CHLOROBUTANOL

Structurally

It is 1,1,1-Trichloro-2-methyl-2-propanol; Tertiary alcohol.

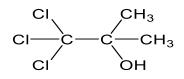


Figure 5.1: Structure of Chlorobutanol.

Some physical properties

- **1.** White or colorless crystalline substance.
- 2. Exists in two forms (anhydrous & hydrated form).
- **3.** It has a characteristic Camphor-like odor & taste.

Chemical stability

Although water is considered theoretically good solvent for crystallization (**why?**) of Chlorobutanol but Hydrolysis will take place in boiled water (the first step in crystallization), so it is best to be crystallized from water-alcohol mixture.

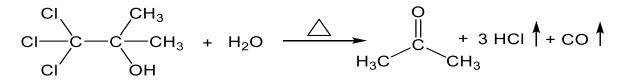


Figure 5.2: Hydrolysis of Chlorobutanol in boiled water.

Pharmaceutical Applications

- **1.** It can be used as preservative in injectable, ophthalmic, otic, and cosmetics preparations at concentration up to 0.5%.
- 2. It has local anesthetic effect so it can be found in dental preparations.

3. It is structurally related to trichloroethanol the active metabolite of chloral hydrate so it will exert similar pharmacological properties to chloralhydrate. *Explain that by chemical structure.....*

Synthesis

Chlorobutanol can be prepared from *acetone* & *chloroform* in *alcoholic KOH* (as catalyst) or KOH (as catalyst) can be added directly without dissolving in absolute ethanol as in the following mechanisms figure 5.3 a and b

1. In case of Ethanolic KOH

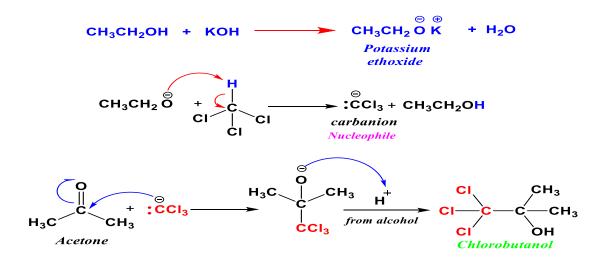


Figure 5.3 a: mechanism of Chlorobutanol synthesis catalyzed by ethanolic KOH.

2. In case of Direct addition of

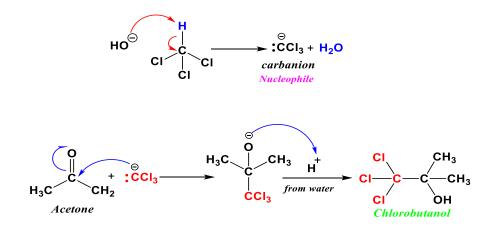


Figure 5.3 b: mechanism of Chlorobutanol synthesis catalyzed by KOH.

LAB 4&5

Procedure

- 1. Mix 33ml acetone (25gm) in a dry conical flask with 7ml chloroform (10gm).
- 2. Cool the mixture. Why?
- **3.** Add powdered KOH (1.75g) gradually through 10 minutes to the cold mixture.
- 4. Stir for 30 minutes and stand for 1hour.
- **5.** Filter the ppt. KCl, its source mentioned in figure 5.4. *during filtration make washing with acetone*, **why?**
- 6. Put the filtrate in beaker containing crashed ice and collect the product.

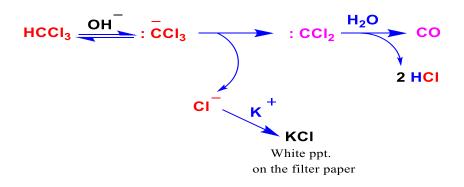


Figure 5.4: source of KCl

Questions:

- 1. How can you synthesize alkyl halide from alcohol?
- 2. Situations for using cooling in organic synthesis