MECHANISM SN_1

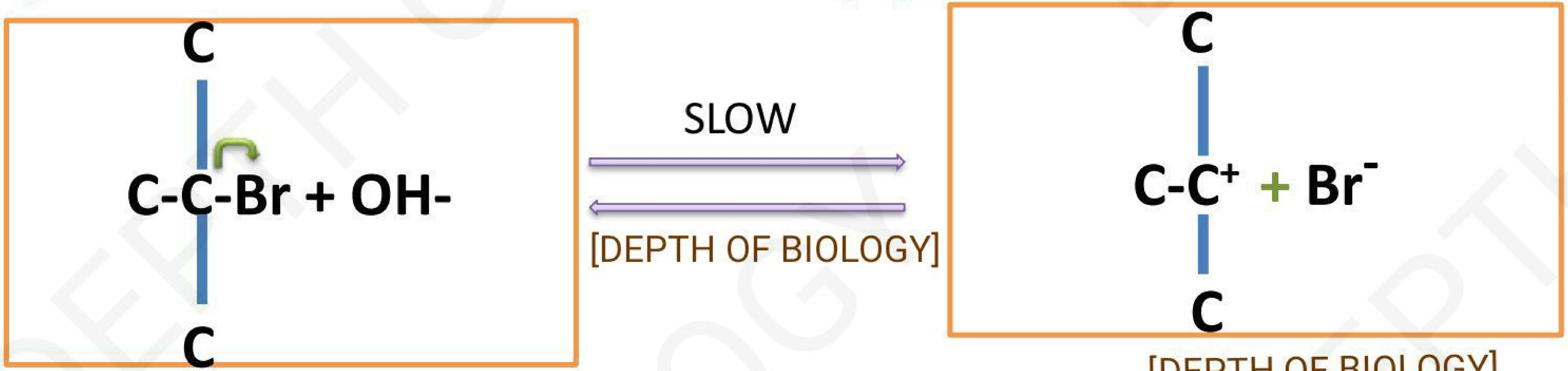
- S_N1 reaction is a nucleophilic substitution reaction where the rate-determining step is unimolecular
- Inversion of configuration takes place as well as retention
- Polar protic solvent (H+)
- Carbocation rearrangement possible
- Partial racemisation takes place
- Reaction follows 1st order kinetics i.e. R.O.R depends upon concentration of alkyl halide only

- Reaction takes place in the presence of polar protic solvent in 2 step

- In 1st step, the formation of carbocation takes place & in 2nd step attack of nucleophile on carbocation takes place.
- Order of reactivity depends upon stability of carbocation and follow the order – $3^o > 2^o > 1^o$

$$(CH_3)_3C\text{-}Br + OH^- \longrightarrow (CH_3)_3C\text{-}OH + Br^-$$

STEP:1



$$\mathrm{C-}\overset{\mathrm{C}}{\underset{\mathrm{C}}{\mathrm{C}^{+}}} + \mathrm{OH}^{-} \xrightarrow{\text{FAST}} (\mathrm{CH}_3)_3\ \mathrm{C-OH}$$

- Allylic & benzylic carbocation show greater stability due to resonance

SN_2

Reaction follow 2nd order kinetics i.e. R.O.R depends upon concentration of R-X as well as nucleophile

- Takes place in single step (inversionof configuration takes place)
- Reactivity order= 1>2>3 (alkyl halide)

Stereochemistry of SN_1 Reaction

Carbocation formed as an intermediate has a **planar structure**

Planar structure allows the Nu^- to attack from either side

Here empty p orbital lies perpendicular to the plane

So in SN1 reaction the optically active halide give almost a racemic mixture

Here complete racemisation is prevented due to the following reasons

Nu^- attack slow

- The ion pair get sufficient time to form carbocation
- Either front or back
- Racemisation takes place

- **Nu^- attack fast**

- Then it occur on ion pair
- In this case front side is sheilded so back side is prefered
- Thus inverted product formation takes place

SN_2 Reaction

Attack of Nu^- is from the back side (side which is opposite to leaving group)

This manner of attack alter the configuration of the C atom.

KINETICS

Depend on both- the concentration of reactant & Nu^-

SN1	SN2
1. Unimolecular	1. Bimolecular
2. Follows 1st order kinetics i.e R.O.R depends only upon concentration of alkyl halides	2. Follows 2nd order kinetics i.e R.O.R depends upon concentration of alkyl halides as well as nucleophile
3. Formation of carbocation takes place	3. Inversion of carbocation takes place
4. Reaction takes place in 2steps	4. Reaction takes place in single step
5. Polar protic solvent is essential (NH_3, H_2O).	5. Polar protic solvent not required.
6. Order of reactivity – $3^{o}>2^{o}>1^{o}$	6. Order of reactivity – $1^{o}>2^{o}>3^{o}$
Depends upon stability of carbocation	Depends upon steric hindrance

FACTORS AFFECTING SN_1 & SN_2

1) *Nature of substrate/ structure of alkyl group-*

SN_1	SN_2
Stability	Steric Hindrance
$3^o > 2^o > 1^o$	$1^o > 2^o > 3^o$

2) *Nature of nucleophile-*

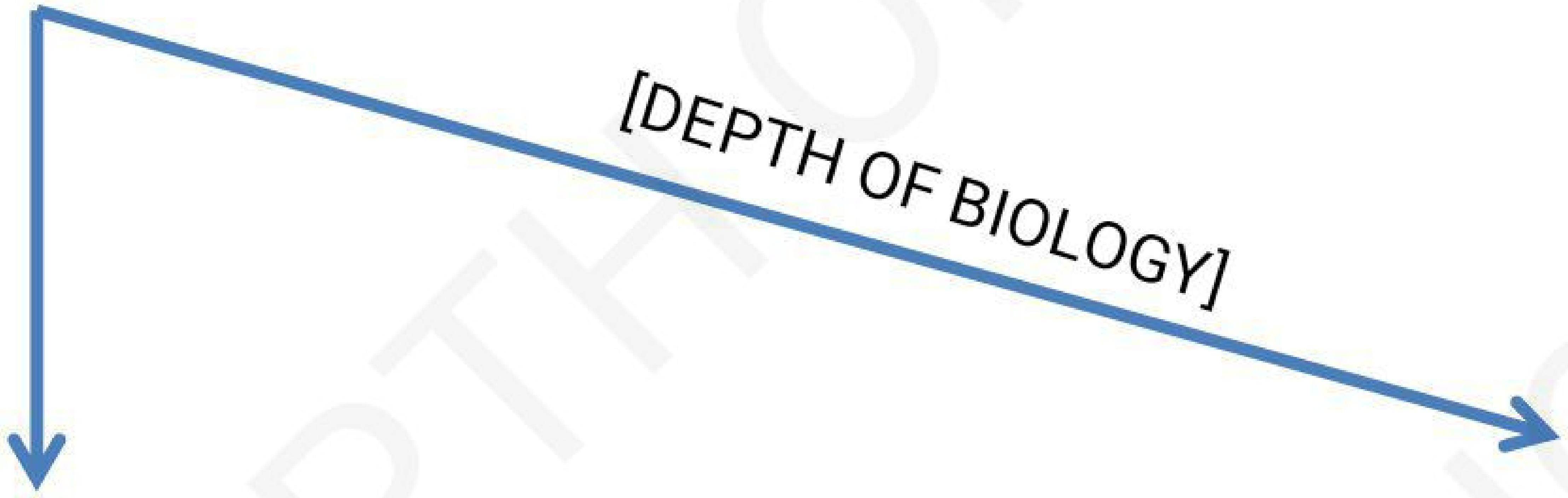
SN_{1-} does not have any effect

SN_{2-} here the concentration of R.O.R affect the nucleophile

3. Nature of solvent

Polar

Non- Polar



Protic	*Aprotic*
-SN_1	- SN_2
-can donate H+ion	*-cannot donate H+ ion*
Eg- CH_3COOH, NH_3 ,$R\text{-}NH_2$	Eg- DMSO, DMF.

4.Nature of halide group

R-I >R-F

5. Effect of leaving group-

When C & leaving group bond break, the leaving group increases the R.O.R.