Board

Alkyl Halide

- Prep^n : ✓
- Properties :
  - Physical
  - Chemical : ✓
    - Fact
    - Fmdg

Mechanism :
- Short Cut ✓
- Detailed Mechanism : ✓

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1). from Alkane :

Photohalogenation:

$CH_4 + Cl_2 \xrightarrow[\text{or heat (dark)}]{\text{Light } (h\nu)} CH_3R + HCl$

R-X

$R-H + X_2 \xrightarrow{h\nu} R-X + H-X$

X_2 : F_2, Cl_2, Br_2, I_2

Fluorination : explosive (never done)

Chlorination : → not used in Lab (Synthesis purpose)
→ commercial production

Bromination : → in Lab ✓
→ commercial ✗✗ (yield is very poor)

$CH_4 \rightarrow CH_3Cl \rightarrow CH_2Cl_2 \rightarrow CHCl_3 \rightarrow CCl_4$

Iodination : ✗ ✗'s not done because iodination is reversible. as HI gets converted into I_2 and it converts R-I back into R-H

$R-H + I_2 \rightleftharpoons R-I + HI$

$2HI^{-1} \longrightarrow I_2^{\circ} + 2H$

$2H + R-I \longrightarrow R-H + I_2$

So do iodination. HNO_3 or HIO_3 is added to remove HI

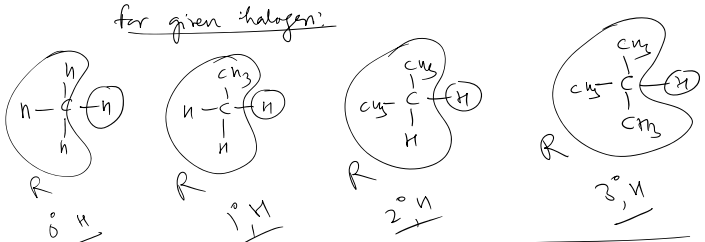
$HI + HIO_3 \longrightarrow I_2 + H_2O$

$R-H + X_2 \xrightarrow{h\nu} R-X + H-X$

for given alkane

rate => $F_2 >>> Cl_2 > Br_2 > I_2$ ✗

for given halogen:



0° H, 1° H, 2° H, 3° H

Rate => $3^{\circ} > 2^{\circ} > 1^{\circ}$

Mechanism:

→ free Radical Mechanism.

$R-H + X_2 \xrightarrow{h\nu} R-X + H-X$

Initiation:

$X_2 \xrightarrow{h\nu} 2X^{\circ}$

Propagation:

$X^{\circ} + R-H \longrightarrow R^{\circ} + H-X$

→ formed in Homolytic cleavage of bond

$Cl-Cl \rightarrow Cl^{\circ} \quad Cl^{\circ}$

$H_3C-H \rightarrow H_3C^{\circ} + H^{\circ}$

Chemical unit or species

Propagation: $X^\cdot + R{-}H \longrightarrow R^\cdot + H{-}X$

alkyl free radical

RDS (Rate determining step) is the slowest step rxn in any mechanism & it decides rate of overall rxn.

chemical unit or species → having odd no. electron → Paramagnetic

$F^\cdot + R{-}H \longrightarrow R^\cdot + HF$

$Br^\cdot + R{-}H \longrightarrow R^\cdot + HBr$

90p/sec → 10p/sec (slowest, RDS) → 40p/sec → 10p/sec → 2/sec.

$F^\cdot$ Unstable

$Br^\cdot$

$F + F \rightarrow F_2$

$Br + Br \rightarrow Br_2$

reacting: $F^\cdot >> Cl^\cdot > Br^\cdot > I^\cdot$

$F_2 >> Cl_2 > Br_2 > I_2$

$1^\circ < 2^\circ < 3^\circ$ => stability for free Radical (due to $+I$ effect)

(Rate of photohalogenation) $\propto$ stability of $R^\cdot$ $\rightarrow F_2 > Cl_2 > Br_2 > I_2$

$\propto \frac{1}{\text{stability of } X^\cdot}$ $\rightarrow 3^\circ > 2^\circ > 1^\circ$

$2^\circ > 1^\circ$