Conjugated Diene

Organic Chemistry

Properties

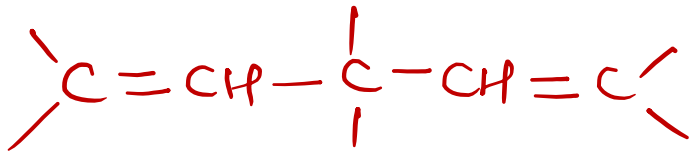
Methods of Preparation

Chemical Reactions

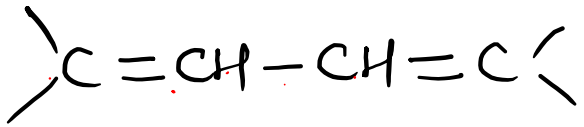
B.Pharm. | POC-I | U 2 | L18

Conjugated Dienes Organic Chemistry

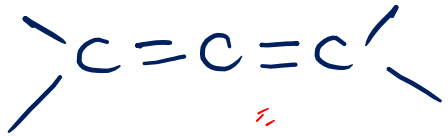
- Alkenes congaing two C=C in alternate is called diene and alkadienes



Non-Conjugated dienes



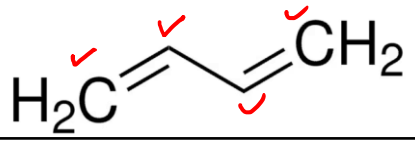
Conjugated dienes "1,3-butadiene"



Cumulated dienes

Conjugated Dienes Organic Chemistry

1,3-Butadiene

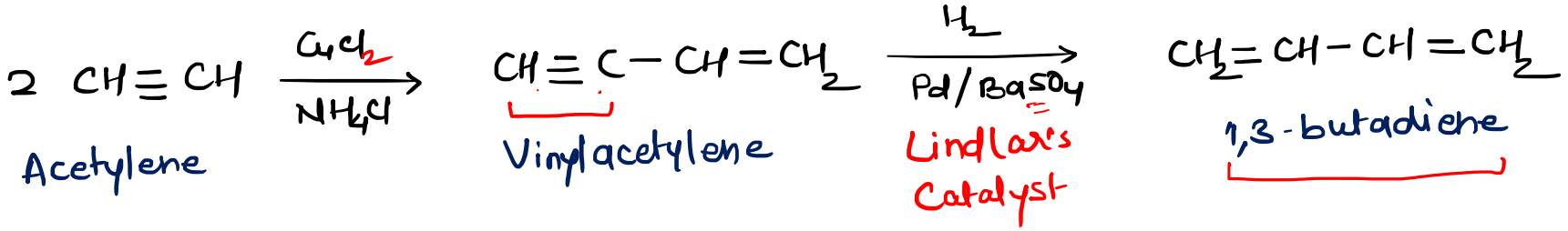


All C-atm – sp^2 hyb.

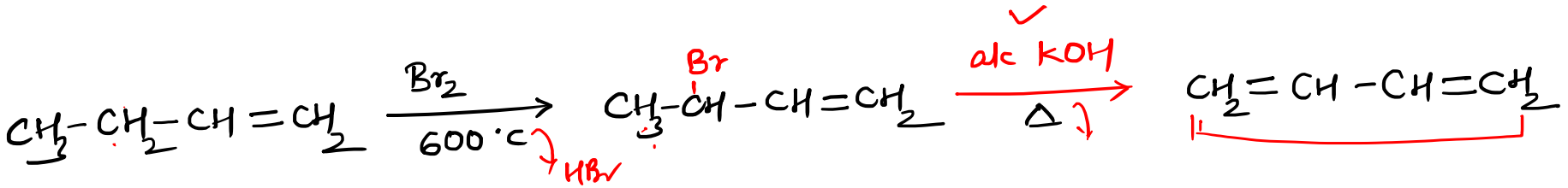
Chemical formula	C_4H_6 $CH_2=CH-CH=CH_2$
Molar mass	54.0916 g/mol
Appearance	Colourless gas or refrigerated liquid
Odor	Mildly aromatic or gasoline-like
Density	•0.6149 g/cm^3 at 25 °C, p>1 atm •0.64 g/cm^3 at −6 °C, liquid
Melting point	−108.91 °C (−164.04 °F; 164.24 K)
Boiling point	−4.41 °C (24.06 °F; 268.74 K)
Solubility in water	1.3 g/L at 5 °C, 735 mg/L at 20 °C
Solubility	•Very soluble in acetone •Soluble in ether, ethanol
Uses	•Most butadiene is used to make synthetic rubbers for the manufacture of tyres and components of many consumer items.

Preparation Methods

1. From Acetylene



2. From 1-Butene

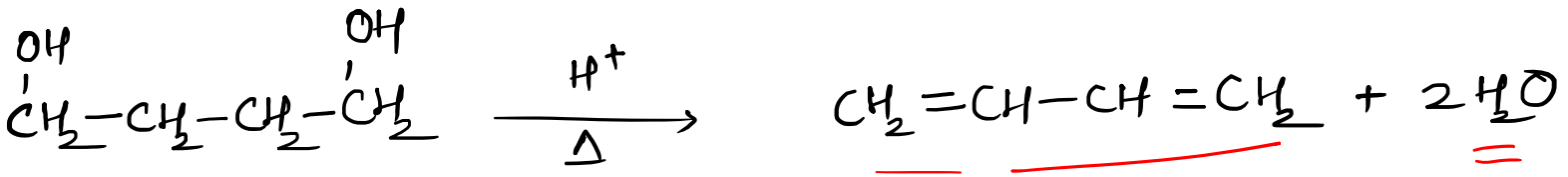


i) Allyl Substitution

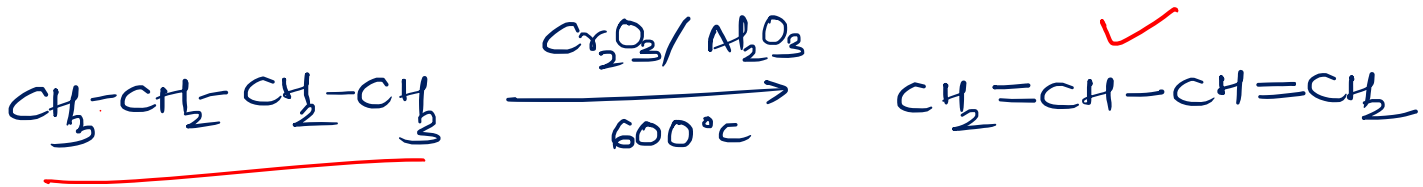
ii) Dehydrohalogenation

Preparation Methods

3. From 1,4-btanediol: by acid catalyzed dehydration

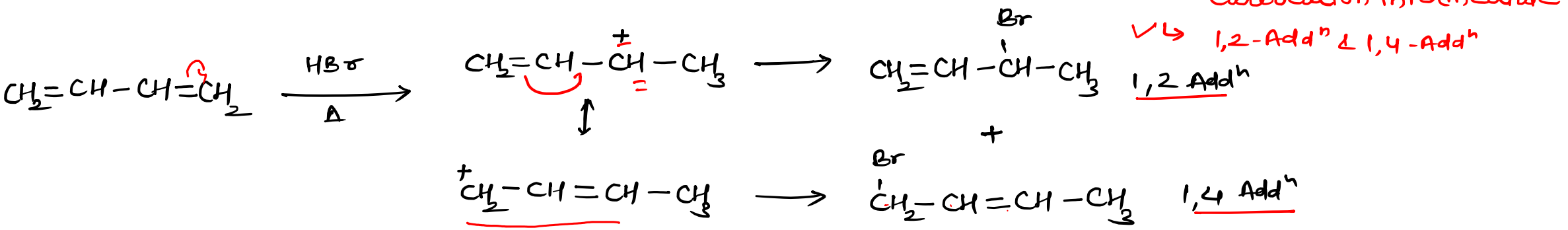


4. From n-Butane: by catalytic dehydrogenation

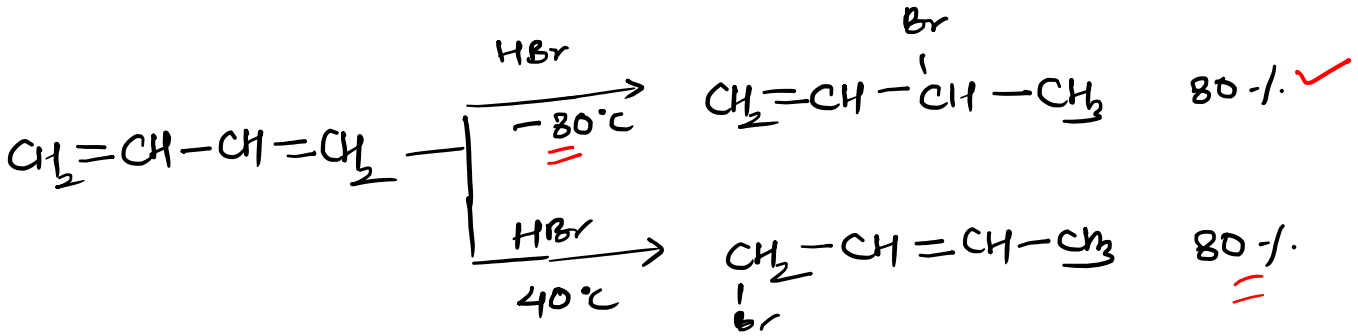


Chemical Reaction

1. Hydrohalogenation

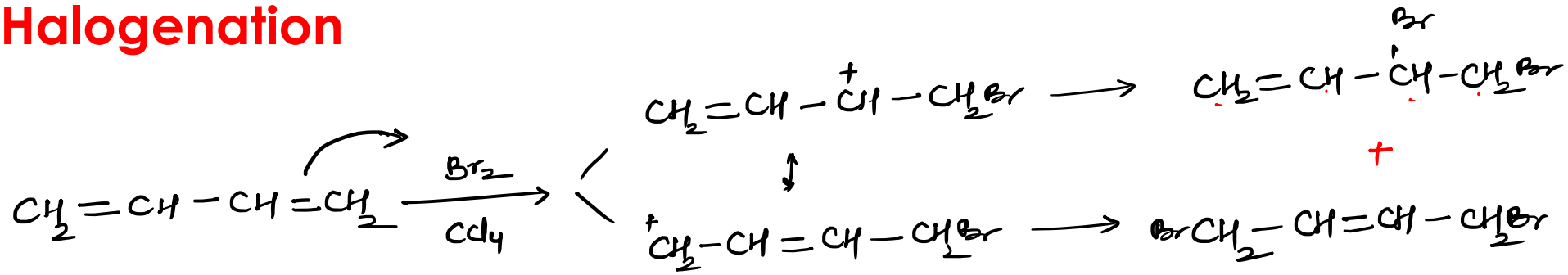


↳ Addⁿ of HX
↳ Carbocation intermediate
↳ 1,2-Addⁿ & 1,4-Addⁿ

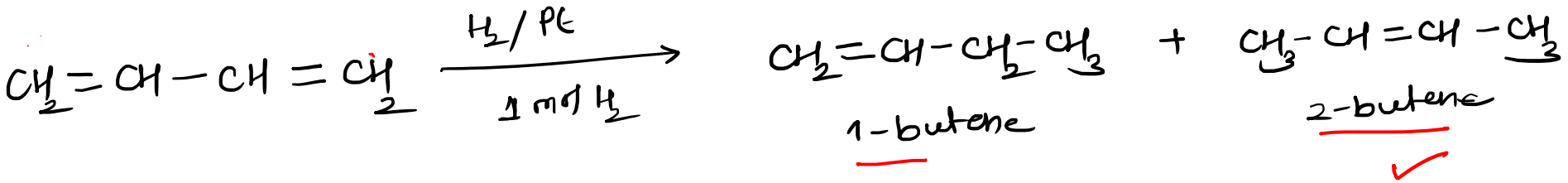


Chemical Reaction

2. Halogenation

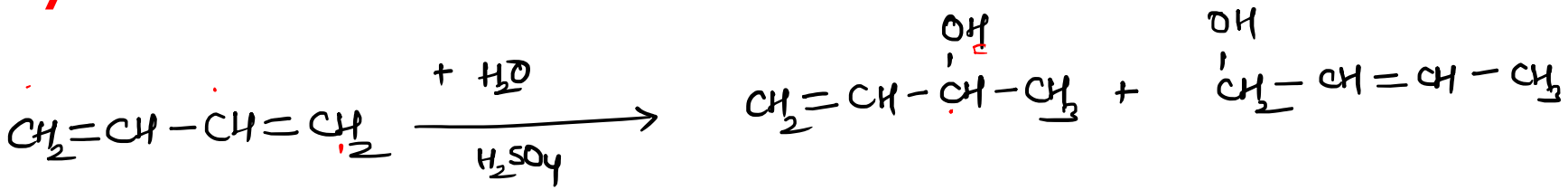


3. Hydrogenation

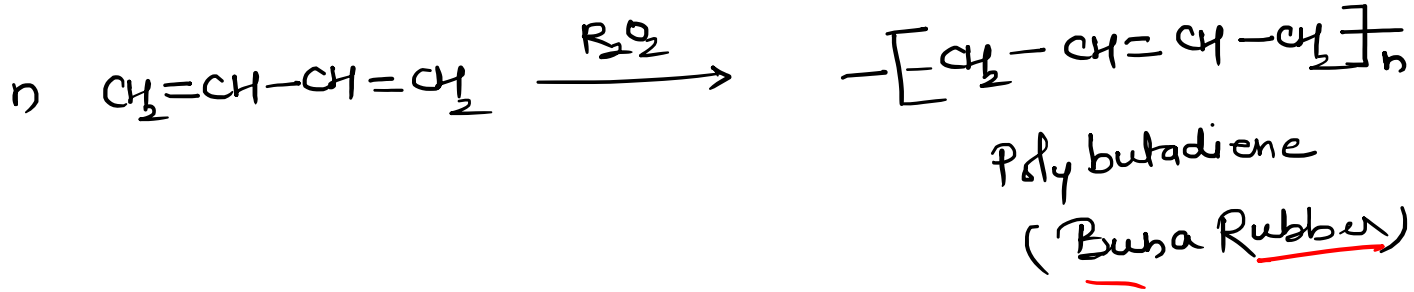


Chemical Reaction

4. Hydration



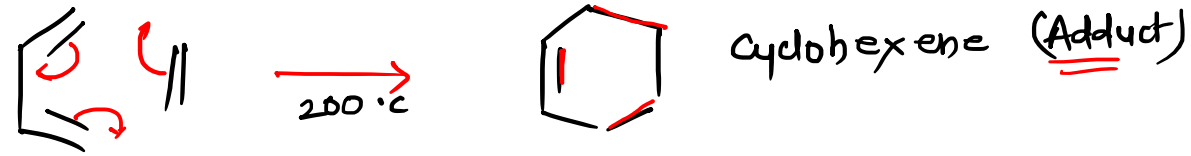
5. Polymerization

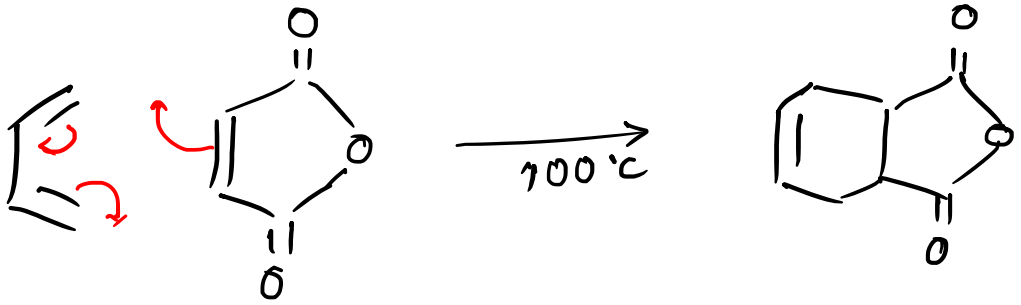


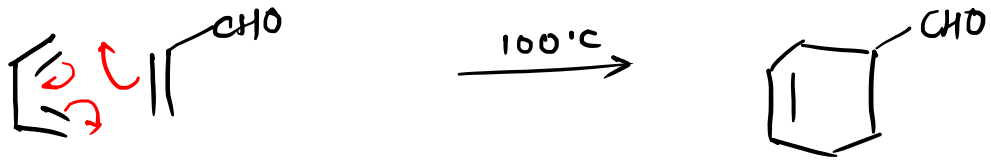
Chemical Reaction

IMP

6. Diels-Alder Reaction- Reaction of conjugation dienes with alkene or alkyne (Dinophile) give to adduct product. Preferred for synthesis in six membered ring







Conjugated Diene

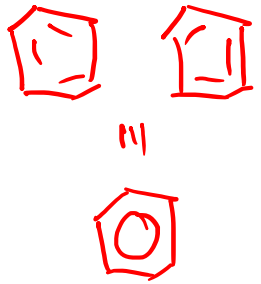
Organic Chemistry

Stability of Conjugated diene

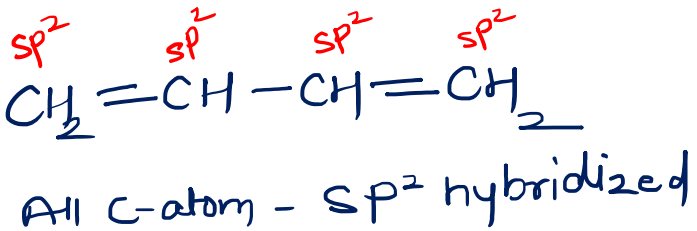
B.Pharm. | POC-I | U 2 | L18

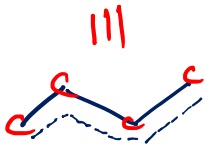
Stability of Conjugated Diene (Alka diene)

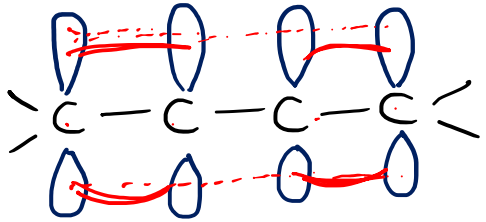
- ✓ Conjugated dienes are more stable than non-conjugated dienes



- ✓ **Resonance:** delocalization of pi electron clouds on Carbon atoms
- ✓ E.g. In conjugated 1,3 Butadiene, all four pi electrons are delocalized over all four Carbon atoms. The delocalization of pi electrons makes the compound more stable.







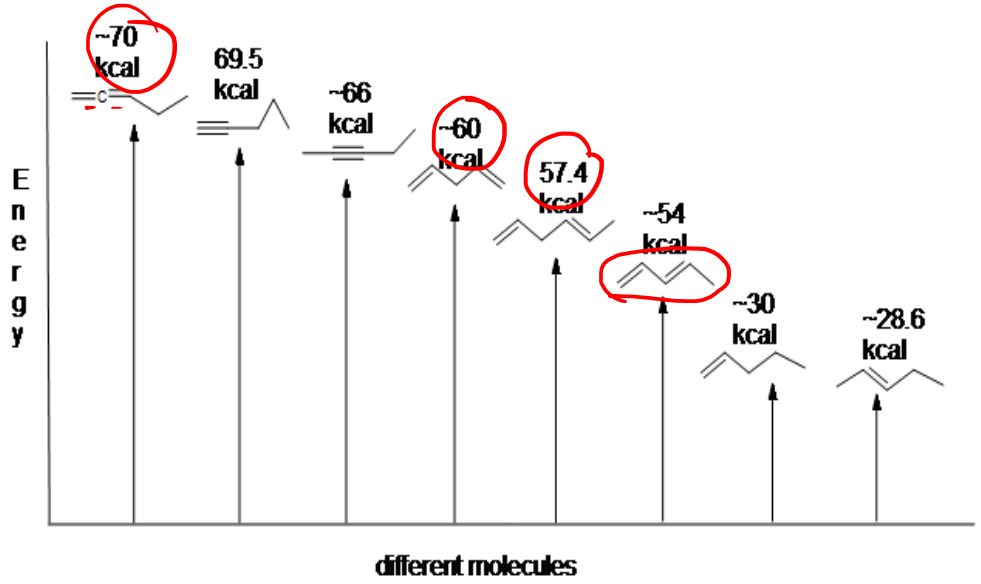
Stability of Conjugated Diene (Alka diene)

✓ **Hydrogenation Energy-** Higher energy – Less Stable

Conjugated diene  54 kcal

Isolated non-conjugated diene  60 kcal

Cumulated diene  70 kcal



Conjugated Diene

Organic Chemistry

Allylic Rearrangement

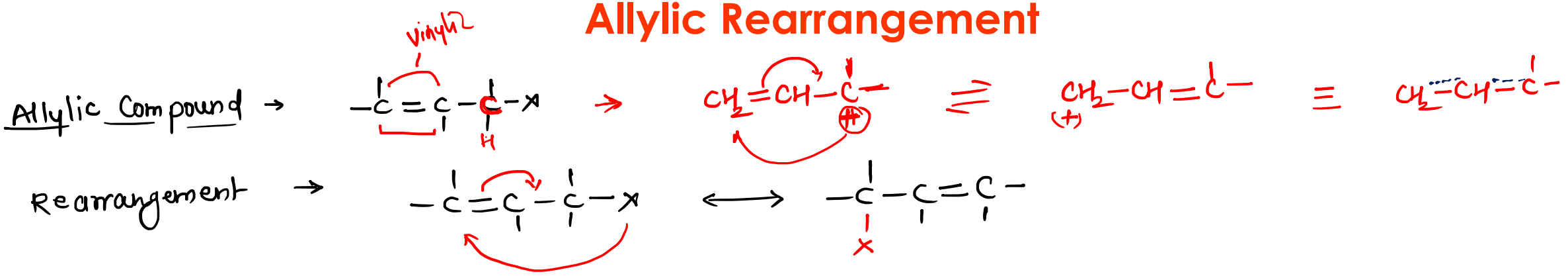
E+ Addition

Free Radical Addition

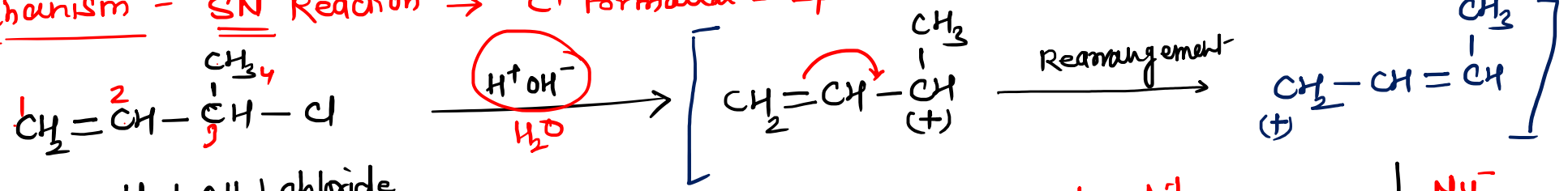
B.Pharm. | POC-I | U 2 | L19

Rearrangement of allylic compound

Allylic Rearrangement



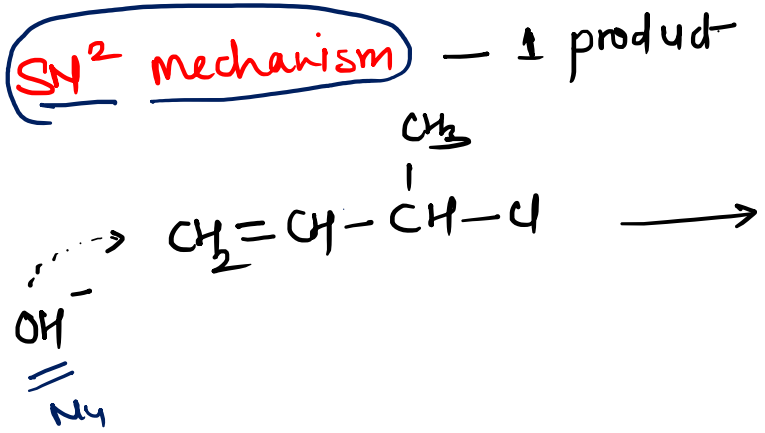
Mechanism - SN' Reaction → C^+ formation - 2 product possibility

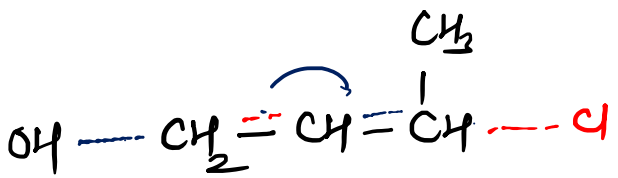


Nu^- : $C_2H_5O^-$
OH^-

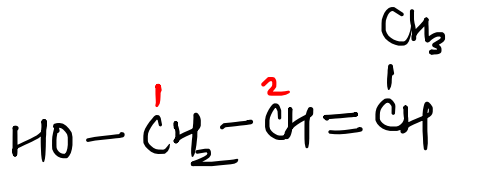
Allylic Rearrangement

S_N2 mechanism — 1 product





Transition state



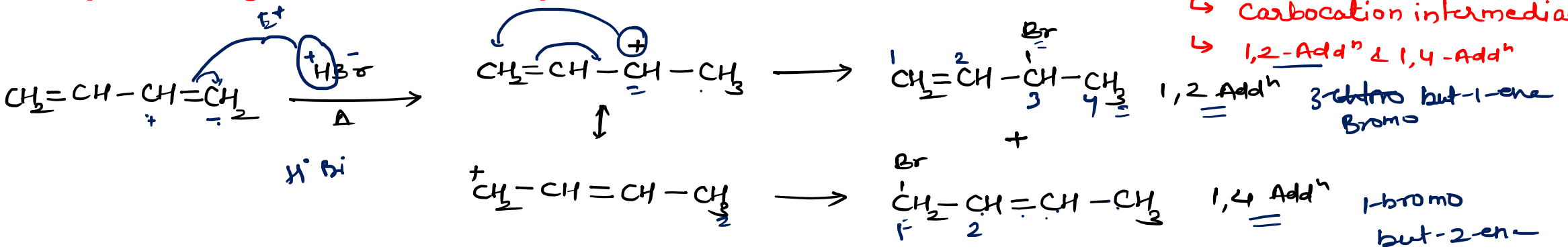
but-2-ene-1-ol

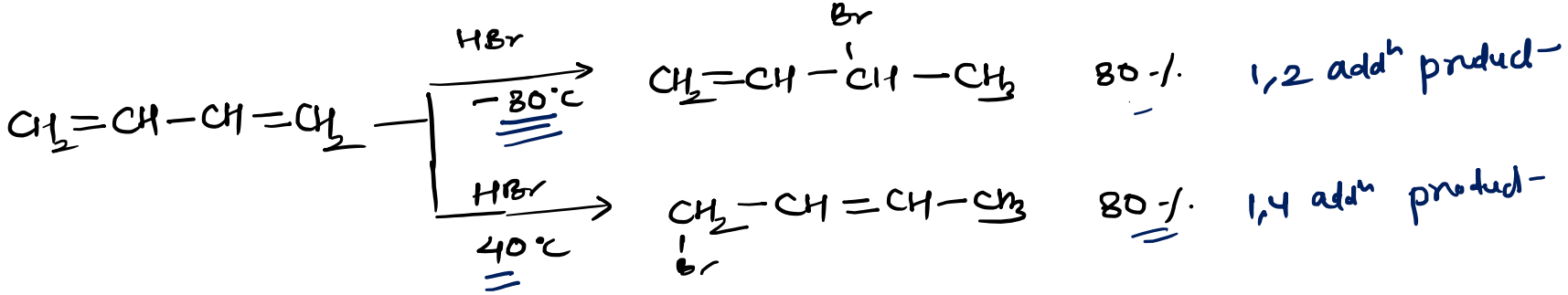
1 product

Electrophilic Addition

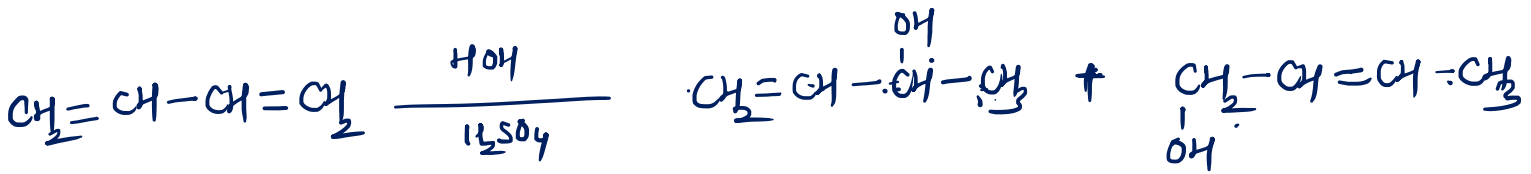
1. Hydrohalogenation- Electrophilic Addition

↳ Addⁿ of HX
↳ Carbocation intermediate
↳ 1,2-Addⁿ & 1,4-Addⁿ



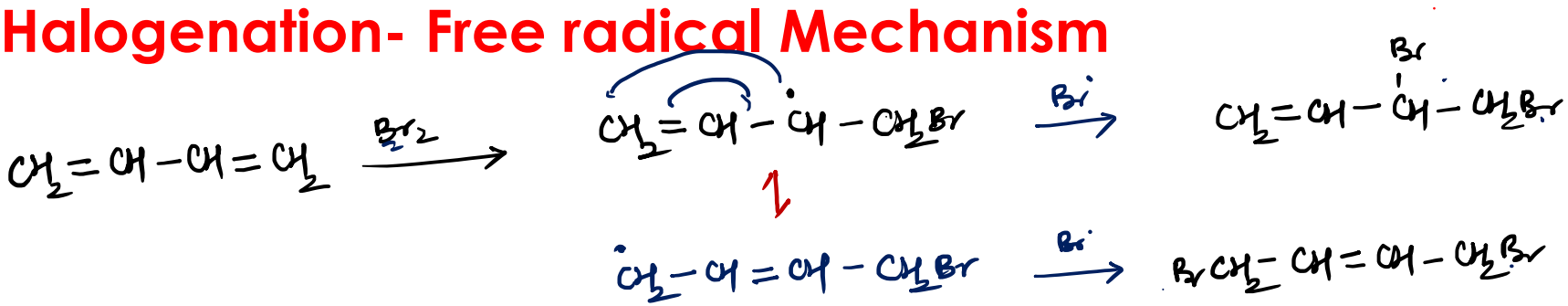


2. Hydration (Addition of water)- E+ Addition



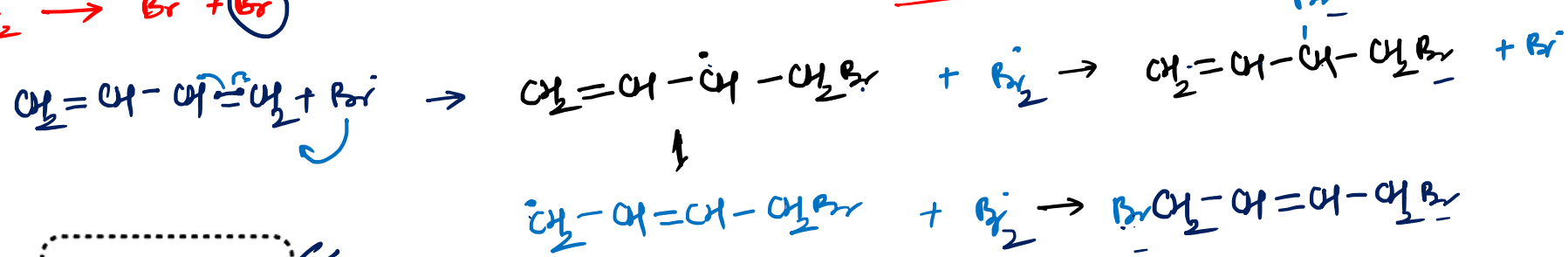
Free Radical Addition Reaction

2. Halogenation- Free radical Mechanism

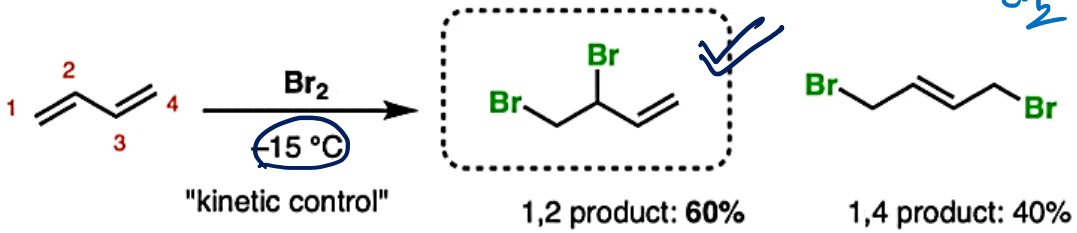


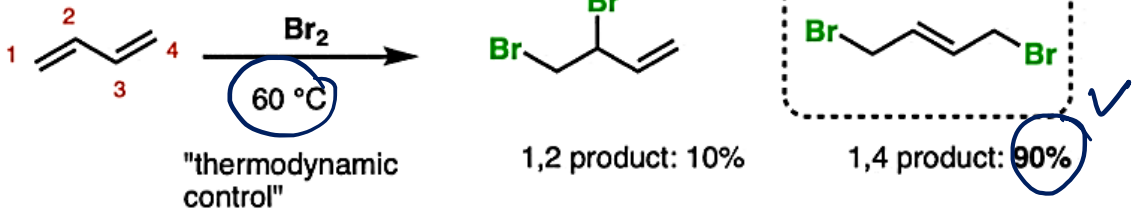
↳ 1) Initiation $Br_2 \rightarrow Br^{\cdot} + Br^{\cdot}$

↳ 2) propogation –



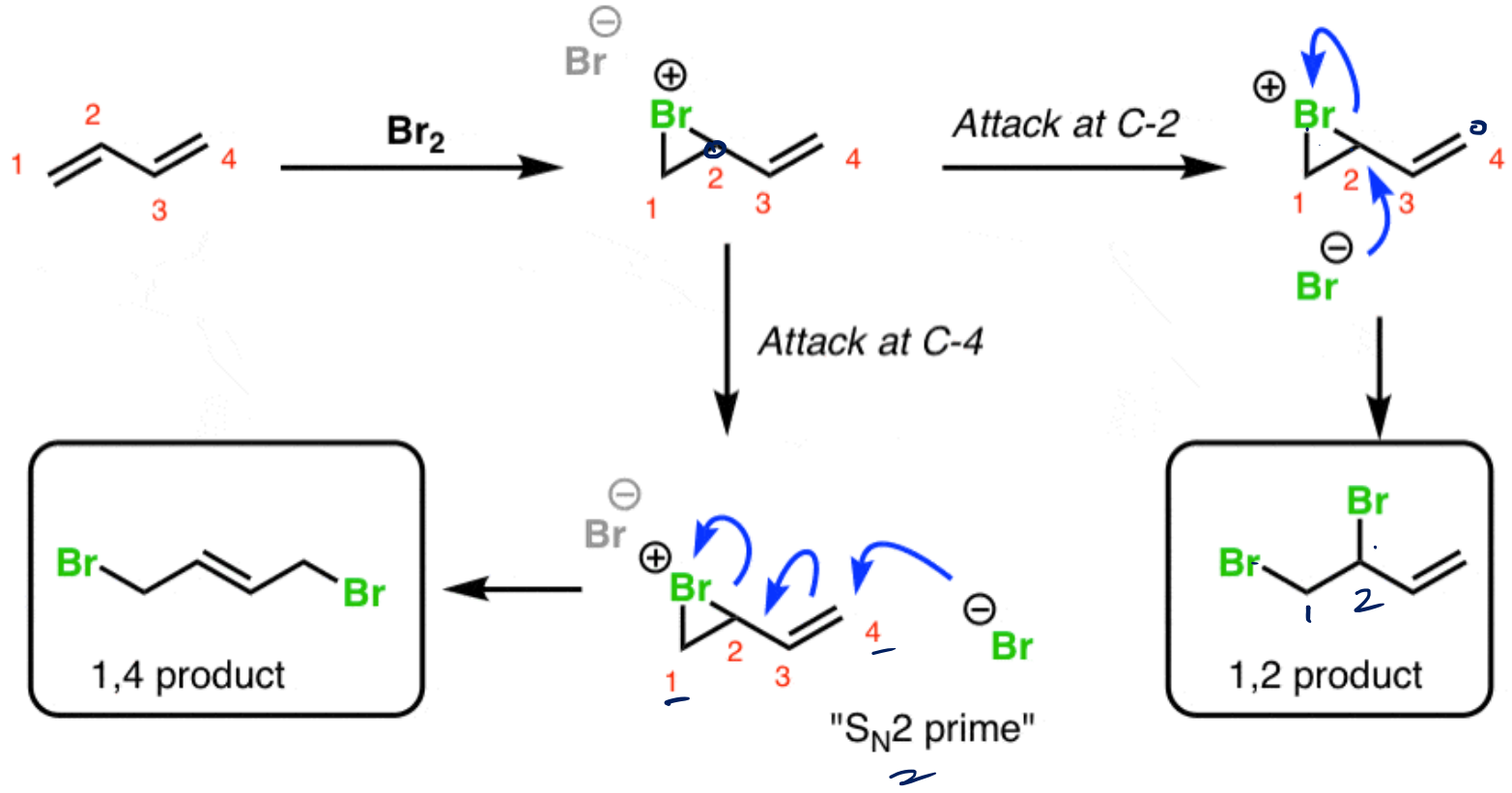
3) termination





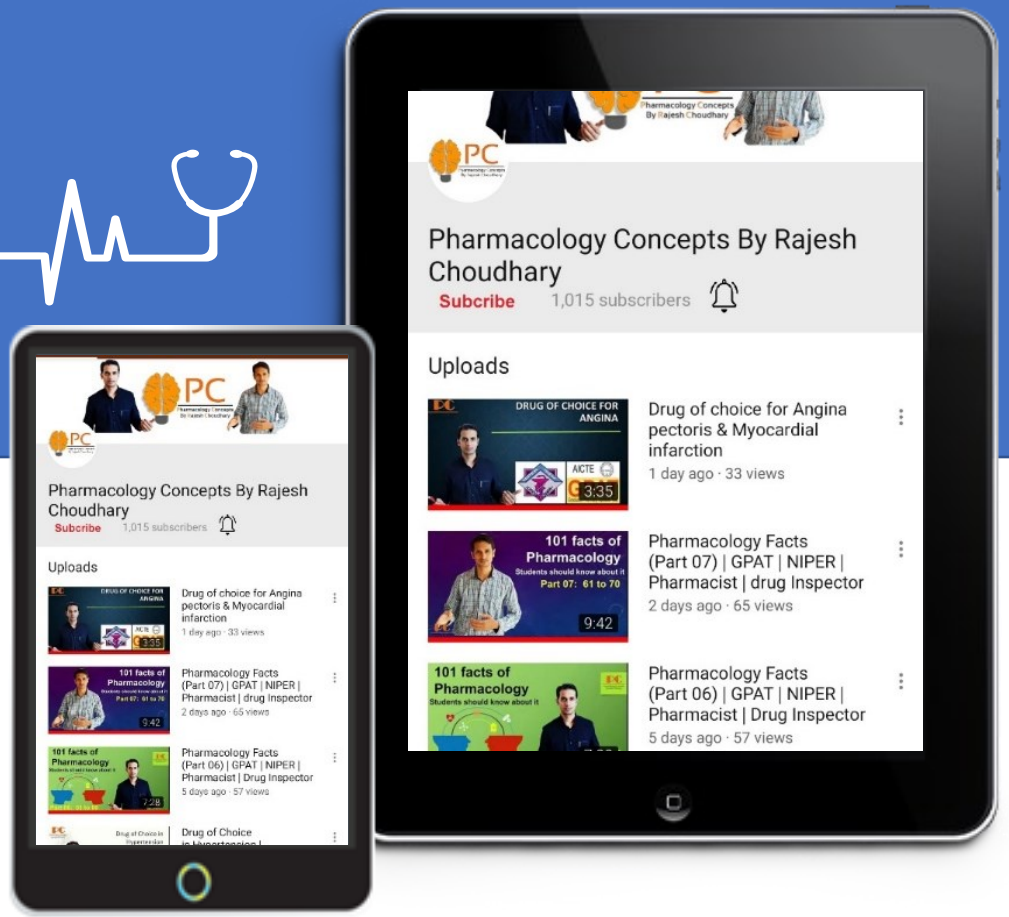
Free Radical Addition Reaction

2. Halogenation



PC
Pharmacology Concepts
By Rajesh Choudhary

Thanks for Watching



Subscribe my YouTube Channel