

Q: In contrast to  $S_N2$  reaction,  $S_N1$  reaction show relatively little nucleophile selectivity. That is when more than 1 Nu. is present in reaction medium,  $S_N1$  reaction show only a slight tendency to discriminate b/w weak Nu. & strong Nu., whereas  $S_N2$  reaction show a marked tendency to discriminate

(a) Provide explanation for this behaviour.

~~In  $S_N2$  reaction, the nucleophile rate depends upon the nature of and power of substrate.~~

In  $S_N2$  reaction, Rate is depends upon:

- Nature of substrate
- Ability of leaving group to leave
- Power of Nucleophile
- Nature of solvent.

In case of Nucleophile, stronger Nucleophile have more tendency to donate electron and have relatively more ability to react with the substrate than that of weaker Nucleophile.

Rate of  $S_N2 \propto$  Power of Nucleophile

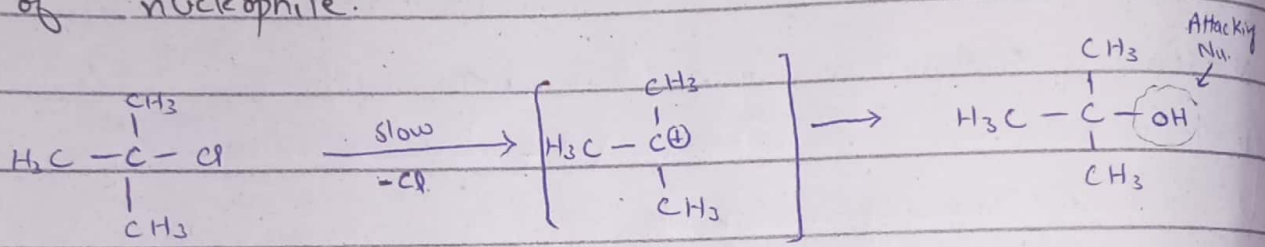
example:

$CN^-$  (cyano group) being a stronger Nucleophile have tendency to react with substrate molecule than that of  $HSO_4^-$  (a weaker Nucleophile)

In  $S_N1$  Reaction: The rate of reaction depends upon:

- Nature of substrate
- Nature of solvent
- Ability of leaving group to leave.

$S_N1$  reaction does not depend upon the power of nucleophile.



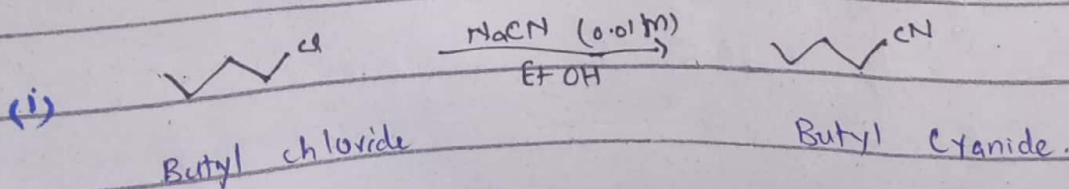
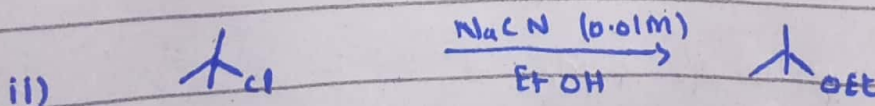
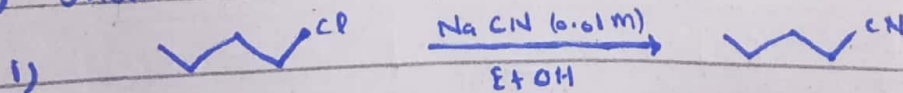
$3^\circ$  Alkyl halide

$3^\circ$  Carbocation (intermediate)

In  $S_N1$  reaction, there is independence of power of nucleophile as rate depends only on the substrate [R-X] while the attacking nucleophile will attack in next step. So, no competition will arise.

Rate of  $S_N1$  Reaction  $\propto$  [Alkyl halide]

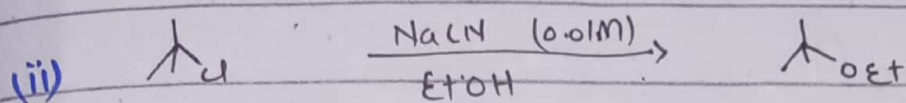
(b) Show how your answer account for:



The given compound is primary alkyl halide, so the preferable nucleophilic substitution reaction is



Nucleophilic Substitution Bimolecular ( $S_N2$ ) Reaction. As discussed earlier that  $S_N2$  reaction depends upon the power of nucleophile. Cyano group is more powerful than Alcohol group. So, both compete and cyanide group will attach to the alkyl group forming Alkyl cyanide (Butyl cyanide)



$3^\circ$ -Butyl chloride

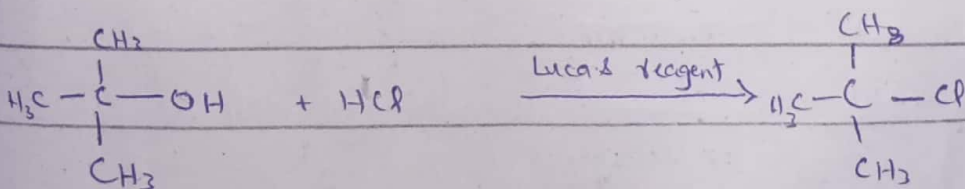
$3^\circ$ -Butylethoxide

The given compound is Tertiary alkyl halide so, for tertiary substrate,  $S_N1$  will be preferable option in which ~~detacking~~ leaving group (Nu) attacks, leaving group leaves at same time. In  $S_N1$  reaction, the <sup>rate of</sup> reaction is independent of power of Nucleophile so that is why a weak Nucleophile (Ethoxide ion) attacks with Carbocation forming tertiary butylethoxide

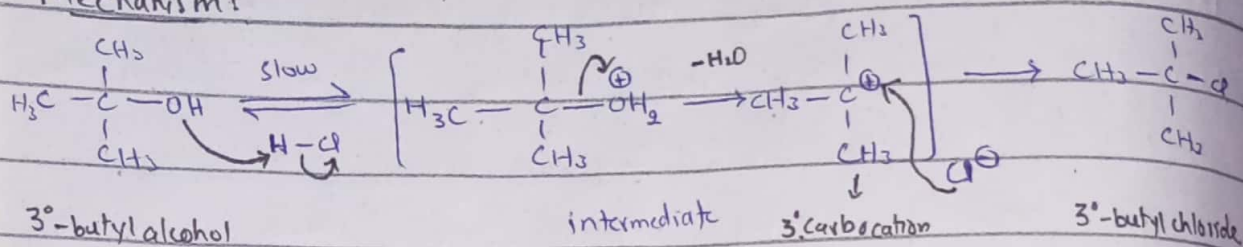
Qno. 2: b)

Process of converting tert-butyl alcohol into tert-butyl chloride, providing detail on the reagents and reaction condition involve.

Reaction:



### Mechanism:



→ First of all, it is observed that the reacting substrate molecule is Tertiary butyl alcohol so, it will follow  $\text{S}_{\text{N}}1$  reaction.

→  $\text{OH}^-$  is a weak / poor leaving group so it has to first react with the Hydrogen of  $\text{HCl}$  to form  $\text{OH}_2^+$  (Good leaving group) then this  $\text{OH}_2^+$  will leave forming water molecule.

→ Remaining molecule will be called as the tertiary carbocation on which chloride ion immediately attack forming tertiary butyl chloride.

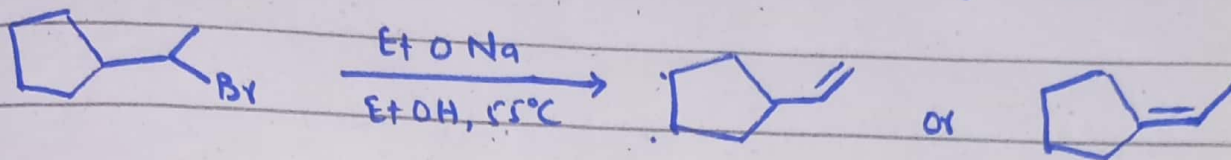
### Reagent:

→ The reagent which is used during this reaction is 'Lucas reagent' with Hydrochloric acid.

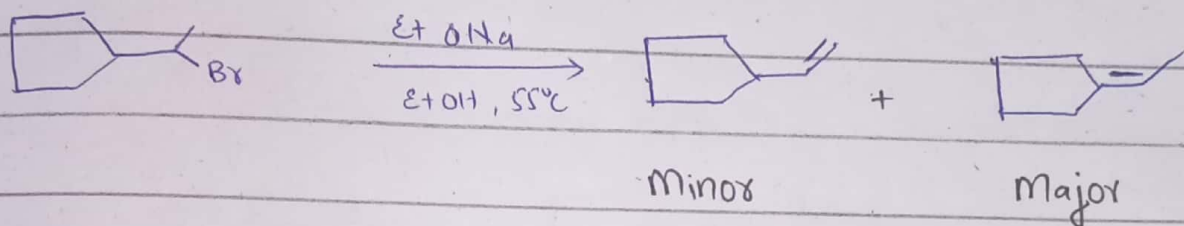
→ This reagent is basically used to determine the given compound is primary, secondary or tertiary alcohol.

Tertiary alcohol	Lucas reagent immediate	Tertiary chloride
Secondary alcohol	Lucas reagent 5-10 min	Secondary chloride
Primary alcohol	Lucas reagent on heating	Primary chloride

Qno, 3: (A) Using Zaitsev rule, predict which would be the major product of following. Justify.



Using Zaitsev rule.



Zaitsev's rule says:

"In elimination of Alkyl Halide (Dehydrohalogenation) that product is formed which will be highly substituted and more stable."

So, in the above reaction, 3-cyclopent-2-ene will be more stable and highly substituted than 1-methylcyclopentane-1-ene.