CONCEPT MAP

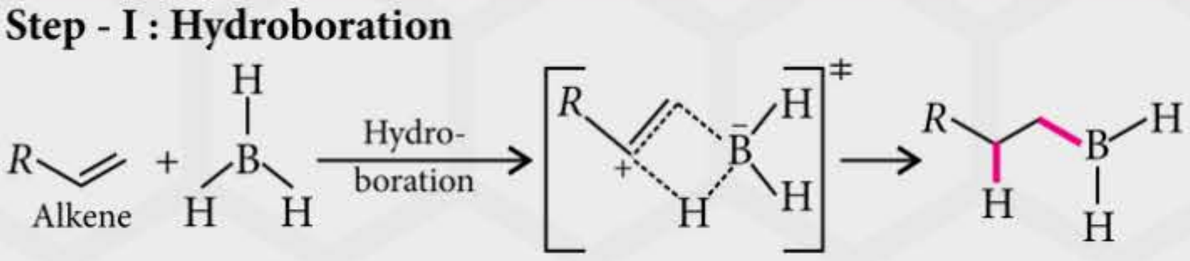
CLASS XI

Mechanistic Approach to Some Name Reactions

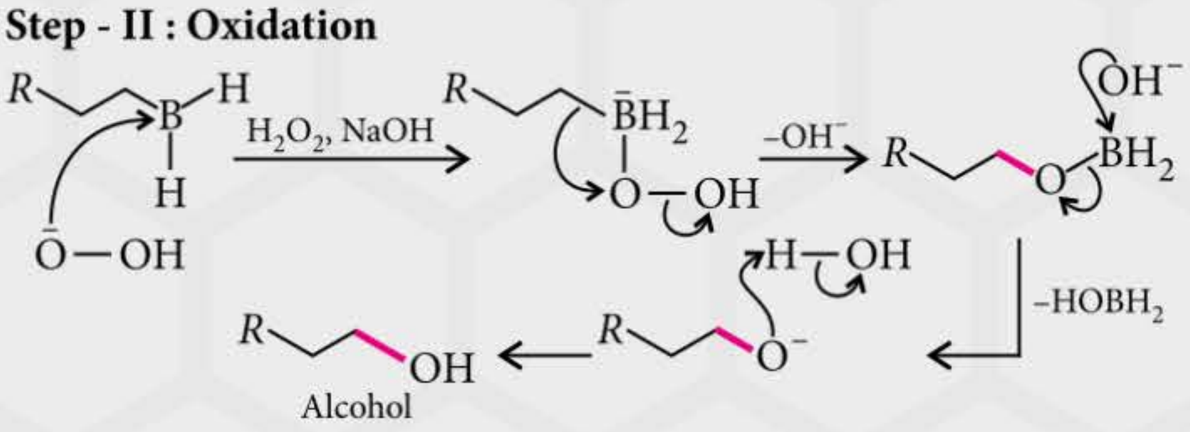
A mechanistic approach to any reaction classifies the reaction according to mechanism rather than by functional group. It explains the stereochemistry involved in a particular reaction, which can either be regioselective, stereoselective or stereospecific.

I Hydroboration – Oxidation Reaction

Step - I : Hydroboration



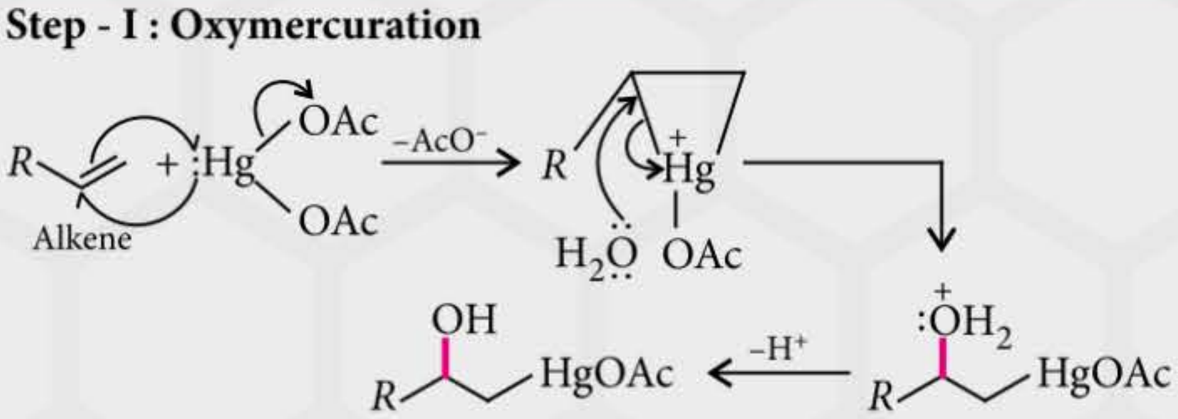
Step - II : Oxidation



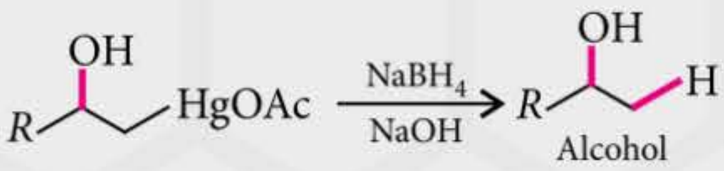
- Rate of formation of the C—B bond > Rate of formation of C—H bond.
- Formation of four-centred transition state.
- Hydroboration is regioselective.
- Hydroboration is a *syn*-addition across the alkene.
- In step-II, boron goes backward and forward between planar neutral structure and anionic tetrahedral structure.
- In step-II, cleavage of O—O single bond is the driving force.
- In step-I, new C—B bond and in step-II new C—O bond are formed.
- The net result of this reaction is addition of water across the double bond.

II Oxymercuration – Demercuration Reaction

Step - I : Oxymercuration



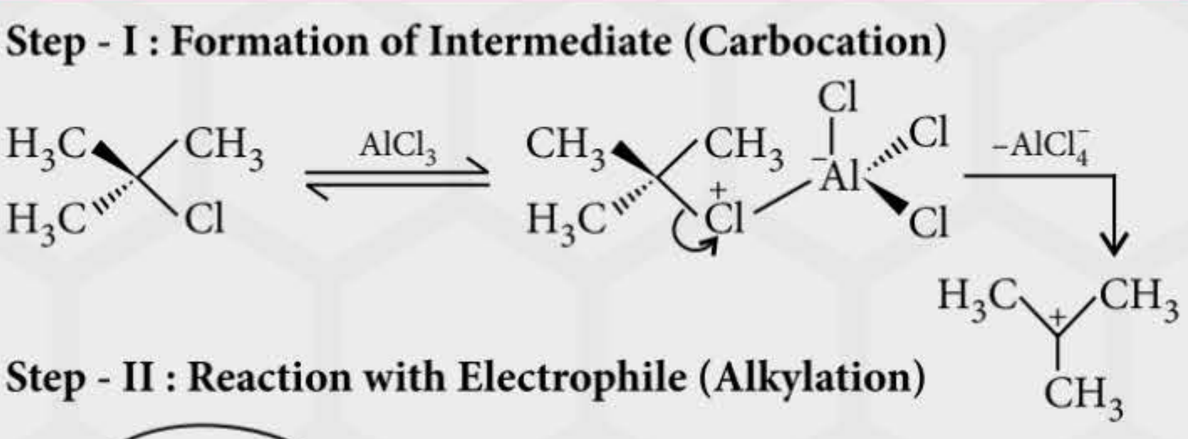
Step - II : Demercuration



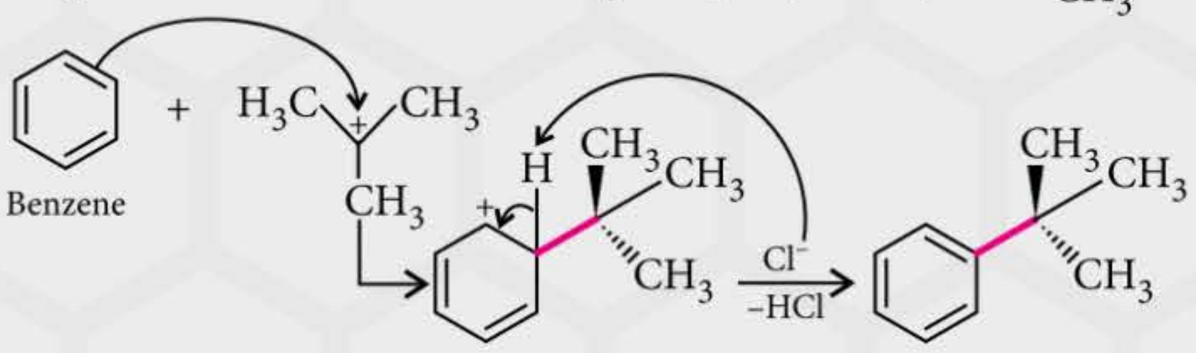
- In step-I, *i.e.*, oxymercuration, —OH and Hg^{2+} are added across the alkene.
- Oxymercuration is regioselective and stereospecific.
- Stereochemically, oxymercuration is an *anti*-addition.
- In step-I, water attacks at the more substituted end of the mercurinium ion (transition state).
- Driving force for demercuration is a weak C—Hg bond.
- To replace Hg with H, $NaBH_4$, a reducing agent is used.
- Oxymercuration-reduction is a popular laboratory technique with Markovnikov selectivity while avoiding carbocation intermediate and thus, rearrangement which can lead to complex product mixture.

III Friedel–Crafts Alkylation Reaction

Step - I : Formation of Intermediate (Carbocation)



Step - II : Reaction with Electrophile (Alkylation)



- This reaction follows S_N1 pathway.
- Species having capability to form carbocation are used.
- Carbocation can be generated by
  - protonation of an alkene.
  - the acid-catalysed decomposition of a tertiary alcohol.
  - Lewis acid catalysed decomposition of a *tert*-alkyl chloride.
- Carbocation rearrangement (to more stable carbocation) takes place whenever possible.
- Friedel—Crafts alkylation with alkyl halides proceeds via a carbocation and chiral alkyl halides are expected to give racemic arene products. The extent of racemisation depends on the Lewis acid and the reaction conditions.