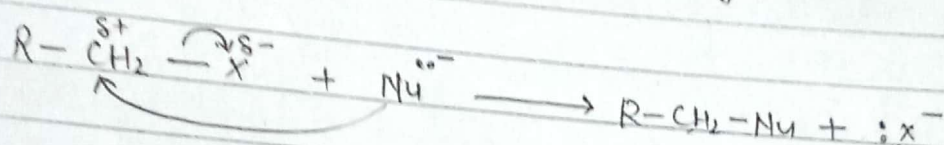


Chemical properties of Alkyl halide :-

Alkyl halide are saturated compounds with electron deficient functional group carbon due to high electronegativity of halogen. Therefore alkyl halide readily undergo to nucleophile substitution reaction.



order of reactivity towards nucleophilic substitution reaction :-
 $1^\circ > 2^\circ > 3^\circ$

Nucleophilic substitution reaction :-

On the basis of kinetics nucleophilic substitution reaction are classified as :-

i) ~~SN~~ SN1 Reaction

ii) SN2 Reaction

1) SN1 Reaction :-

It is unimolecular nucleophilic substitution reaction follows 1st order kinetic. chemical kinetics studies reveal that rate of this reaction depend only on the concentration of alkyl halide and independent with the concentration of the nucleophile.

$$\text{Rate} \propto [\text{Alkyl halide}]$$

$$\frac{dx}{dt} = k [R-X]$$

where k is the rate constant.

The reaction is completed in two steps in which 1st step is the ionisation and second step is the bond formation between nucleophile and carbon.

Ionisation is highly endothermic process with high energy of activation therefore it is rate determining step.

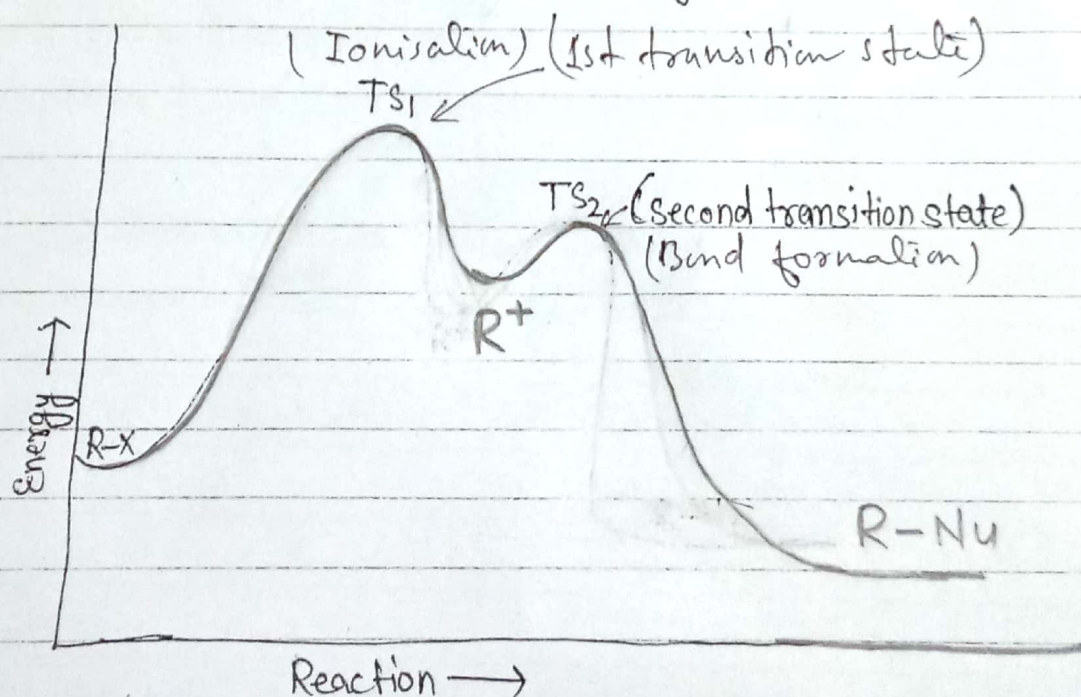


Fig: Illustration of two steps including intermediate of the ~~rea~~ SN1 reaction.

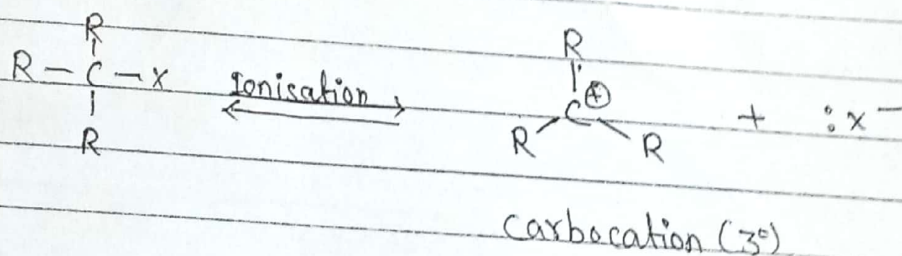
Mechanism of S_N1 Reaction :-

Following two steps are involved in this type of nucleophilic substitution reactions.

STEP 1 :- Ionisation and formation of carbocation intermediate:-

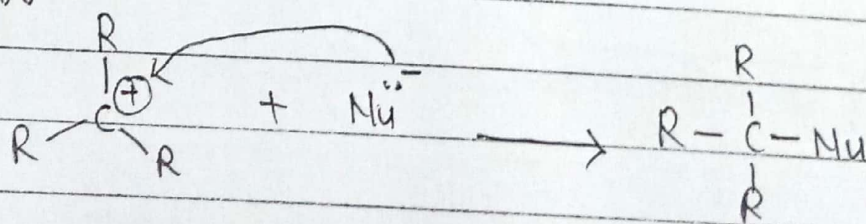
Ionisation have high free energy of activation but it occurs due to ionising ability of the solvent. The energy required for ionisation is supplied by the formation of many ion dipole bonds between the ion produced and polar solvent molecule.

S_N1 reaction is the characteristics of 3° alkyl halides hence a relatively stable 3° carbocation and a halide ion are produced.



STEP-2 :- Bond formation by nucleophile with cationic carbon:-

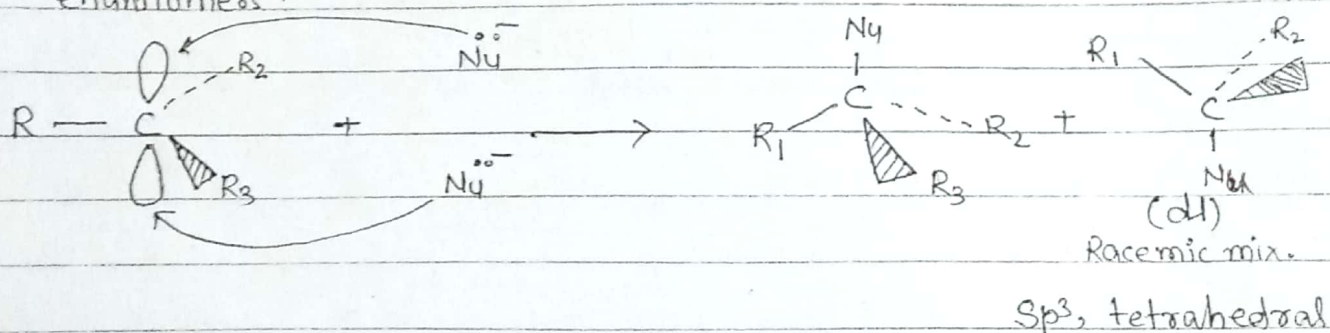
In this step carbocation rapidly reacts with nucleophile this step is faster than 1st step due to lower activation energy.



Stereochemistry of S_N1 reaction:-

S_N1 Reaction is nonstereospecific due to formation of planar carbocation as reaction intermediate in which empty p-orbital lies perpendicular to the plane. Nucleophile can be attack equal and easily at lobes of its empty p-orbital.

If substrate is a chiral molecule, its product will be a racemic mixture of the two possible enantiomers.



2) S_N2 Reaction :- It is bimolecular nucleophilic substitution reaction follows second order kinetics.

$$\text{Rate} \propto [\text{Alkyl halide}] [\text{Nucleophile}]$$

$$\frac{dx}{dt} = k [R-X] [Nu^-]$$

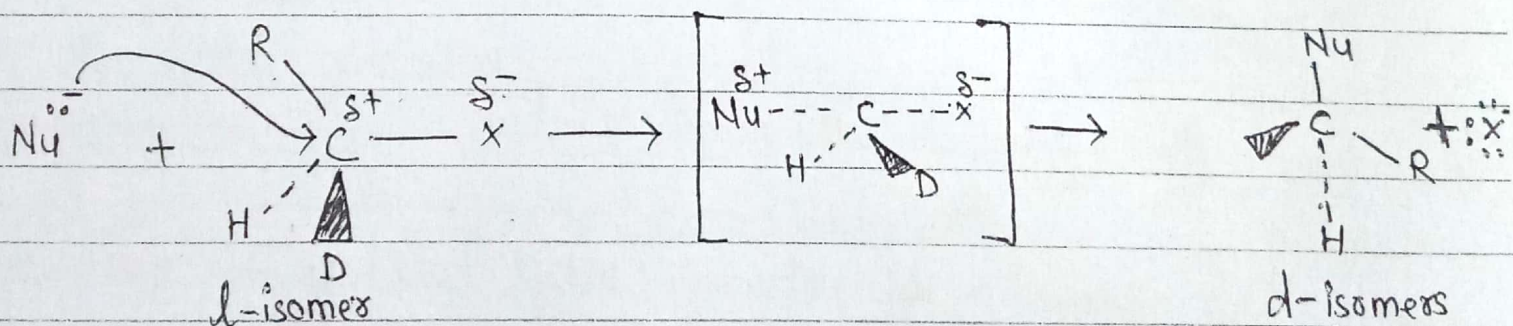
It is character of primary alkyl halides. The reaction is completed in single step by formation of activated complex as transition state of the reaction.

Mechanism of S_N2 Reaction :-

The transition state is the fleeting arrangement of the atom in which the nucleophile and the leaving group are both partially bonded to the carbon atom undergoing attack. The transition state has an extremely brief existence.

Stereochemistry of the Reaction :-

In reaction nucleophile attacks on electron deficient carbon from opposite side of the alkyl group. This results in the inversion of configuration. Such inversion is called Walden inversion in case of optically active compound.



Difference between S_N1 and S_N2 reactions.

Feature	S_N1 reaction	S_N2 reaction.
i) Step	<p>Reaction is completed in two steps by formation of carbocation intermediate in which step 1 is Rate determining step.</p> <p>i) $R-X \rightleftharpoons R^+ + X^-$ (slow)</p> <p>ii) $R^+ + Nu^- \xrightarrow{\text{fast}} R-Nu$</p>	<p>Reaction is completed in one step by formation of activated complex as transition state.</p> <p>$R-X + Nu^- \rightarrow [Nu-R-X] \rightarrow Nu-R + X$</p>
ii) Molecularity	It is unimolecular reaction.	It is bimolecular reaction.
iii) Kinetics	<p>It follows 1st order kinetic.</p> <p>Rate $= k[R-X]$</p>	<p>It follows 2nd order kinetic.</p> <p>Rate $= k[R-X][Nu^-]$</p>
iv) Rate determination	Rate of reaction is determined by stability of carbocation.	Rate of reaction is determined by steric factor in transition state.
v) Stereochemistry.	Inversion and racemization takes place due to planar nature of carbocation.	Inversion takes place without racemization because nucleophile attacks on opposite side of the leaving group.

vi) Solvent	Polar, protic solvent such as alcohol, water, acids and high dielectric constant favour S_N1 reaction.	There is no much importance on solvent factor place There without is no much importance of nature of the solvent. Generally aprotic solvent like acetone, acetonitrile etc. has high dielectric constant are used.
vii) Nucleophile	It is favoured by weak nucleophile with low concentration.	It is favoured by strong nucleophile with high concentration.
viii) Nature of Alkyl halide	It is character of 3° alkyl halides. The order of reactivity is $3^\circ > 2^\circ > 1^\circ > \text{methyl}$.	It is character of 1° alkyl halides. The order of reactivity is $\text{methyl} > 1^\circ > 2^\circ > 3^\circ$.
ix) The nature of halide	Iodo group is the best leaving group. The order is $R-I > R-Br > R-Cl > R-F$.	Iodo group is the best leaving group. The order $R-I > R-Br > R-Cl > R-F$.