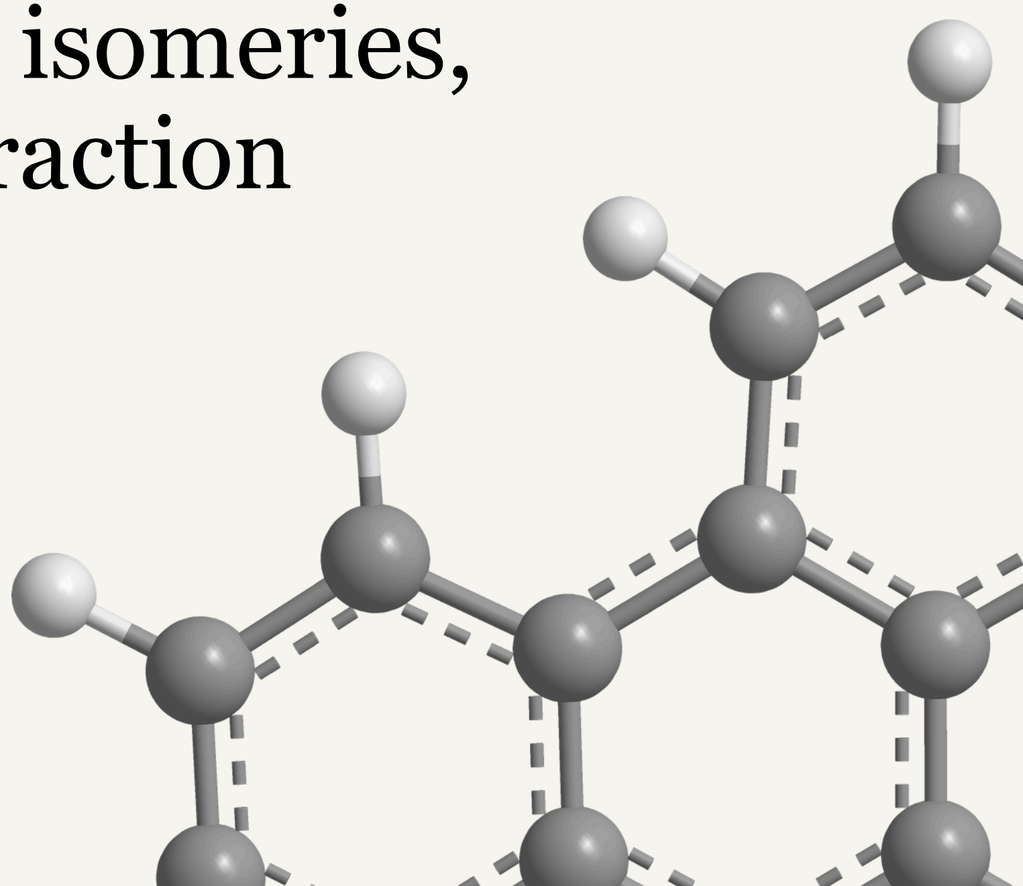
Lecture 7

Alkenes: structure and isomeries, nomenclature, extraction



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Aim and objectives

Aim: study structure, isomerism, nomenclature and preparation of alkenes and their importance in chemistry and industry

1. Define alkenes and their general formula
2. Structure and bonding of C=C
3. sp^2 hybridization and geometry
4. Structural and geometrical isomerism
5. IUPAC nomenclature
6. Laboratory preparation
7. Industrial production
8. Practical applications

What are alkenes?

$$C_nH_{2n}$$

One C=C bond, n ≥ 2

- Unsaturated hydrocarbons with C=C
- More reactive than alkanes
- Characteristic addition reactions
- sp^2 carbons at the double bond
- Raw materials for synthesis and polymers

Ethene $CH_2=CH_2$ · Propene $CH_2=CH–CH_3$ · But-1-ene $CH_2=CH–CH_2–CH_3$

Homologous series

Members differ by $–CH_2–$; the step $C_nH_{2n} \rightarrow C_{n+1}H_{2n+2}$ is a formula change, not a reaction

C atoms	Alkene	Formula
2	Ethene	C_2H_4
3	Propene	C_3H_6
4	Butene	C_4H_8
5	Pentene	C_5H_{10}
6	Hexene	C_6H_{12}

Structure of the C=C bond

- σ bond from sp^2 overlap
- π bond from sideways p overlap
- Attached atoms lie in one plane
- Rotation about C=C is restricted

$$C{=}C = 1\sigma + 1\pi$$

The reactive π bond drives addition reactions

sp^2 hybridization

1 s + 2 p

↓

3 sp^2 orbitals

+ 1 unhybridized p

- Trigonal planar geometry
- Bond angles ≈ 120°
- Forms σ and π bonds

$CH_2=CH_2$

Isomerism of alkenes

Same molecular formula, different structure or spatial arrangement

Chain

Different carbon skeletons

Position

Different double-bond positions

Geometrical

Different spatial configurations

Functional-class

Alkenes and cycloalkanes

Structural isomers of C_4H_8

But-1-ene

$CH_2{=}CH{-}CH_2{-}CH_3$

Double bond at C1

But-2-ene

$CH_3{-}CH{=}CH{-}CH_3$

Double bond at C2

2-Methylpropene

$CH_2{=}C(CH_3)_2$

Branched skeleton

Geometrical isomerism

Restricted rotation about C=C; each double-bonded carbon needs two different groups

cis-But-2-ene

Methyl groups on the same side

trans-But-2-ene

Methyl groups on opposite sides

Geometrical isomers may differ in physical properties

E/Z nomenclature

Based on Cahn–Ingold–Prelog priority rules

Z

Zusammen: higher priorities on the same side

E

Entgegen: higher priorities on opposite sides

(Z)-But-2-ene = cis · (E)-But-2-ene = trans

IUPAC nomenclature

1. Choose the parent chain with the most double bonds
2. Give the double bond the lowest locant
3. Change -ane to -ene
4. Show the double-bond position
5. Name substituents
6. Add E/Z when needed

Formula	Name
$CH_2=CH_2$	Ethene
$CH_2=CH–CH_3$	Propene
$CH_3–CH=CH–CH_3$	But-2-ene
$CH_2=C(CH_3)_2$	2-Methylpropene
$CH_2=CH–CH(CH_3)_2$	3-Methylbut-1-ene

Physical properties

- Lower alkenes are gases
- Medium chains are often liquids
- Heavier alkenes may be solids
- Nonpolar, poorly soluble in water
- Boiling point rises with size

Alkene	b.p. (approx.)
Ethene	−104 °C
Propene	−48 °C
But-1-ene	−6 °C
Pent-1-ene	30 °C
Hex-1-ene	63 °C

Laboratory preparation

Dehydration of alcohols

$CH_3CH_2OH \rightarrow (H_2SO_4, \Delta)\ CH_2{=}CH_2 + H_2O$

Dehydrohalogenation

$CH_3CH_2Br + KOH \rightarrow (\text{ethanol}, \Delta)\ CH_2{=}CH_2 + KBr + H_2O$

Dehalogenation

$BrCH_2CH_2Br + Zn \rightarrow CH_2{=}CH_2 + ZnBr_2$

Elimination removes groups from adjacent carbons to form C=C

Industrial production

Steam cracking

$C_6H_{14} \rightarrow (\Delta)\ C_2H_4 + C_4H_{10}$ (illustrative; real output is a mixture)

Dehydrogenation

$CH_3CH_3 \rightarrow (\text{catalyst}, \Delta)\ CH_2{=}CH_2 + H_2$

Fluid catalytic cracking

Petroleum fractions → lighter products incl. propene and butenes

Applications

Alkene	Main uses
Ethene	Polyethylene, ethanol, ethylene oxide
Propene	Polypropylene, propan-2-ol, propylene oxide
Butenes	Polymers, fuel components, intermediates
Higher alkenes	Detergents, lubricants, plasticizer intermediates

$$n\ CH_2{=}CH_2 \rightarrow [-CH_2-CH_2-]_n$$

Conclusion

- Acyclic alkenes with one C=C: C_nH_{2n}
- C=C = one σ bond + one π bond; sp^2 carbons
- Chain, position and geometrical isomerism
- IUPAC names give chain, position, substituents, E/Z
- Preparation: dehydration, dehydrohalogenation, dehalogenation
- Industry: cracking and dehydrogenation; products feed polymers and chemicals