



Pharmaceutical Organic Chemistry-I

UNIT - III

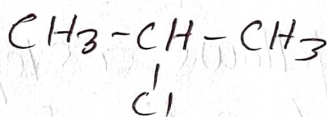
* Alkyl halides :-

- Alkyl halides also called haloalkanes or halogenoalkanes are chemical compounds that are often derived from alkanes that contain one or more halogens.
- Alkyl halides or haloalkanes are formed by the replacement of hydrogen atoms in an aliphatic hydrocarbon by halogen atoms (Fluorine, chlorine, bromine or iodine).

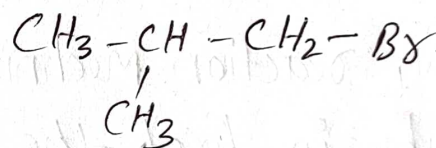
Example:-



(Iodoethane)



(2-chloropropane)



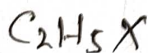
1-bromo-2-methylpropane

* Classification :-

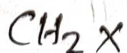
1. Classification based on the number of halogen atoms:

They may be classified as mono, di, or polyhalogen compounds depending on whether they contain one, two or more halogen atoms in their structure.

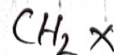
Example:-



(monohaloalkane)



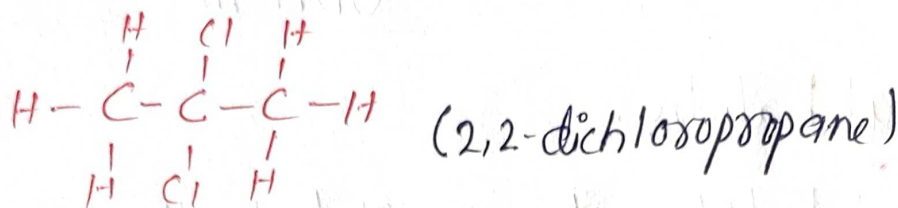
(Dihaloalkane)



(Trihaloalkane)

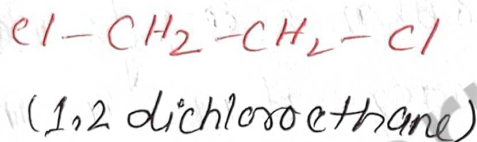
(ii) Gem-dihalides: The two halogen atoms are attached to the same Carbon atom in gem-dihalides.

Example :-



(iii) Vic-dihalides :-

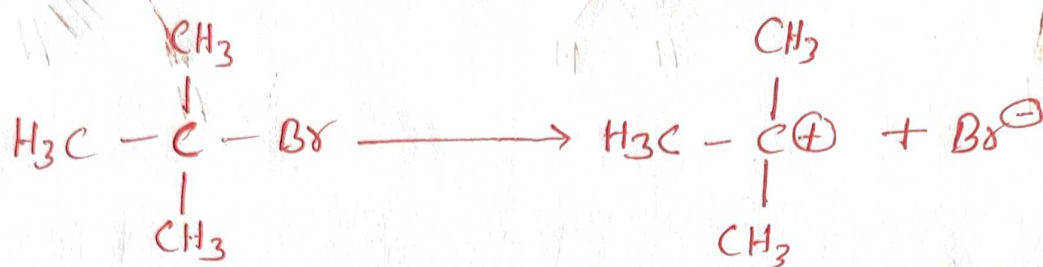
In these Compounds, the two halogen atoms are attached to adjacent Carbon atoms.



★ SN₁ REACTION :-

- The SN₁ reaction is a nucleophilic Substitution reaction where the rate-determining step is unimolecular.
- SN₁ reaction mechanism follows a step by-step process wherein first the Carbo cation is attacked by the nucleophile.
- Finally, the deprotonation of the protonated nucleophile takes place to give the required product.
- The reaction involves the formation of a Carbo cation intermediate.
- It is generally seen in the reactions of tertiary or secondary alkyl halide with secondary or tertiary alcohols under strongly acidic or strongly conditions.

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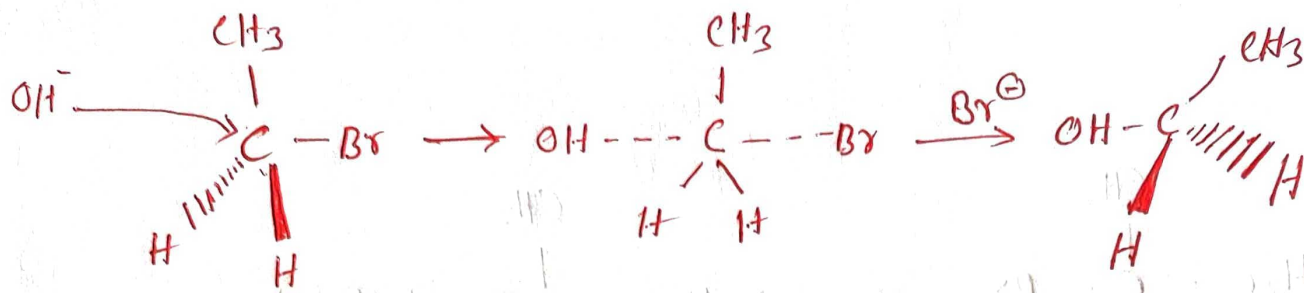


① SN₂ REACTION:-

- SN₂ stand for bimolecular Nucleophilic Substitution Reaction.
- The reaction follows Second order of kinetics.
- The Reactivity order $1^\circ > 2^\circ > 3^\circ$.
- It is one step process.
- Formation of Transition State take place.

Mechanism:-

- In SN₂ reaction the nucleophile attacks on Carbon atom of Alkyl halide from backside which results in the formation of transition state & ultimately give product of opposite / inverted Configuration to that of initial Alkyl halide.



S_N1 REACTION	S_N2 REACTION
• It is a unimolecular Reaction • It follows 1st order kinetics • It is a two step process • Reactivity order: $3^\circ > 2^\circ > 1^\circ$	• It is a bimolecular Reaction • It follows second order kinetics • It is a one step process • Reactivity order: $1^\circ > 2^\circ > 3^\circ$

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★ Factor affecting S_N1 & S_N2 Reaction :-

(i) Nature of Substrate :-

- As a result, S_N2 mechanism is favored in primary halides and least favored in tertiary halides.
- Reactivity order of alkyl halide towards S_N2 Mechanism



(ii) Nucleophilicity of the reagent :-

- S_N2 Mechanism: A more powerful nucleophile attacks the substrate faster and favours the S_N2 Mechanism.
- S_N1 Mechanism: The rate of the S_N1 Mechanism is independent of the nature of nucleophile as nucleophile does not react in the slow step of S_N1 .

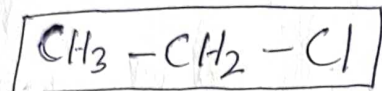
(iii) Solvent polarity :-

- S_N2 Mechanism: polar protic Solvents Usually decrease the rate of an S_N2 reaction.
- In the rate-determining step of the S_N2 Mechanism the substrate, as well a nucleophile, is involved.
- Thus S_N1 reaction proceeds more rapidly in polar protic solvent than in aprotic solvent.

★ Structure and uses of different Compounds :-

① ETHYL CHLORIDE (C_2H_5Cl) :-

Structure

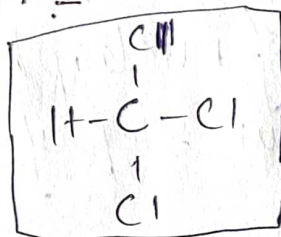


Uses :-

1. Use as a refrigerant.
2. Used as chemical promoter
3. Used to prepare tetra ethyl lead.
4. used for industrial purpose.
5. Used as an anesthetic.
6. used as a inhalant drug,
7. Used in dentistry

② CHLOROFORM :-

Structure :-



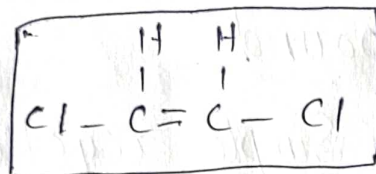
Uses :-

1. use as reagent
2. Used for the preparation of teflon.
3. As a industrial solvent.
4. use as general anesthetic.

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③ TRICHLORO ETHYLENE:-

Structure:-

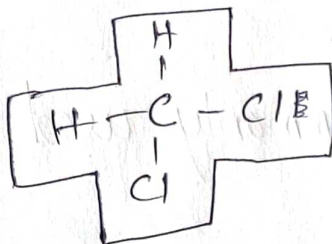


Uses:-

1. Use as anaesthetic
2. Use as solvent.
3. Dry Cleaning Solvent.

④ DICHLORO METHANE:-

Structure:-

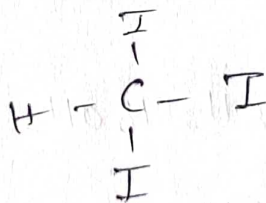


Uses:-

1. used as solvent + plastic welding adhesive
2. ~~As an ana~~
2. used in garment printing industry.

⑤ IODOFORM:-

Structure:-

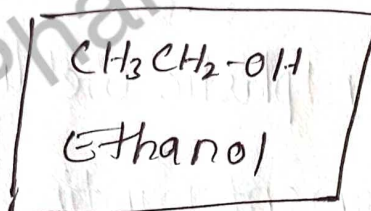
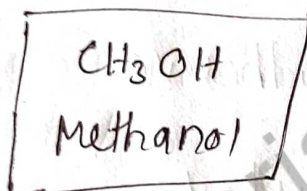


Uses:-

1. Used for poisoning
2. used as disinfectant
2. For removing hair.

★ Alcohols:

- Alcohols are organic Compounds that have one or more hydroxy (OH) groups bonded to the Carbon atoms in aliphatic Compounds.
- The General formula for a Simple acyclic alcohol is $\text{C}_n\text{H}_{2n+1}\text{OH}$, Where $n=1,2,3$ etc.
- Alcohol Can be Viewed as organic analogues of water in which one hydrogen atom is replaced by an alkyl groups.
- In alcohols, OH group is attached to sp^3 hybridised Carbon.
- The Simplest and most Commonly used alcohols are Methanol and Ethanol.



Classification:

① Monohydric Alcohols: $\text{CH}_3\text{CH}_2\text{OH}$, $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$

② Dihydric Alcohols: $\begin{array}{c} \text{CH}_2\text{OH} \\ | \\ \text{CH}_2\text{OH} \end{array}$

③ Trihydric Alcohols: $\begin{array}{c} \text{CH}_2\text{OH} \\ | \\ \text{CH}-\text{OH} \\ | \\ \text{CH}_2-\text{OH} \end{array}$

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NOMENCLATURE :-

- According to the IUPAC system of nomenclature, alcohols are called alkanols.
- They are named as the derivatives of the corresponding alkanes in which the -e of the alkane is replaced by -ol.

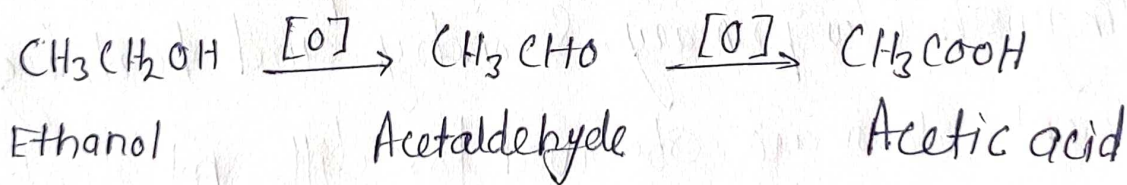
★ Qualitative test :-

Distinction between primary, Secondary and Tertiary Alcohols.

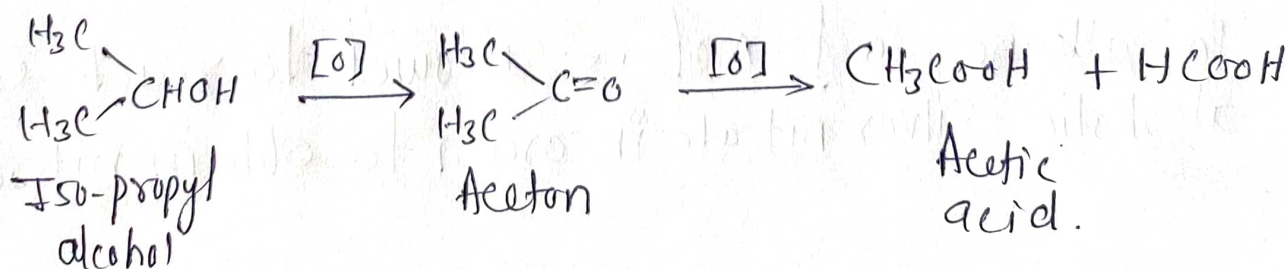
① Oxidation :-

Oxidation of alcohols involves the formation of a Carbon-oxygen double bond with the cleavage of an O-H and C-H bond.

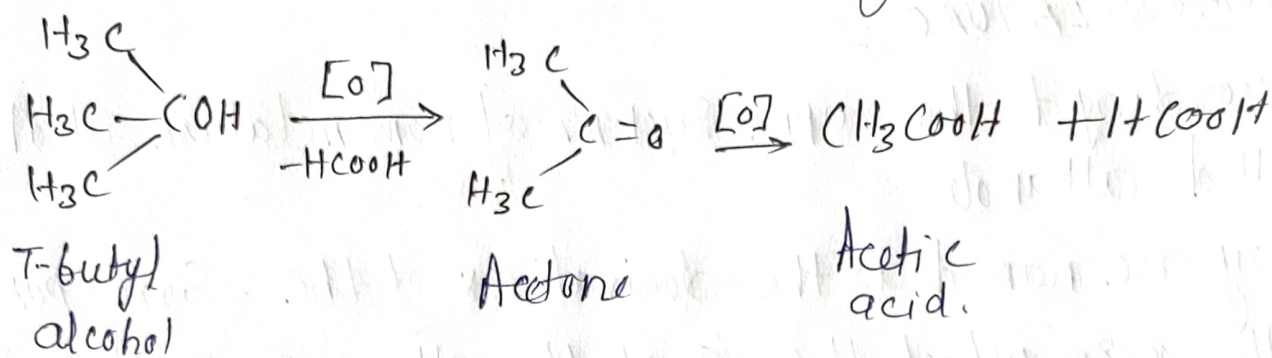
- Primary alcohol on oxidation gives aldehyde and on further oxidation yield Carboxylic acid.



- Secondary alcohol on oxidation gives ketone which upon further oxidation yield Carboxylic acid.

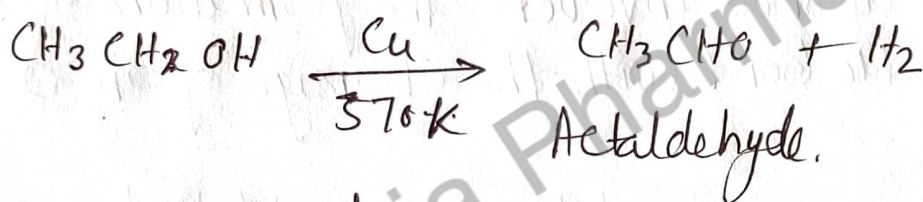


+ Tertiary alcohol on oxidation gives ketone which upon further oxidation yield Carboxylic acid.



② Dehydrogenation of alcohol by the action of hot reduce Copper:-

All three Class of alcohol behave differently with hot reduce Copper at 570K.



③ Victor Mayer Method:-

Victor Meyer's Test is one of the prominent test to distinguish b/w primary, secondary and tertiary alcohols.

- Different Colour are observed for different alcohols.
- The alcohol is treated with Iodine in presence of red Phosphorus to obtain iodoalkane.
- Iodoalkane so formed is allowed to react with alcoholic Silver nitrate in order to obtain nitroalkane.



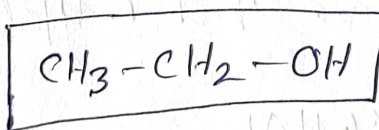
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- The nitroalkane is treated with nitrous acid (Mixture of NaNO_2 and HCl and the resulting solution is made ~~alkali~~ alkaline by the addition of Caustic Soda.
- The Colour of the resulting solution is observed in which following observation are made.
- The Primary alcohol gives blood red colour.
- The Secondary alcohol gives the blue colour.
- And the tertiary alcohol does not produce any colour.

★ Structure and uses of different alcohols :-

① ETHYL ALCOHOL :-

Structure :-

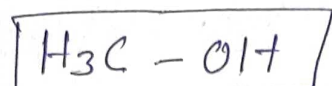


uses :-

1. use as antiseptic
2. Manufacturing of alcoholic beverage
3. For preservative for biological specimens.

② METHYL ALCOHOL :-

Structure :-

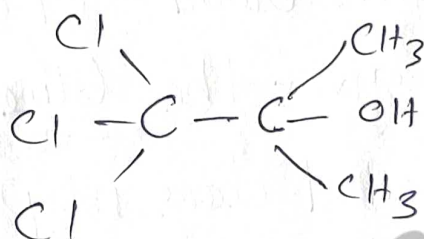


uses :-

1. In the production of Synthesis gas.
2. Raw Material for Synthesis of formaldehyde.
3. Use as fuel for vehicles.

③ CHLOROBUTANOL :-

Structure :-

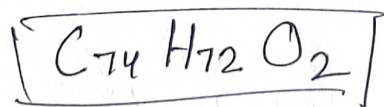


uses :-

1. used as antibacterial agent.
2. used as preservatives in eye drop, Injection, Creams and Mouthwash.
3. uses as Sedative and hypnotics.

④ CETOSTERYL ALCOHOL :-

Structure :-



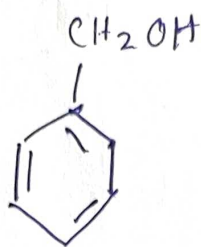
uses :-

1. preparation of emulsifying wax.
2. opacifying agent, and foam boosting Surfactant.

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⑤ Benzyl Alcohol :-

Structure :-

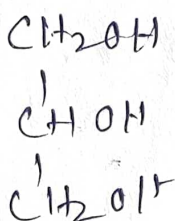


Uses :-

1. used as antiseptic
2. used to treat asthma and whooping Cough.

⑥ Glycerol :-

Structure

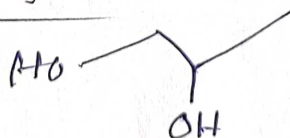


Uses :-

1. used as humectants, Solvent and Sweetener.
2. used in Soaps, hand lotion, toothpaste and bakery product.

⑦ Propylene Glycol :-

Structure :-



Use :-

1. used as drug Solubiliser in topical, oral and injection.
2. pharmaceutical additives.
3. used as a antifreeze agent.