HALOALKANES & HALOARENES

By-Dr.Rinky

06-07-2020

Chemistry
Class-XII

Lecture-12

Topic :- Mechanism of Nucleophilic Substitution Reaction Continued..

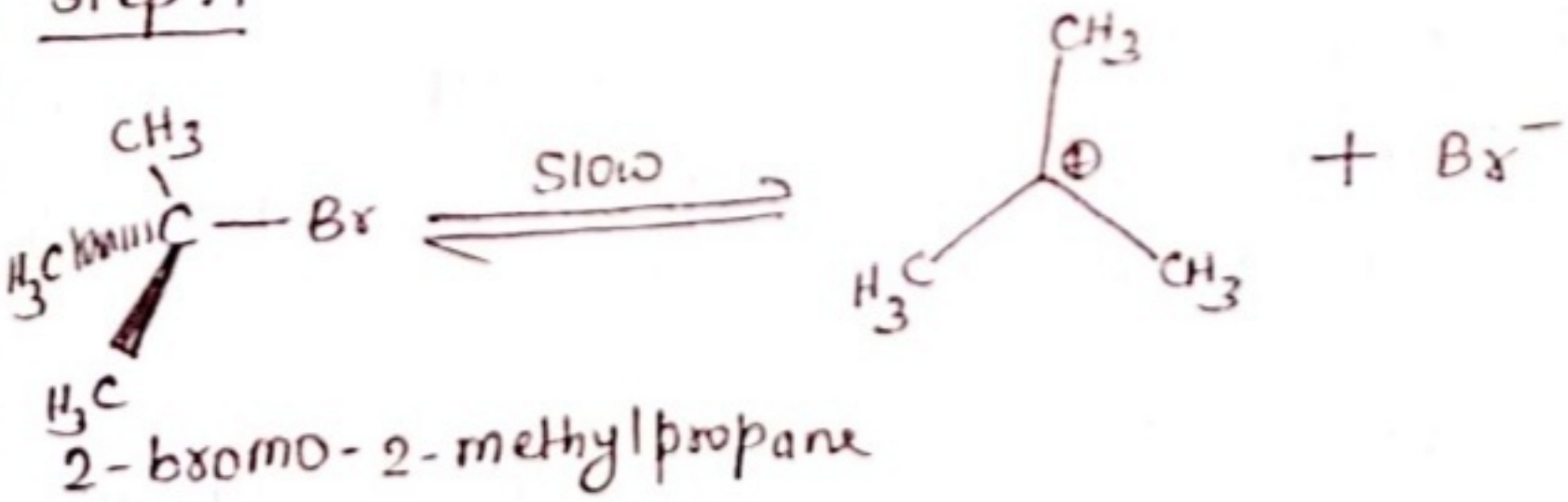
Substitution Nucleophilic Unimolecular SN1 Reaction

* SN1 reaction are generally carried out in polar protic solvents (like water, alcohol, acetic acid etc.)

$$(CH_3)_3CBr + OH^- \longrightarrow (CH_3)_3COH + Br^-$$

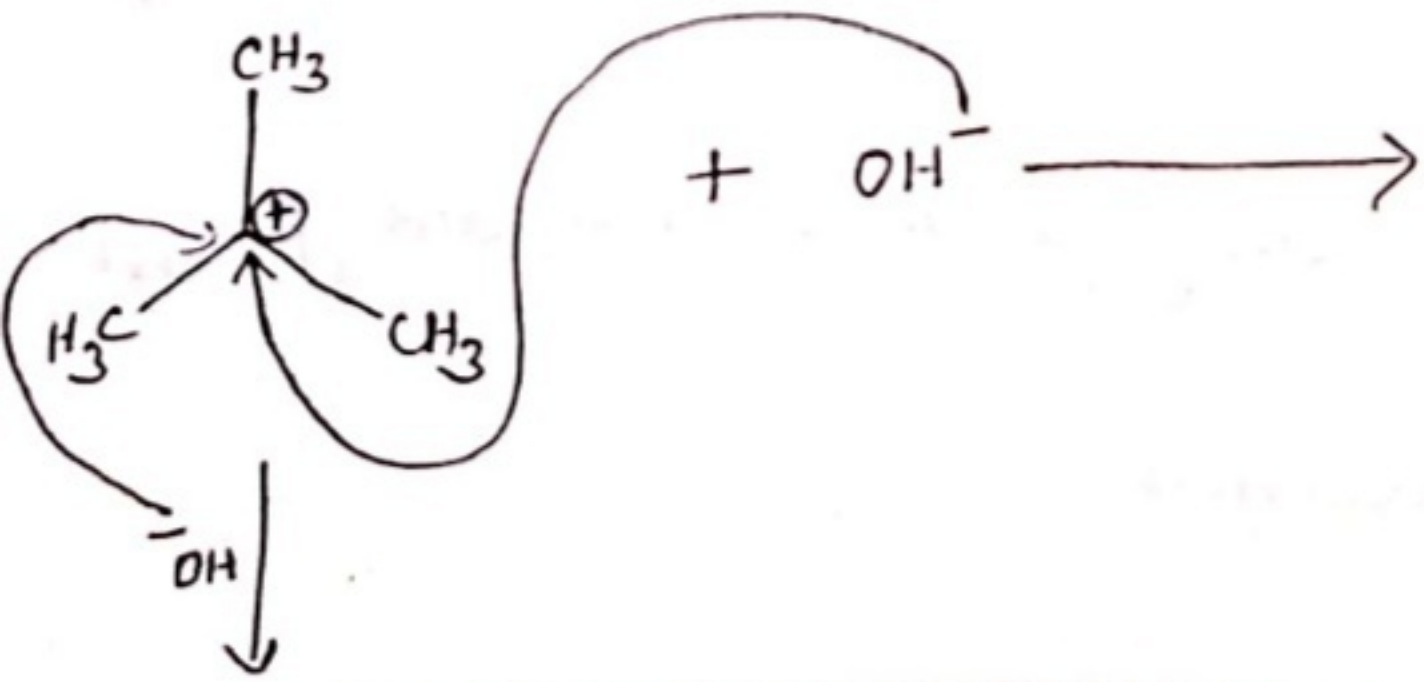
MECHANISM

Step : 1



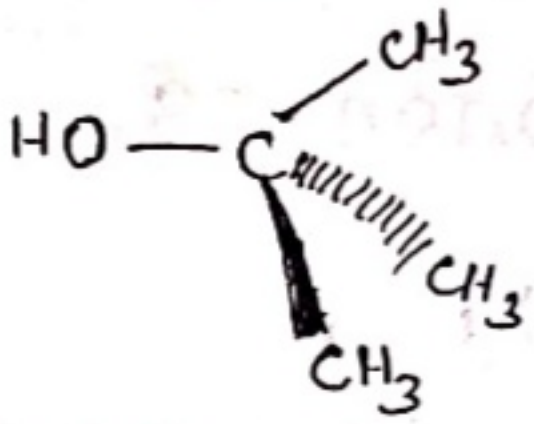
2-bromo-2-methylpropane

Step : 2



(–) 2-methylpropan-2-ol

2.



(+) 2-methyl propan-2-ol

Rate of reaction $r = K[(CH_3)_3CBr]$

Order = 1st order reaction

* S_N1 reaction occurs in two steps.

1st step is formation of carbocation (slow step)

2nd step is formation of product (fast step)

* Greater the stability of carbocation, greater will be its ease of formation from alkyl halide and faster will be the rate of reaction.

* In case of alkyl halides, 3° alkyl halides undergo S_N1 reaction very fast because of the high stability of 3° carbocation.

Formation of carbocation is basic criteria of S_N1 reaction.

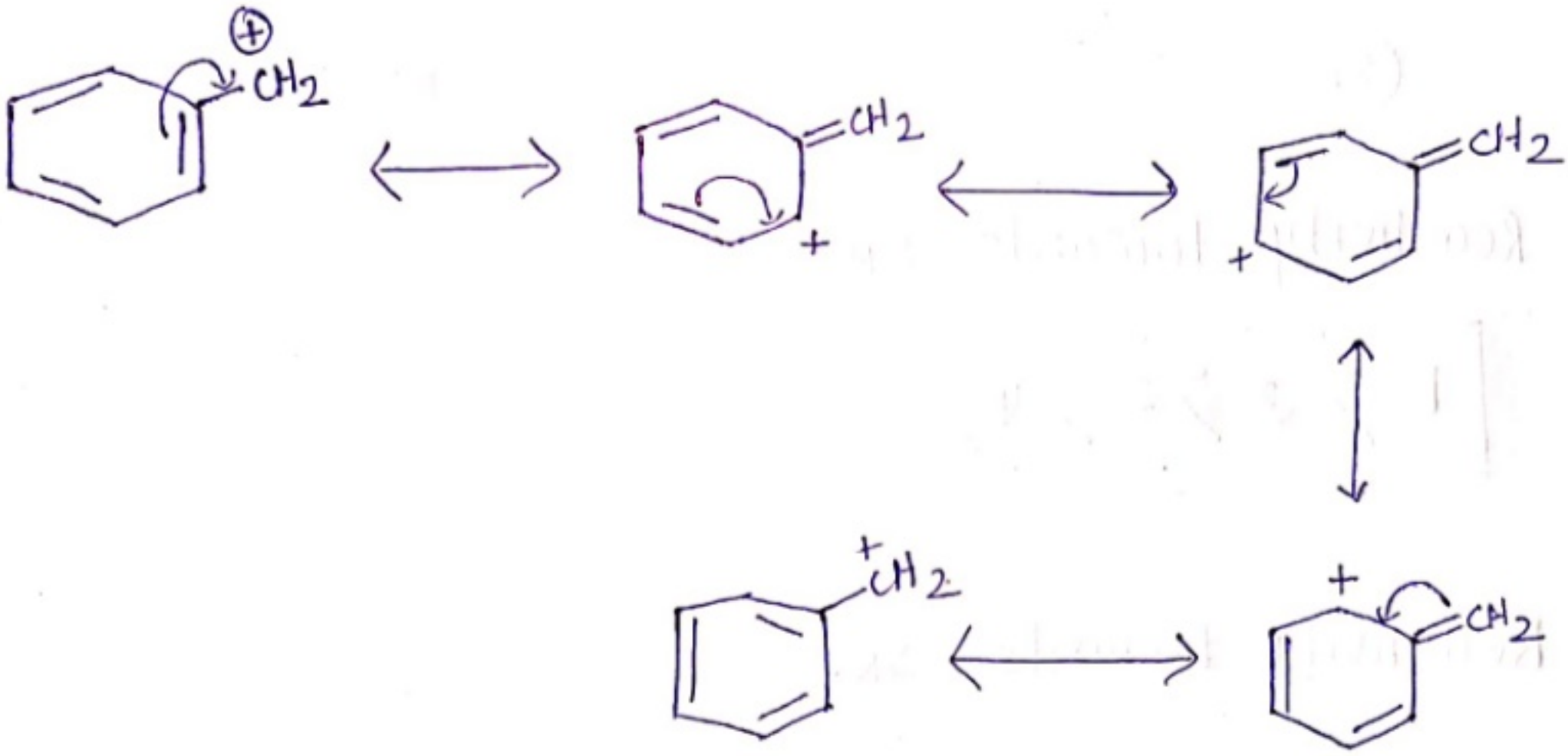
Racemisation of configuration occurs, during S_N1 reaction.

The order of reactivity for S_N1 reaction is, **3.**

$$3^\circ > 2^\circ > 1^\circ > CH_3X$$

* Allylic halide and benzylic halides show high reactivity towards the S_N1 reaction, because, Allylic carbocation and benzylic carbocation is resonance stabilised.

Allyl carbocation



For a given alkyl group, the reactivity of the halide. R-X follows the same order in both the mechanism.

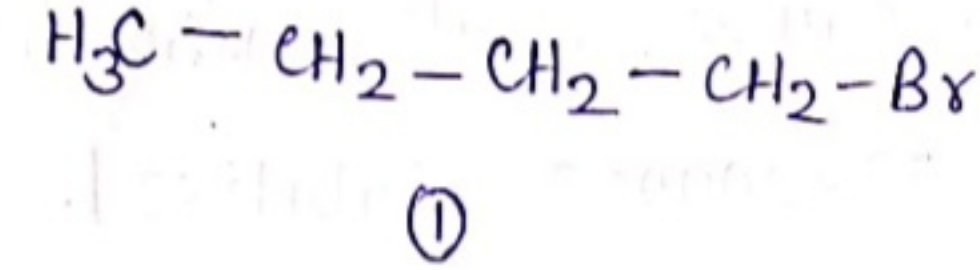
$$R-I > R-Br > R-Cl >> R-F$$

NCERT BOOK

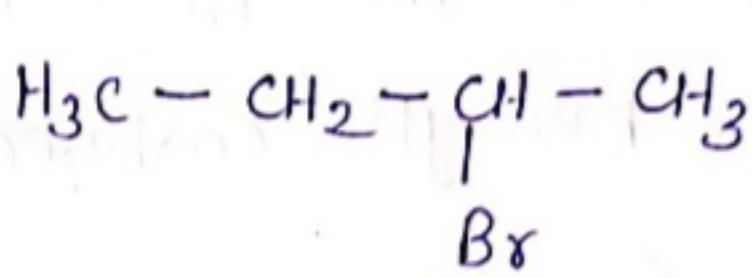
4.

Example 10.7

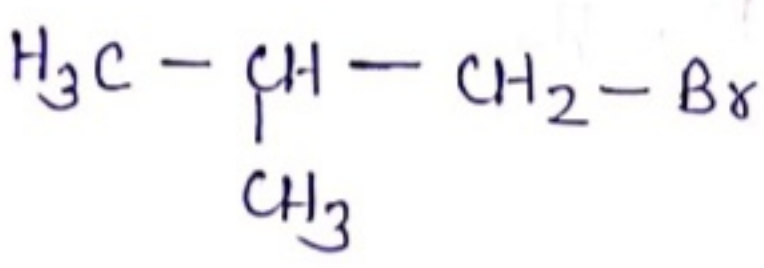
(i) The four isomeric bromobutanes are:--



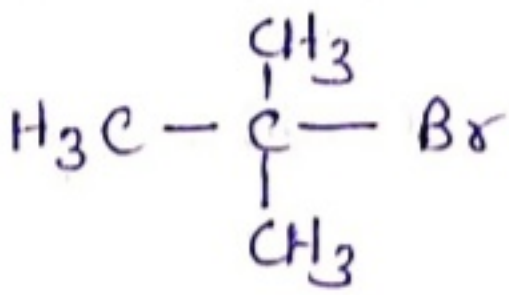
(1)



(2)



(3)



(4)

Reactivity towards S_N2

1 > 3 > 2 > 4

Reactivity towards S_N1

4 > 2 > 3 > 1

(ii) $C_6H_5-CH_2Br$ (1) $C_6H_5-CH(C_6H_5)Br$ (2), $C_6H_5-CH(CH_3)Br$ (3)

$C_6H_5-C(CH_3)(C_6H_5)Br$ (4)

Reactivity towards S_N2	Reactivity towards S_N1
1 > 3 > 2 > 4	4 > 2 > 3 > 1