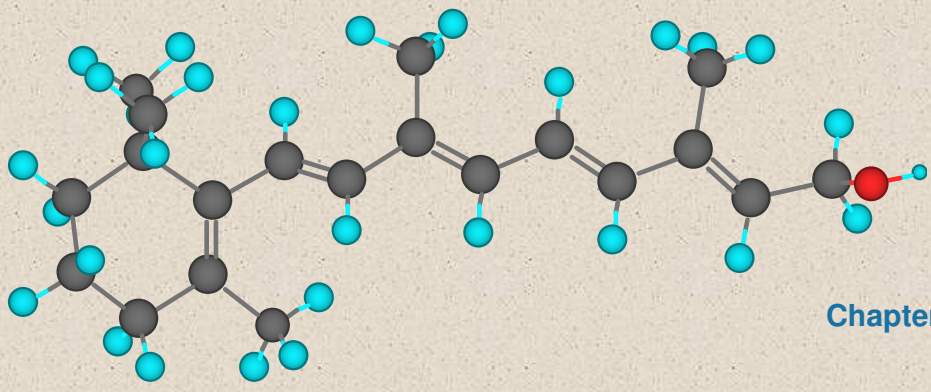
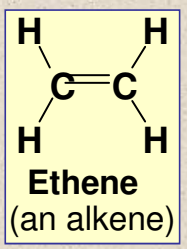
Alkenes: Structure and Nomenclature



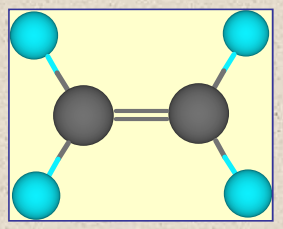
Chapter 5

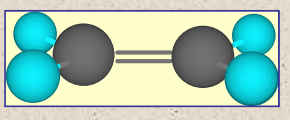
Unsaturated Hydrocarbons

- Unsaturated hydrocarbon: Contains one or more multiple bonds.
- Alkene: Contains a carbon-carbon double bond and has the general formula C_nH_{2n}.



Ethene
(an alkene)



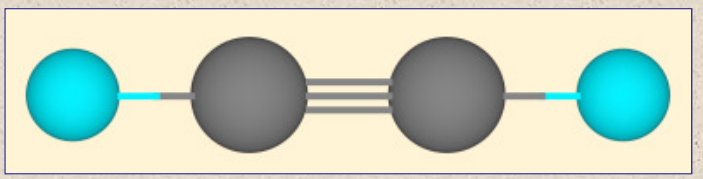


Unsaturated Hydrocarbons

- Alkyne: Contains a carbon-carbon triple bond and has the general formula C_nH_{2n-2}.

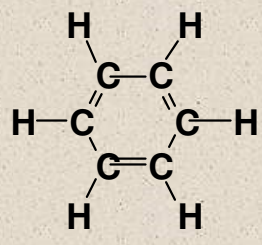
H-C≡C-H

Ethyne
(an alkyne)

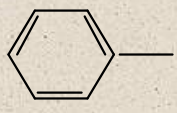


Unsaturated Hydrocarbons

- Arenes: Benzene and its derivatives (Ch 21-22)



Benzene

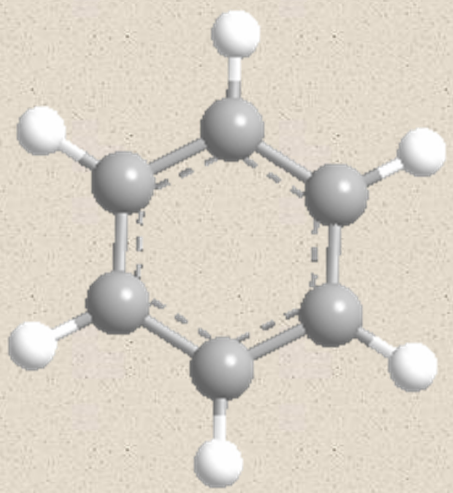


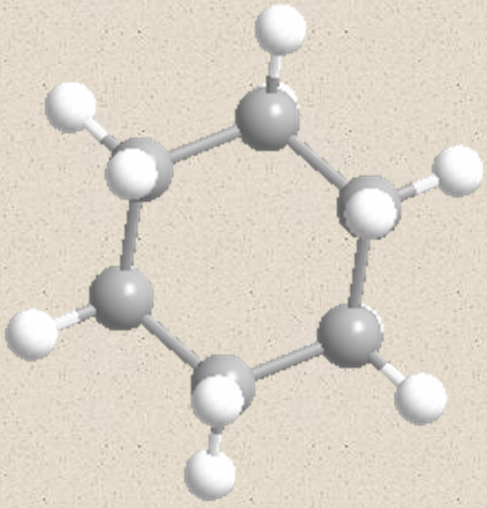
C_6H_5- **Ph-**

Alternative representations for the phenyl group

  - The phenyl group is not reactive under any of the conditions described in Ch 6-20.

Benzene

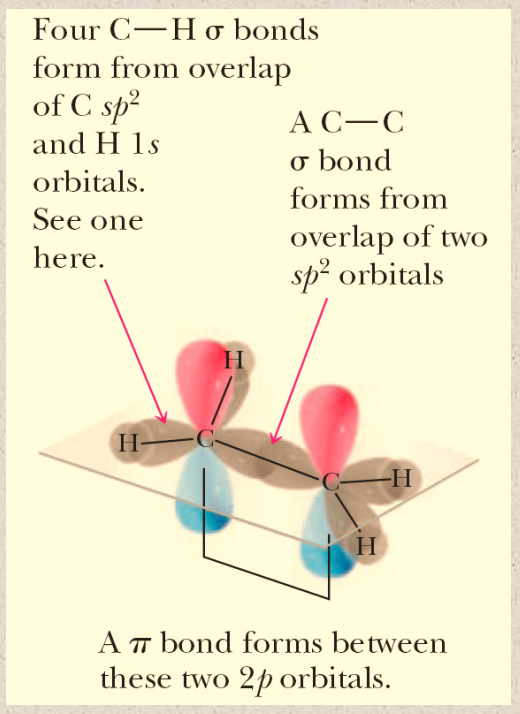




Cyclohexane

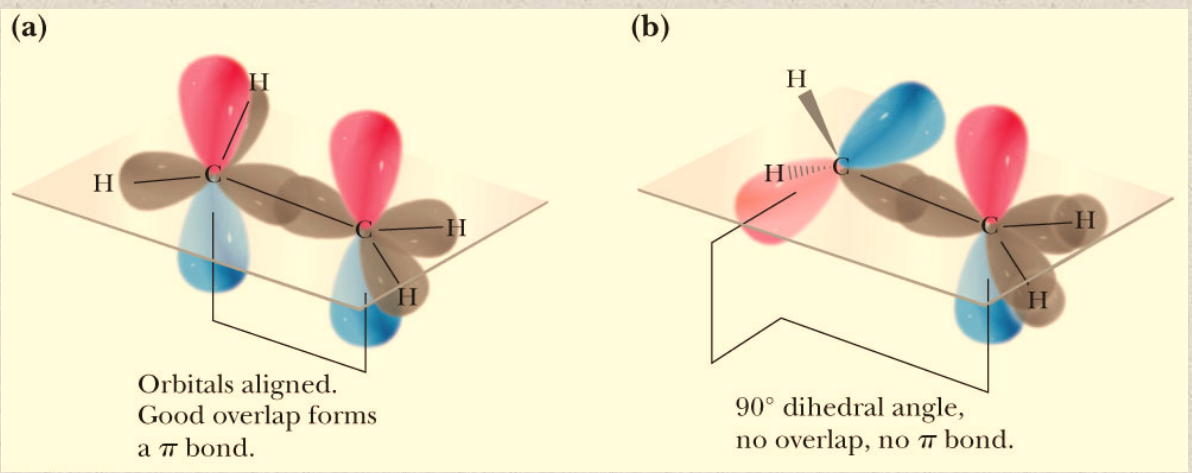
Structure of Alkenes

- A double bond consists of
  - one sigma bond formed by the overlap of sp^2 hybrid orbitals and one pi bond formed by the overlap of parallel 2*p* orbitals.
  - the two carbon atoms of a double bond and the four atoms bonded to them lie in a plane, with bond angles of approximately 120°.



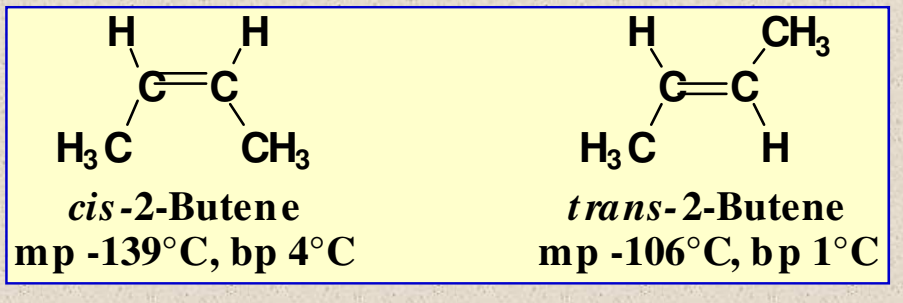
Structure of Alkenes

– it takes approximately 264 kJ (63 kcal)/mol to break the pi bond in ethylene; that is, to rotate one carbon by 90° with respect to the other so that there is no overlap between 2*p* orbitals on adjacent carbons.



Cis,Trans Isomerism in Alkenes

- *Cis,trans* isomers: Isomers that have the same connectivity but a different arrangement of their atoms in space due to the presence of either a ring (Chapter 2) or a carbon-carbon double bond.



Index of Hydrogen Deficiency

- Index of hydrogen deficiency (IHD): The sum of the number of rings and pi bonds in a molecule.
- To determine IHD, compare the number of hydrogens in an unknown compound with the number in a reference hydrocarbon of the same number of carbons and with no rings or pi bonds.
  - the molecular formula of the reference hydrocarbon is C_nH_{2n+2}.

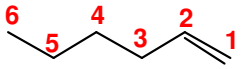
Index of Hydrogen Deficiency

$$\text{IHD} = \frac{(H_{\text{reference}} - H_{\text{molecule}})}{2}$$

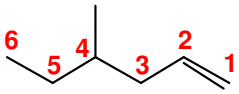
1. for each atom of a Group 7 element (F, Cl, Br, I), add one H.
2. no correction is necessary for the addition of atoms of Group 6 elements (O,S) to the reference hydrocarbon.
3. for each atom of a Group 5 element (N, P), add one hydrogen.

IUPAC Nomenclature

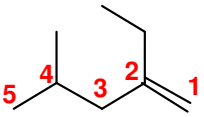
1. Number the longest chain of carbon atoms that contains the double bond in the direction that gives the carbons of the double bond the lowest numbers.
2. Locate the double bond by the number of its first carbon.
3. Name substituents.
4. Number the carbons, locate and name substituents, locate the double bond, and name the main chain.



1-Hexene



4-Methyl-1-hexene



2-Ethyl-4-methyl-1-pentene

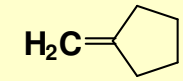
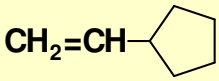
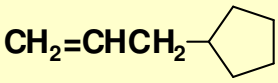
Common Names

- Despite the precision and universal acceptance of IUPAC nomenclature, some alkenes, particularly low-molecular-weight alkenes, are known almost exclusively by their common names.

	$CH_2=CH_2$	$CH_3CH=CH_2$	$CH_3C(CH_3)=CH_2$
IUPAC:	**Ethene**	**Propene**	**2-Methylpropene**
Common:	**Ethylene**	**Propylene**	**Isobutylene**

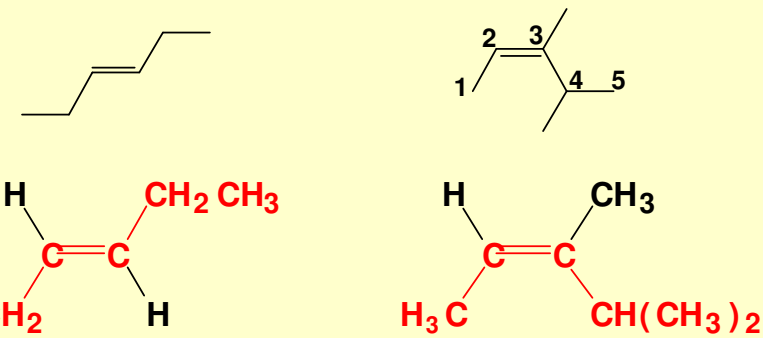
Common Names

– the common names methylene, vinyl, and allyl are often used to show the presence of the following alkenyl groups:

Alkenyl Group	Common Name	Example	IUPAC Name (Common name)
$CH_2=$ Methylidene	Methylene		Methylidenecyclopentane (Methylenecyclopentane)
$CH_2=CH-$ Ethenyl	Vinyl		Ethenylcyclopentane (Vinylcyclopentane)
$CH_2=CHCH_2-$ 3-Propenyl	Allyl		3-Propenylcyclopentane (Allylcyclopentane)

The *Cis,Trans* System

- Configuration is determined by the orientation of atoms of the main chain.



trans -3-Hexene

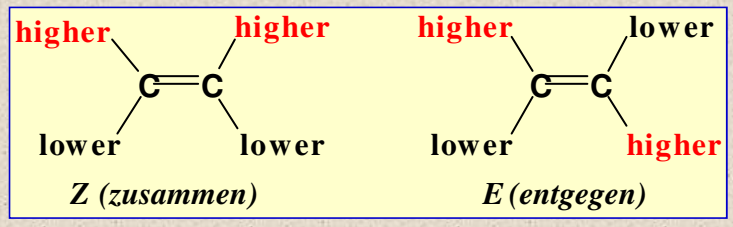
cis -3,4-Dimethyl-2-pentene

The *E,Z* System

– Uses priority rules (Chapter 3).

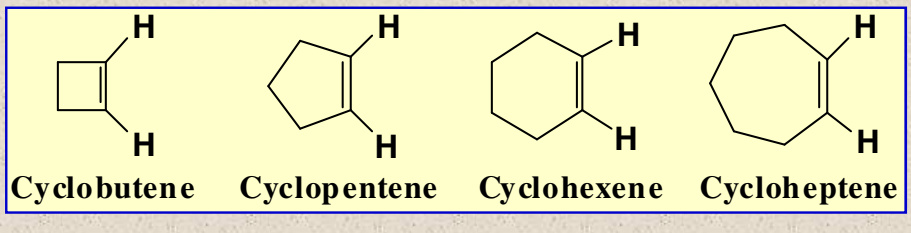
– If groups of higher priority are on the same side, the configuration is *Z* (German, *zusammen*).

– If groups of higher priority are on opposite sides, the configuration is *E* (German, *entgegen*).



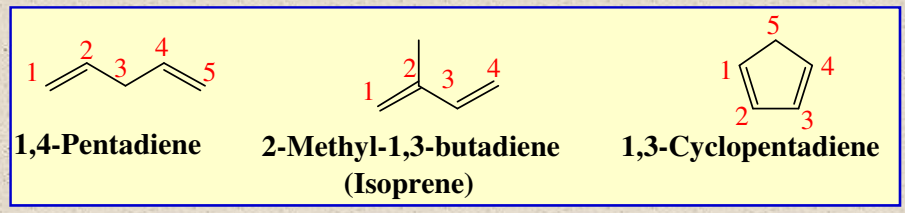
The *Cis,Trans* Isomerization

- Cycloalkenes
  – In small-ring cycloalkenes, the configuration of the double bond is *cis*.
  – These rings are not large enough to accommodate a *trans* double bond.



Dienes, Trienes, and Polyenes

- For alkenes containing two or more double bonds, change the infix -en- to -adien-, -atrien-, etc.
  - Those containing several double bonds are often referred to more generally as polyenes.
  - Following are three dienes.



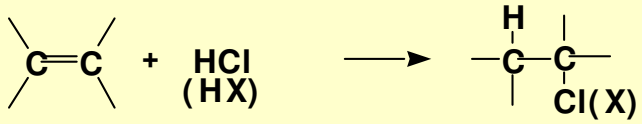
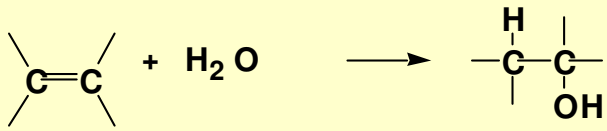
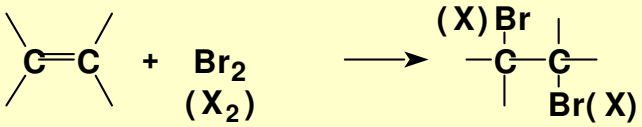
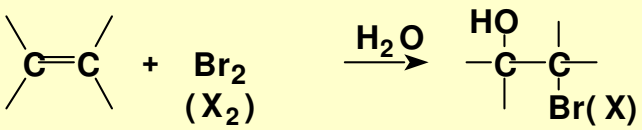
Physical Properties

- Alkenes are nonpolar compounds.
- The only attractive forces between their molecules are dispersion forces.
- The physical properties of alkenes are similar to those of alkanes.

Reactions of Alkenes

- The most characteristic reaction of alkenes is addition to the carbon-carbon double bond.
  - The pi bond is broken.
  - In its place, sigma bonds form to two new atoms or groups of atoms.

Reactions of Alkenes

Reaction	Descriptive Name(s)
	Hydrochlorination (hydrohalogenation)
	Hydration
	Bromination (halogenation)
	Halohydrin formation (Bromohydrin formation)