Programme: Bachelor of Science

Subject: Chemistry

Semester: I

Course Code: CHC 101

Course Title: Inorganic and Organic Chemistry Section B

Title of the unit: Alkanes Alkenes and Alkynes

Module Name: Dehydrohalogenation of Alkyl Halides

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OUTLINE

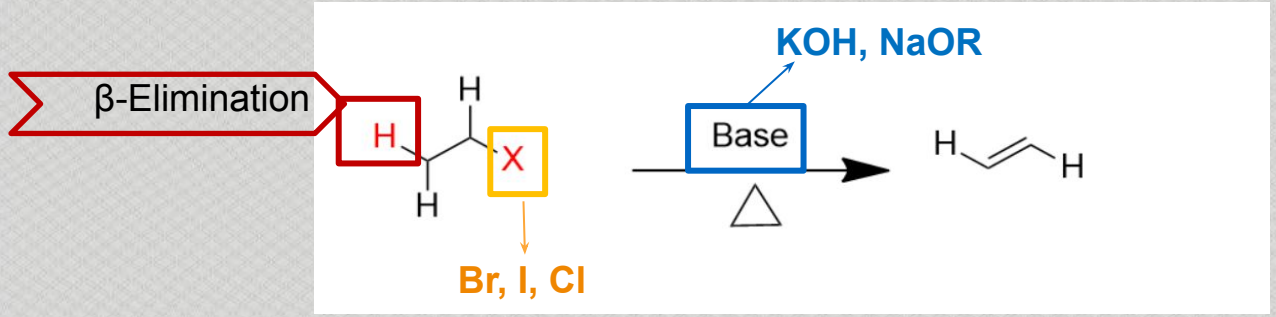
- Dehydrohalogenation of Alkyl halides
- Saytzeff's Rule
- Mechanistic pathway for dehydrohalogenation (E1/E2)

LEARNING OUTCOMES

- Understand dehydrohalogenation of Alkyl halides
- Apply Saytzeff's Rule
- Understand the mechanistic pathway for dehydrohalogenation (E1/E2)

DEHYDROHALOGENATION OF ALKYL HALIDES

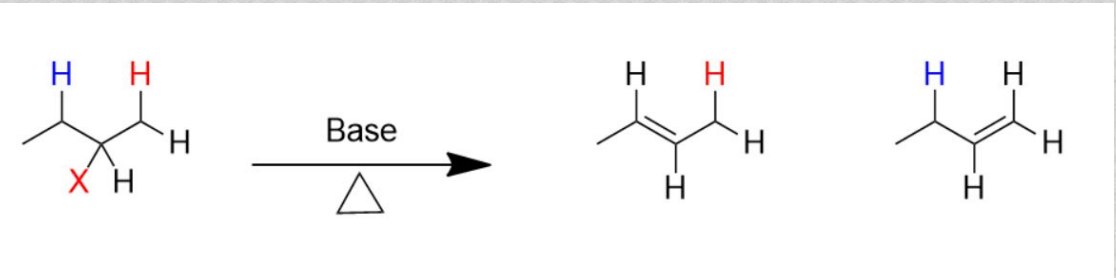
*Alkenes can be obtained from **alkyl halides** by the **loss of hydrogen halide** in the presence of base.*



Alkyl halides: 3º 2º 1º

DEHYDROHALOGENATION OF ALKYL HALIDES

Unsymmetrical alkenes



Major product explained by Saytzeff's rule

DEHYDROHALOGENATION OF ALKYL HALIDES

Saytzeff's Rule

Alkene is obtained when a proton is removed from the β-carbon that is bonded to the fewest number of hydrogen atoms.

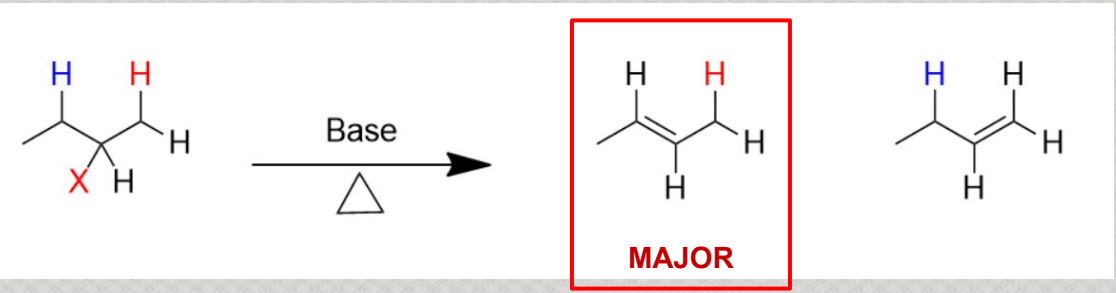
$$CH_2 = CHR < RCH = CHR < R_2C = CHR < R_2C = CR_2$$

Mono < di < Tri < Tetra

- *The **most substituted product** would be the most stable and most **preferred one**.*

DEHYDROHALOGENATION OF ALKYL HALIDES

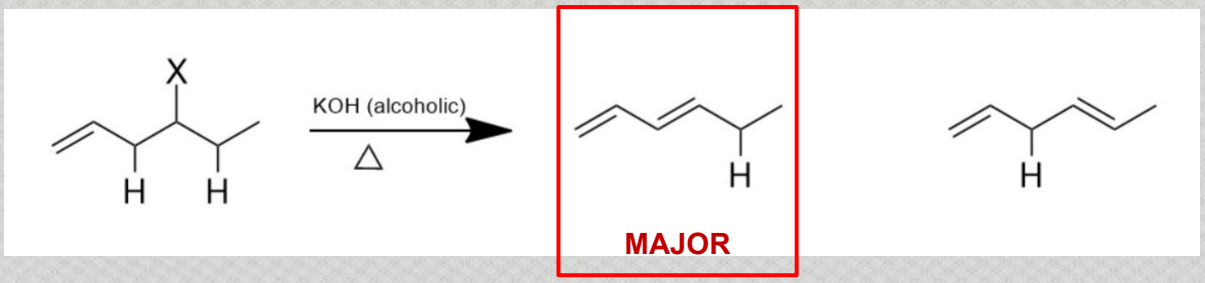
Unsymmetrical alkenes



*Thus the reaction is **regioselective.***

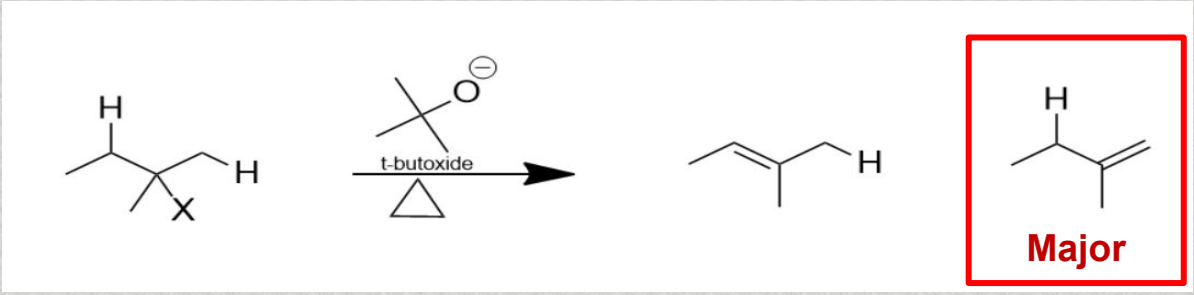
DEHYDROHALOGENATION OF ALKYL HALIDES

Conjugated Alkenes preferred

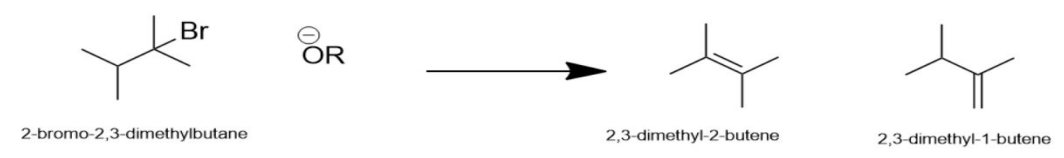


DEHYDROHALOGENATION OF ALKYL HALIDES

Influence of Steric hindrance



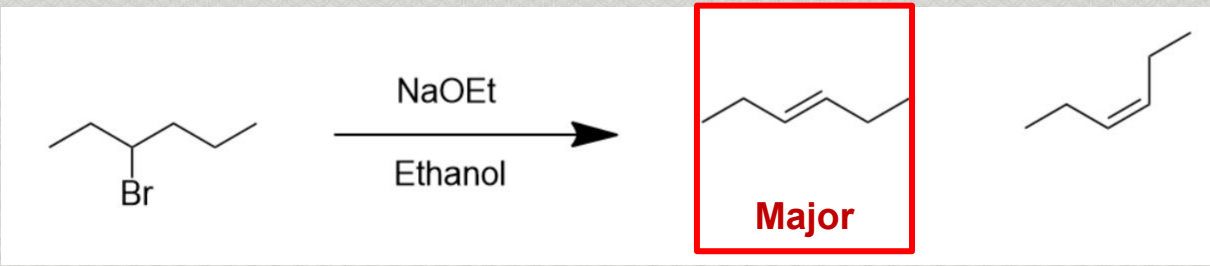
Effect of steric properties of base on the distribution of product



Base	More substituted product	Less substituted product
$CH_3CH_2O^-$	79%	21%
$CH_3CH_2C(CH_3)_2O^-$	27%	73%
$CH_3CH_2C(CH_3)(CH_2CH_3)O^-$	19%	81%
$(CH_3CH_2)_3CO^-$	8%	92%

DEHYDROHALOGENATION OF ALKYL HALIDES

Stereoselectivity



3-bromobutane

trans-3-hexene

Cis-3-hexene

DEHYDROHALOGENATION OF ALKYL HALIDES

MECHANISM

E1

E2

The E2 mechanism

Key Points:

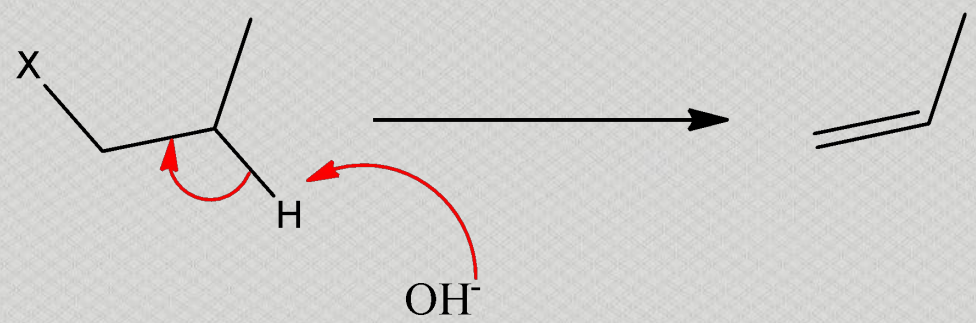
- Rate depends on the alkyl halide as well as base bimolecular.
- 2nd order kinetics
- Rate depends on the abstraction of proton and cleavage of C-X bond.

Order of reactivity of different halogens

Cl > Br > I

Concerted mechanism 1 step

The E2 mechanism



The E1 mechanism

- Some 2º and 3º alkyl halides elimination in a solution of low base concentration.

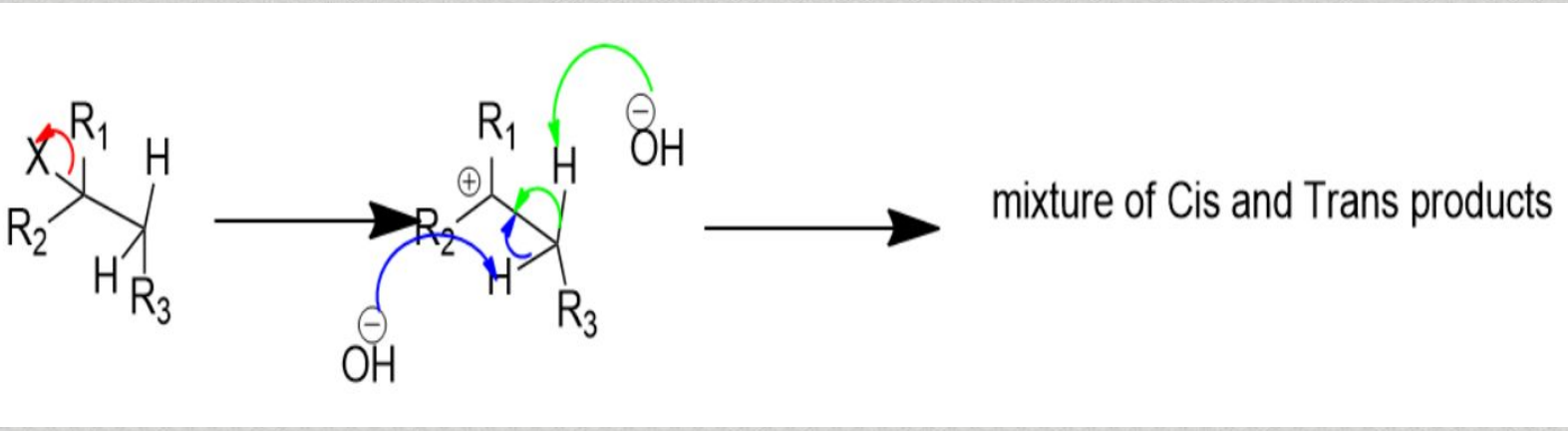
- Unimolecular.

- 2 step mechanism.

- Rate depends **only** on the substrate (Alkyl halide)
  depends on cleavage of C-X bond

- Reactivity of halogen I>Br>Cl

- Reactivity of Alkyl halides 3º and some 2º alkyl halides


R1
X
H
R2
H
R3
R1
H
OH
R2
H
R3
OH
mixture of Cis and Trans products

References

- Boyd, Robert N., and Robert T. Morrison. *Organic Chemistry*. seventh ed., Pearson, 2010
- Francis Carey, Organic Chemistry; 3rd Edition, Tata McGraw Hill India
- , R.L. Madan Chemistry for degree students; CBCS, S. Chand

Thank you