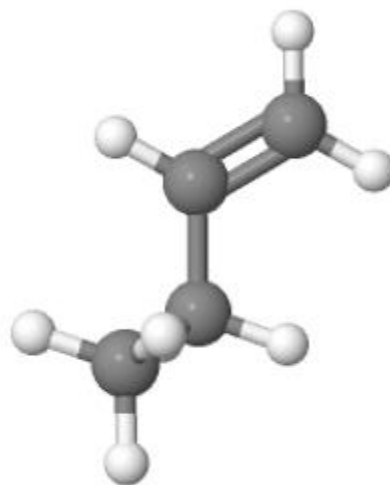


Alkenes – Structures and Nomenclature



Instructor: Asst. Prof. Dr. Tanatorn Khotavivattana

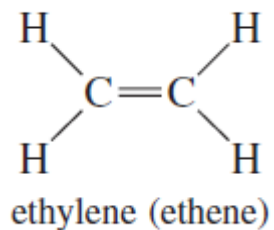
E-mail: tanatorn.k@chula.ac.th

Recommended Textbook:

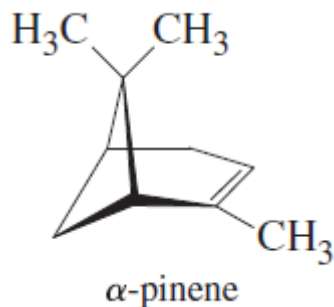
Chapter 7 in *Organic Chemistry*, 8th Edition, L. G. Wade, Jr., 2010, Prentice Hall (Pearson Education)

What is alkene?

Hydrocarbons with carbon-carbon double bonds



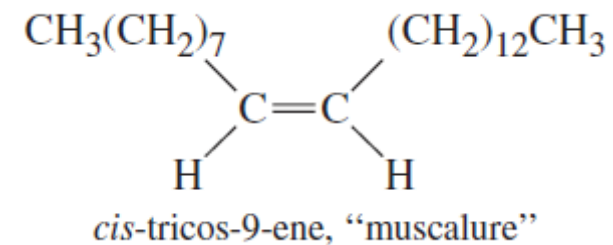
Preparation of polyethylene and a variety of other industrial and consumer chemicals.



Major component of turpentine, the paint solvent distilled from extracts of evergreen trees



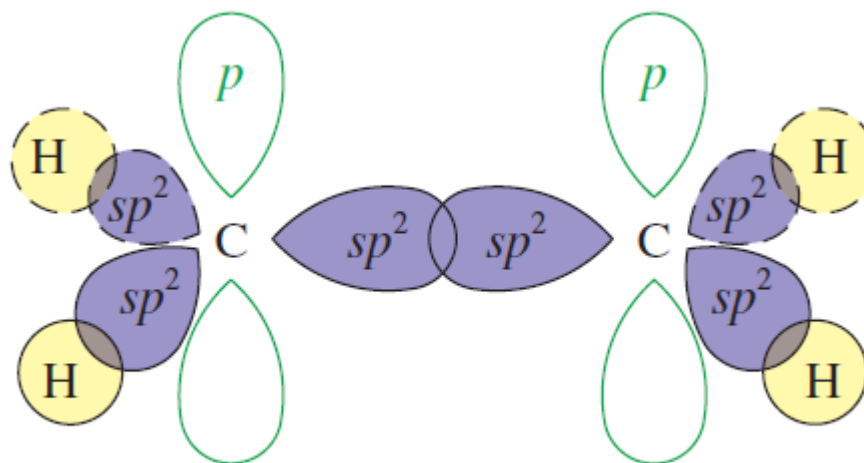
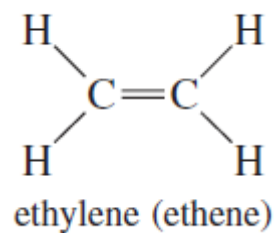
double-bond dissociation energy	611 kJ/mol
subtract sigma bond dissociation energy	<u>(-)347 kJ/mol</u>
pi bond dissociation energy	264 kJ/mol



Sex attractant pheromone of the common housefly.

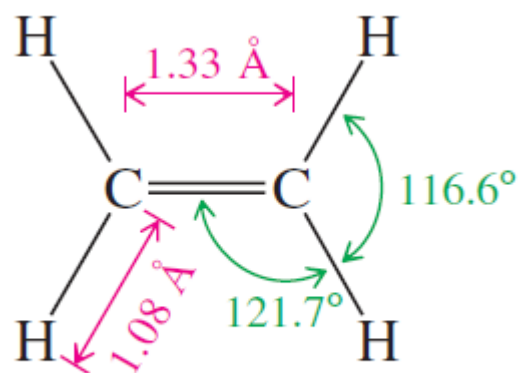


Orbital Description of the Alkene Double Bond

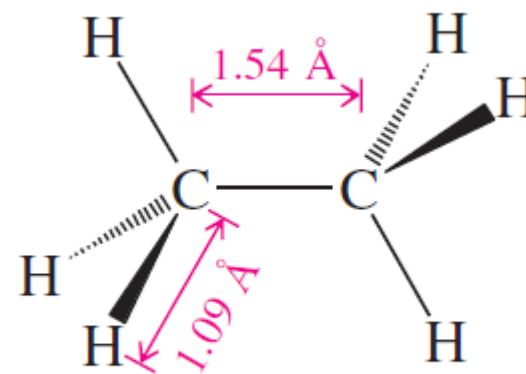


sigma bonding orbitals of ethylene

1) Sigma bond



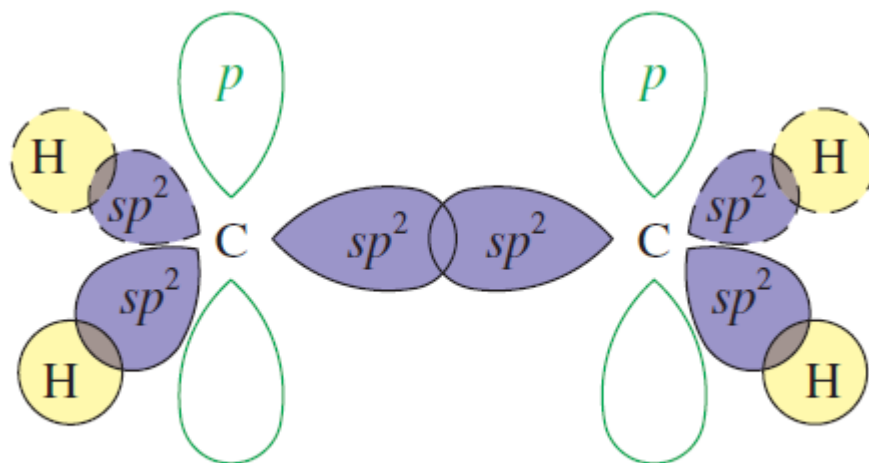
ethylene



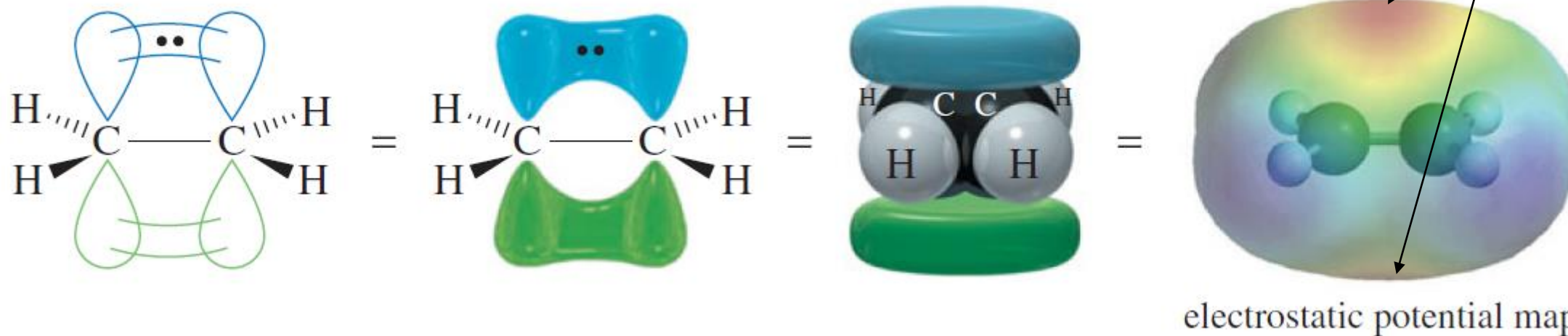
ethane

Orbital Description of the Alkene Double Bond

2) Pi bond



sigma bonding orbitals of ethylene



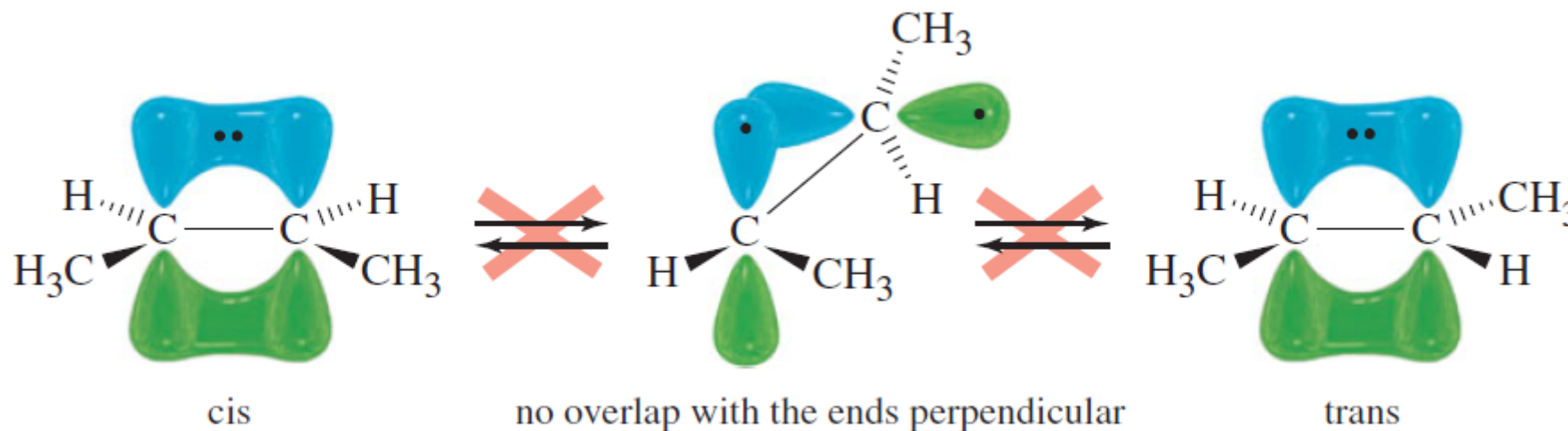
High electron density

electrostatic potential map

Orbital Description of the Alkene Double Bond

2) Pi bond

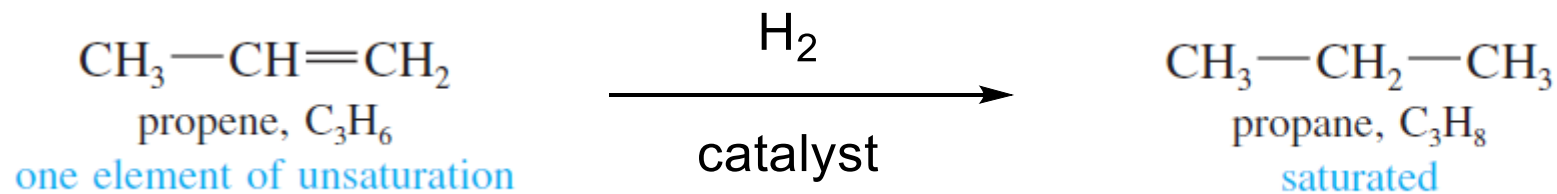
Unlike single bonds, a carbon–carbon double bond **does not permit rotation**. **Six atoms**, including the double-bonded carbon atoms and the four atoms bonded to them, must **remain in the same plane**.



Cis - trans isomerism

If two groups are on the **same side** of a double bond (**cis**), they cannot rotate to **opposite sides** (**trans**) without breaking the pi bond.

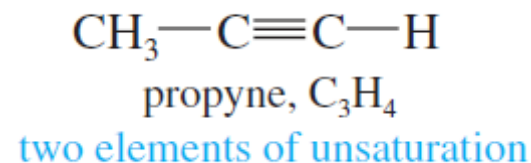
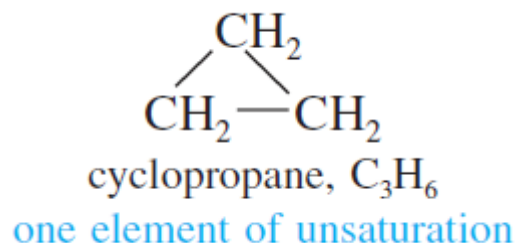
Degree of Unsaturation in Hydrocarbons



An **alkane**, is called **saturated** because it **cannot react with any more hydrogen**

The presence of a **pi bond** of an alkene (or an alkyne) or the **ring** of a cyclic compound decreases the **number of hydrogen atoms** in a molecular formula. = **“Degree / Element of unsaturation”**

Each degree of unsaturation corresponds to **two fewer hydrogen atoms** than in the “saturated” formula.



Calculate the maximum number of hydrogen atoms from the saturated formula **“C_nH_{2n+2}”** and see how many are missing.

Degree of Unsaturation in Hydrocarbons

Example 1

Determine the number of elements of unsaturation in the molecular formula C_4H_6 . Give all 9 possible structures having this formula.

***Note**

1 **double bond** = 1 degree of unsaturation

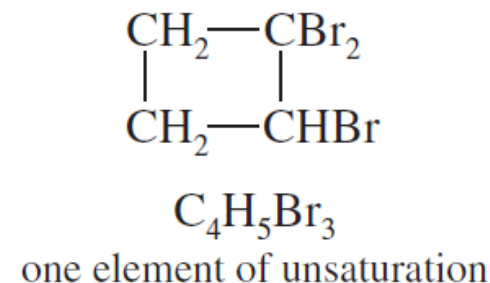
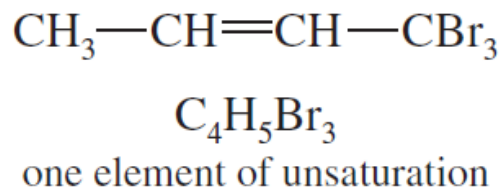
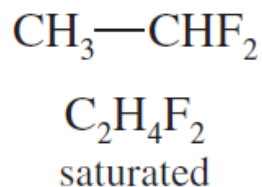
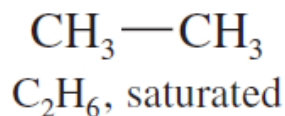
1 **ring** = 1 degree of unsaturation

1 **triple bond** = 2 degree of unsaturation

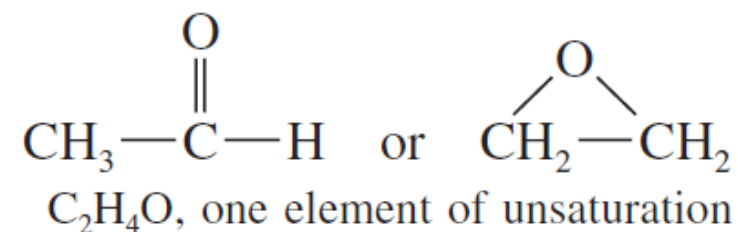
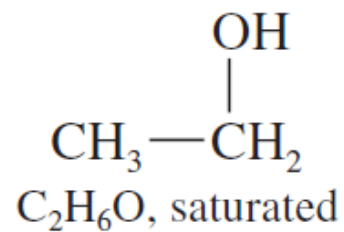
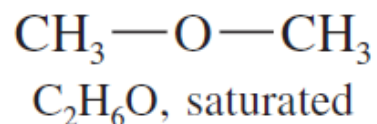
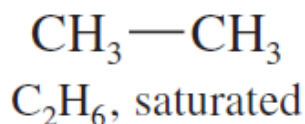
Degree of Unsaturation with Heteroatoms

Heteroatoms = any atoms other than carbon and hydrogen

- Halogens:** Halogens can substitute for hydrogen atoms in the molecular formula: **count halogens as hydrogen atoms**

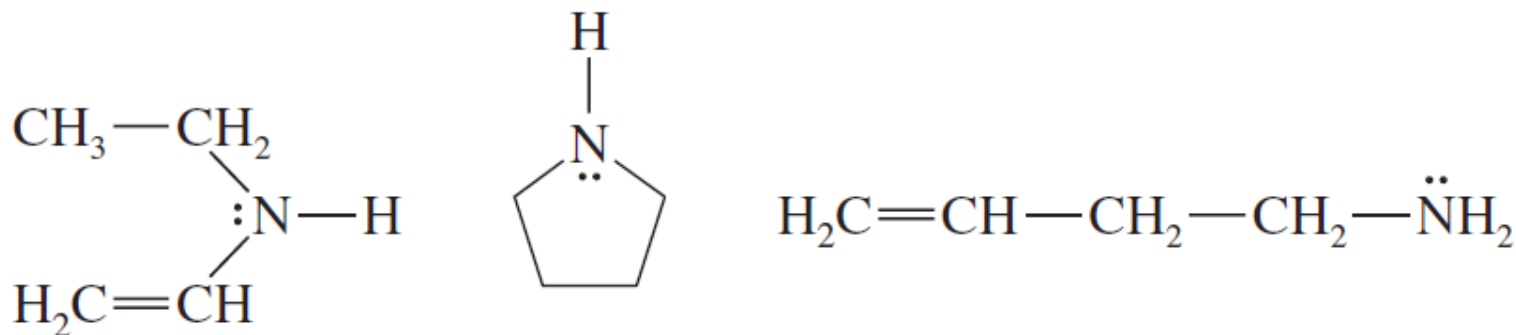
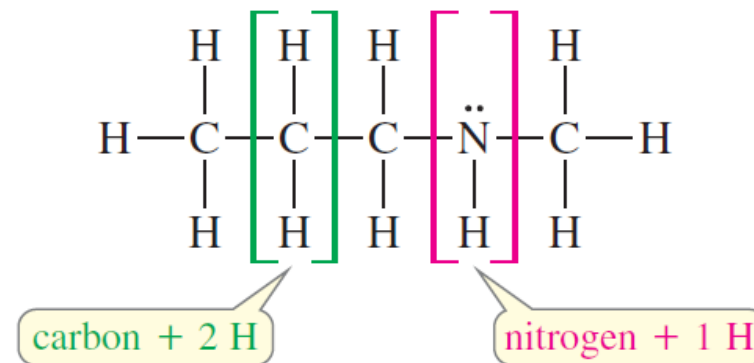


- Oxygens:** An oxygen atom can be added to the chain without changing the number of hydrogen atoms or carbon atoms: **ignore the oxygen atoms**



Degree of Unsaturation with Heteroatoms

- Nitrogen:** A nitrogen atom can take the place of a carbon atom, but nitrogen has only one additional hydrogen atom (compared with two hydrogens for each additional carbon atom): **count nitrogen as half a carbon atom.**



examples of formula $\text{C}_4\text{H}_9\text{N}$, one element of unsaturation

Degree of Unsaturation in Hydrocarbons

Example 2 Draw at least four compounds of formula C_4H_6NOCl

***Note**

halogen = counts as H
oxygen = ignores
nitrogen = counts as $\frac{1}{2}$ C

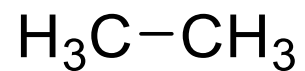
***Note**

1 double bond = 1 degree of unsaturation
1 ring = 1 degree of unsaturation
1 triple bond = 2 degree of unsaturation

IUPAC Nomenclature

Alkanes

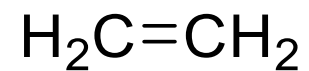
Suffix: -ane



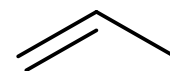
ethane

Alkenes

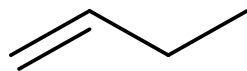
Suffix: -ene



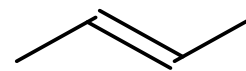
ethene



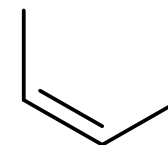
propene



but-1-ene

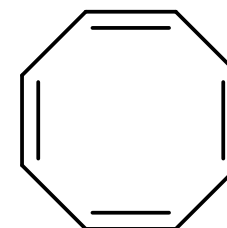
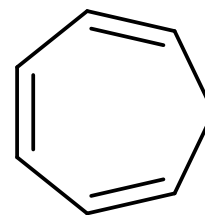
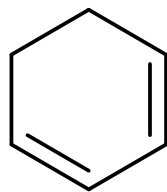
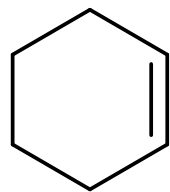
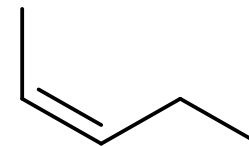
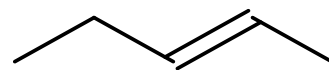
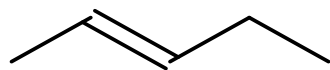
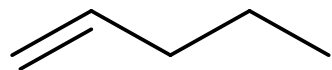


trans-but-2-ene

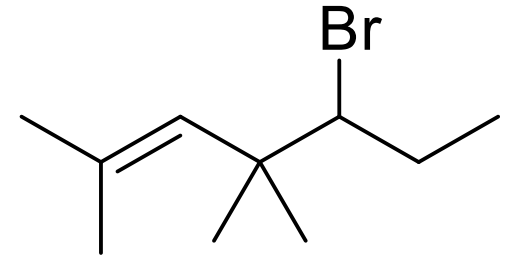
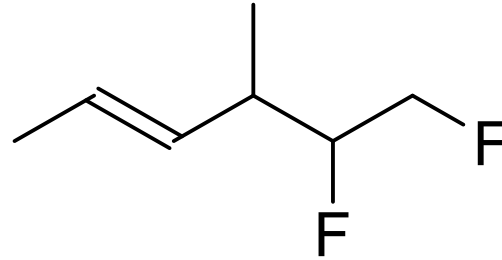
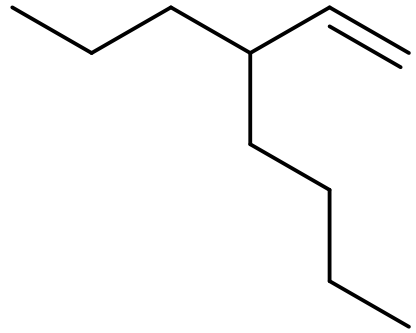
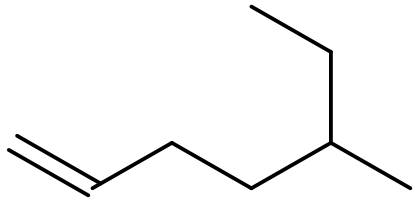


cis-but-2-ene

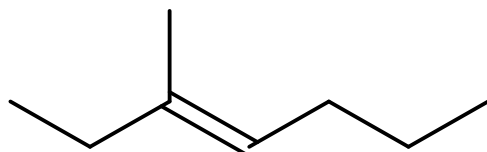
IUPAC Nomenclature and *cis-trans*



IUPAC Nomenclature and *cis-trans* nomenclature



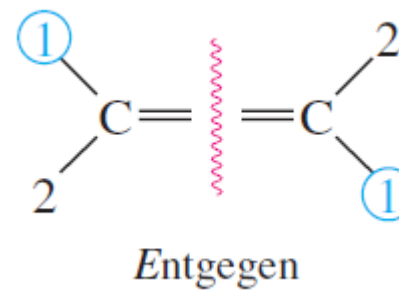
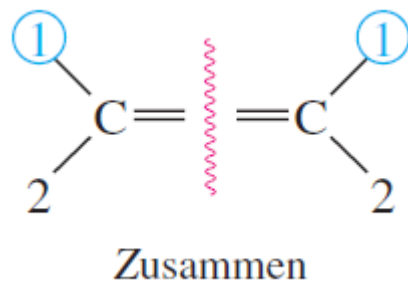
IUPAC Nomenclature and *E-Z* nomenclature



Use Cahn–Ingold–Prelog convention

If the two first-priority atoms are **together on the same side** of the double bond, you have the **Z** isomer.

If the two first-priority atoms are on **opposite sides** of the double bond, you have the **E** isomer.



IUPAC Nomenclature and *E-Z* nomenclature

