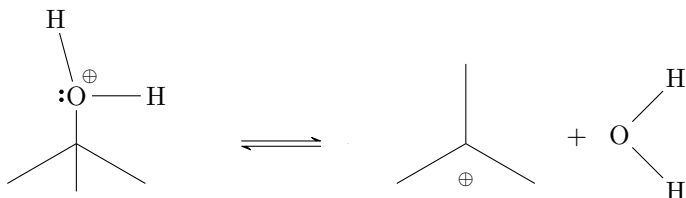
In the halogenation reactions (part A), all the isomers appeared to react almost immediately, but only the tertiary alcohol (2-methylpropan-2-ol) released a significant amount of smoke.

There are differences in the reaction mechanisms between tertiary and primary alcohols, leading to the differences in reactions.

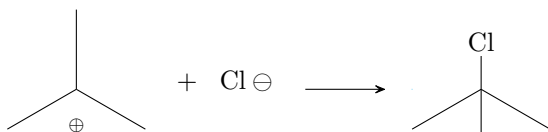
When tertiary alcohols react with HCl, they undergo a S_n1 reaction [1]. First, the hydroxyl group protonates in the presence of a H^+ , in this case, from the dissolution of HCl.



The protonation forms H_2O which is a good leaving group, forming a carbocation and water.

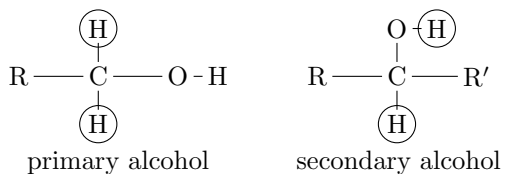


The carbocation is an electrophile, and the remaining Cl^- from the acidic solution jumps in to finish the reaction, forming an alkylhalide.



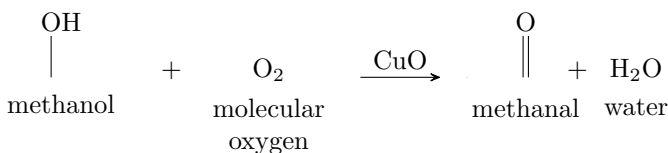
Although primary and secondary alcohols would like to undergo a similar reaction, they would form primary and secondary carbocations, which are very unstable[2]. With these unstable cations, the chloride ions are not strong enough to force this reaction to take place, and it proceeds very slowly via the S_N2 mechanism instead[1]. As secondary carbocations are more stable than primary, the reaction can use both the S_N1 and S_N2 mechanism, which allows it to react slightly faster. This may be the reason why propan-2-ol produced slightly more smoke than propan-1-ol, while both being dwarfed by the smoke produced by 2-methylpropan-2-ol. However, the smoke and reaction speed of propan-1-ol and propan-2-ol may have been inaccurate due to the miniscule amount of smoke seen (observational error).

In the elimination reactions (part B), propan-1-ol reacted faster than propan-2-ol, which in turn reacted faster than 2-methylpropan-2-ol. The hydroxyl carbon (α carbon) in a primary alcohol is bonded to 2 hydrogens, making it more readily removed in the oxidation reaction, to form H_2O . In a secondary alcohol, only one hydrogen is bonded to the α carbon, so the other hydrogen must be removed from the $\text{O}-\text{H}$ bond, which requires more energy[7], making the reaction proceed slower.



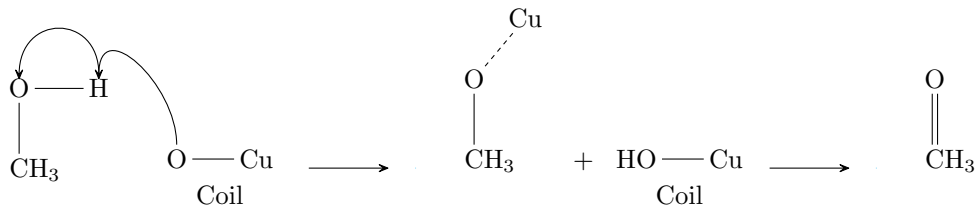
Application

When methanol undergoes an oxidation reaction, it forms formaldehyde (interestingly enough, this is why methanol is toxic – liver enzymes oxidize methanol into formaldehyde). If methanol is passed through a heated copper coil, atmospheric oxygen is able to act as this oxidation agent. When heated, copper undergoes the following reaction to produce copper(II) oxide: $2\text{Cu} + \text{O}_2 \longrightarrow 2\text{CuO}$. Heat from the wire also contributes to the vaporization of methanol. As vapors of methanol rise through the copper wire, the copper(II) oxide acts as a catalyst for the following oxidation reaction, where the oxidizer is atmospheric oxygen.



Although the reason for copper(II) oxide acting as a catalyst is under debate, the following mechanism has been proposed and is in agreement with Poreddy *et al.*[3], Abad *et al.*[4], and Fristup *et al.*[5]. The methanol's hydroxyl hydrogen reacts with the oxygen in CuO on the surface of the wire, allowing Cu(II) to break the O—H bond, forming a carbonyl group. The Cu(II) then bonds with the released H⁺, forming a copper(II) hydride anion. The atmospheric oxygen then bonds with the Cu(II), reforming CuO, and the hydrogen joins with an oxygen to form a hydroxide ion, which then bonds with a hydrogen from another simultaneous reaction, creating water.

This mechanism is best shown when only considering the core methanol reaction.



Since formaldehyde is a carcinogen and an irritant to the eyes, skin, nose, and throat, it must be made and stored carefully[6]. It should always be handled in an area with sufficient ventilation, in order to minimize inhalation of formaldehyde. Eye protection should always be worn to minimize splashes or vapors coming into contact with the eyes. In terms of storage, formaldehyde should be stored in large containers, which are labeled. Large containers should be stored on a low-shelf so that it is not accidentally knocked over. Additionally it should never be stored in an area where it may drain into the sewage system.

References

- [1] I. Hunt, *University of Calgary*, 2008, **Ch. 8**.
- [2] N. Turro, *Columbia University*, 2014, **Ch. 14**.
- [3] R. Poreddy, Christian Engelbrekt, and Anders Riisager, *Catal. Sci. Technol.*, 2015, **5**, 2467.
- [4] A. Abad, A. Corma and H. Garcia, *Chem. - Eur. J.*, 2008, **14**, 212.
- [5] P. Fristrup, L. B. Johansen and C. H. Christensen, *Catal. Lett.*, 2008, **120**, 184.
- [6] Office of Environment, Health & Safety, *University of California: Berkeley*, 2012.
- [7] W. Mosher, D. Preiss, *J. Amer. Schem. Soc.*, 1953, **75**, 5605-5607,