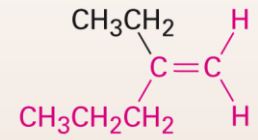
Alkene
1 - Nomenclature and Properties

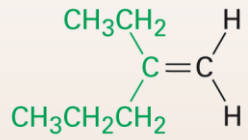
Dr. Sapna Gupta

Nomenclature

- Name the parent hydrocarbon

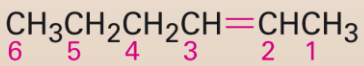


Named as a *pentene* *NOT*

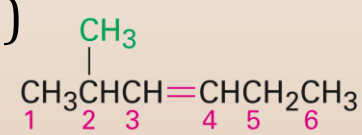


as a hexene, since the double bond is not contained in the six-carbon chain

- Number the carbons in chain so that double bond carbons have lowest possible numbers.
- **Write the full name-** Number substituents according to: 1) Position in chain, 2)Alphabetically

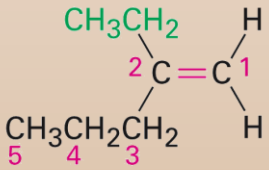


2-Hexene

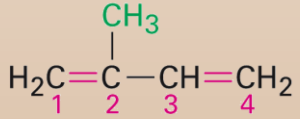


2-Methyl-3-hexene

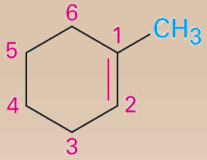
- Rings have "**cyclo**" prefix



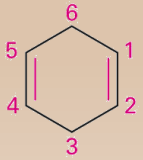
2-Ethyl-1-pentene



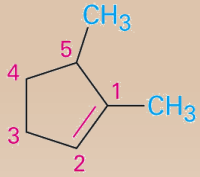
2-Methyl-1,3-butadiene



1-Methylcyclohexene



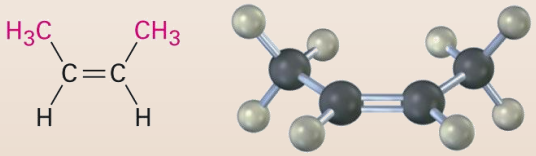
1,4-Cyclohexadiene
(New: Cyclohexa-1,4-diene)



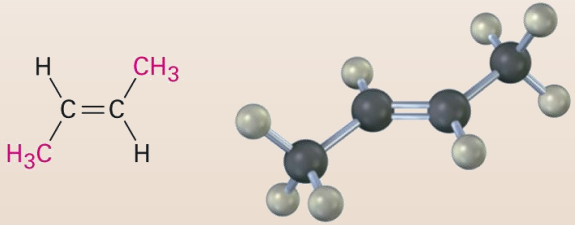
1,5-Dimethylcyclopentene

More on Nomenclature

- Cis and Trans isomerism (geometric isomers)
- This isomerism occurs because double bonds cannot rotate

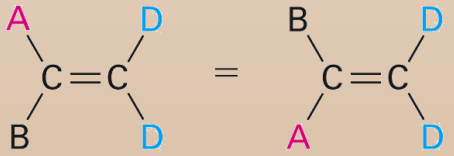


cis-2-Butene



trans-2-Butene

- Cis and trans is usually referred to only for two hydrogen atoms are on the same side.
- Cis and trans is not possible when two terminal atoms are the same.



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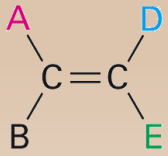
These two compounds are identical; they are not cis–trans isomers.



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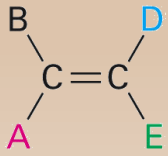
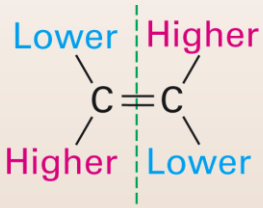


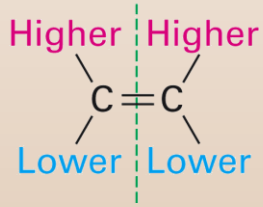
These two compounds are not identical; they are cis–trans isomers.

E/Z Nomenclature

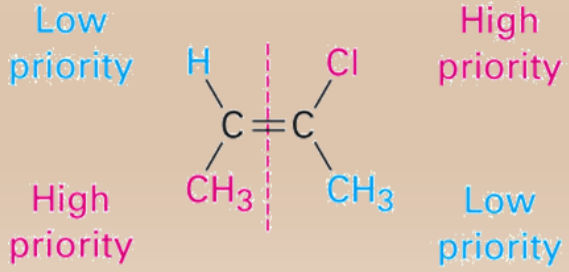
- Cahn-Ingold-Prelog nomenclature is used when two or more atoms around the double bond are not hydrogen
- Compare where higher priority groups are with respect to bond and designate as prefix
- **E -*entgegen*,** opposite sides
- **Z - *zusammen*,** same side
- Priority rules are the same as in stereochemistry. (see next slide for a review)



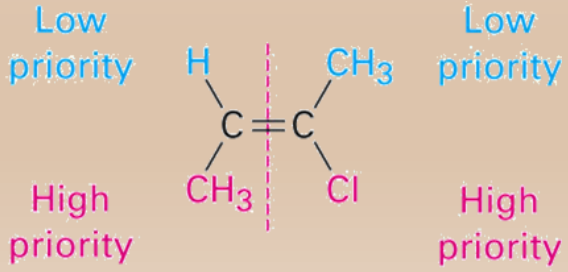
E double bond
(Higher-ranked groups are on opposite sides.)



Z double bond
(Higher-ranked groups are on the same side.)



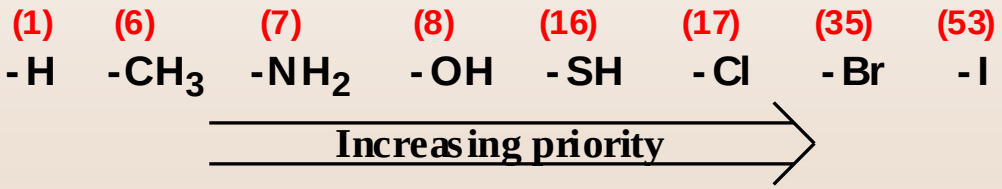
(a) (*E*)-2-Chloro-2-butene



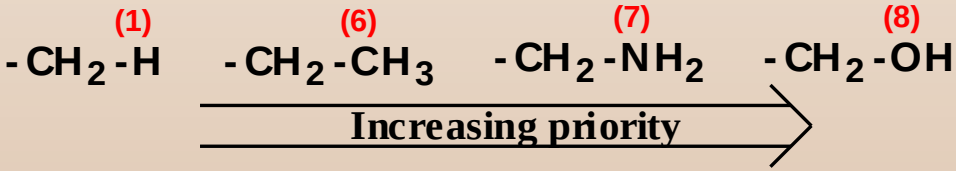
(b) (*Z*)-2-Chloro-2-butene

Assigning Priority

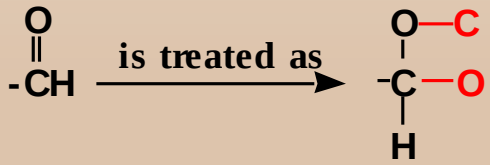
1. Look at the atom (not the group) directly attached to the carbon and arrange according to atomic weight

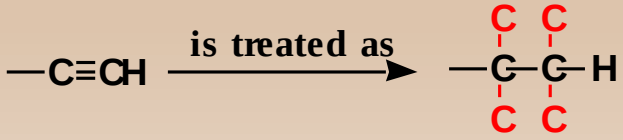


2. If priority cannot be assigned per the atoms bonded to the chiral center, look to the next set of atoms; priority is assigned at the first point of difference



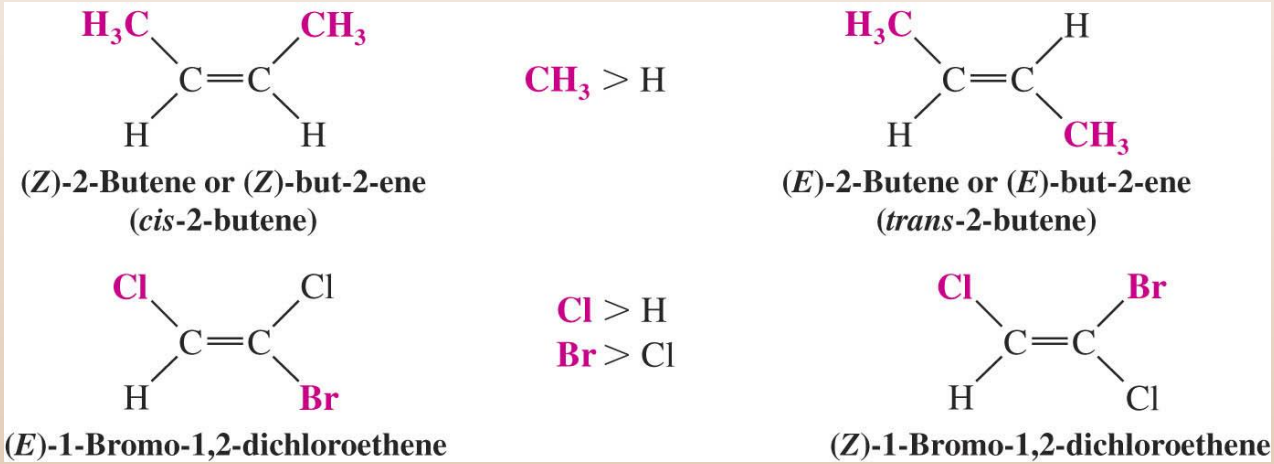
3. Groups with double or triple bonds are assigned priorities as if their atoms were duplicated or triplicated





More Example of E/Z Nomenclature

- Alkenes with two hydrogens (typically assigned as cis or trans) can be named as E/E also.

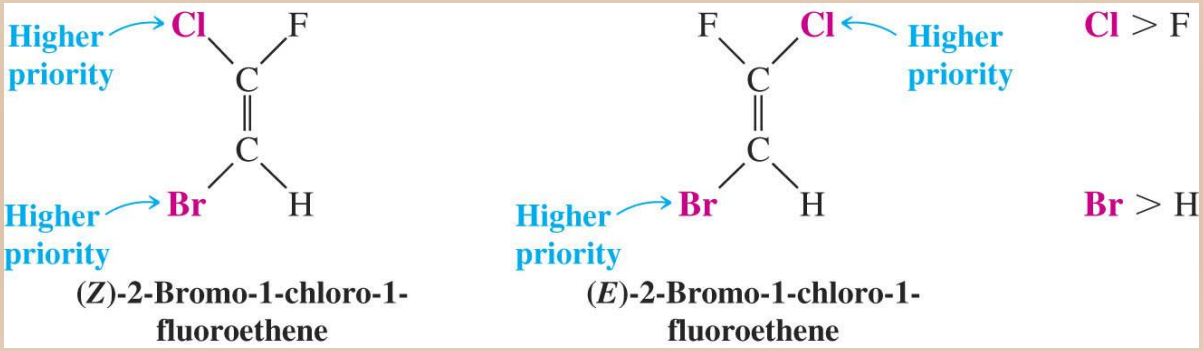


(*Z*)-2-Butene or (*Z*)-but-2-ene (*cis*-2-butene)

(*E*)-2-Butene or (*E*)-but-2-ene (*trans*-2-butene)

(*E*)-1-Bromo-1,2-dichloroethene

(*Z*)-1-Bromo-1,2-dichloroethene

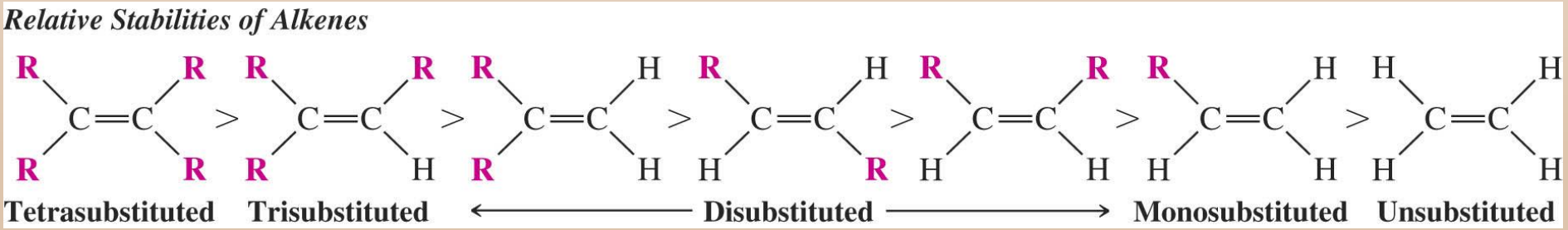


(*Z*)-2-Bromo-1-chloro-1-fluoroethene

(*E*)-2-Bromo-1-chloro-1-fluoroethene

Stability of Alkenes

- *Cis* alkenes are less stable than *trans* alkenes
- Less stable isomer is higher in energy and gives off more heat during combustion.
- So general rule – more substituted the double bond the more stable it is
- tetrasubstituted > trisubstituted > disubstituted > monosusbtituted



Degree of Unsaturation

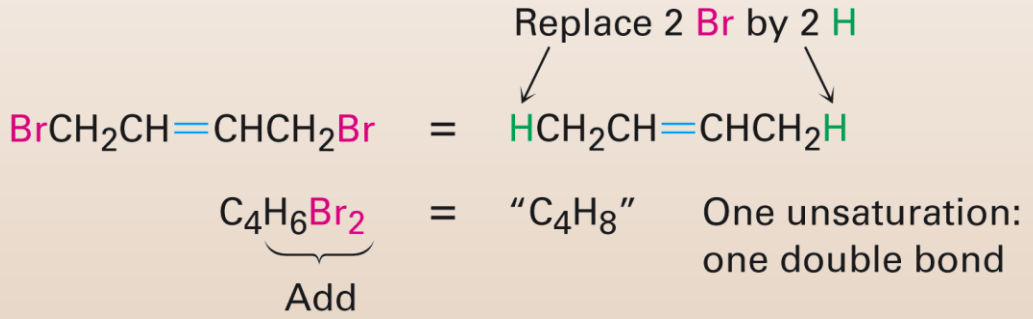
- Alkanes are C_nH_{2n+2} and alkenes are C_nH_{2n} so alkenes are two less H than alkanes.
- 2 less H in a formula is known as one degree (1^o) of unsaturation or Hydrogen Deficiency Index (HDI)

$$\frac{\#\ of\ H\ in\ alkane - \#\ of\ H\ in\ compound}{2} = \text{HDI}$$

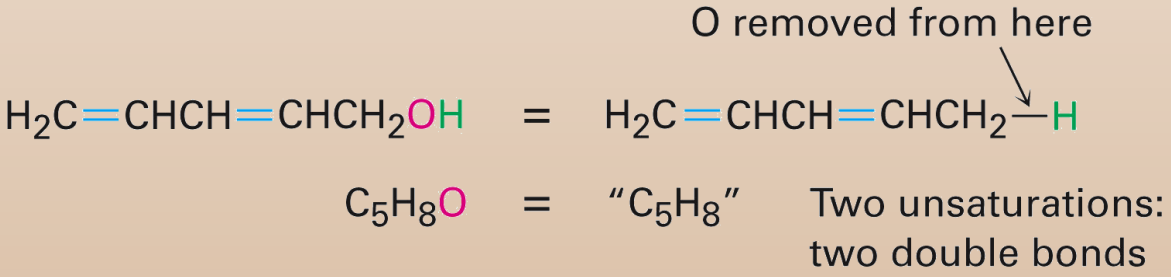
- 1^o of unsaturation is equivalent to either a presence of one double bond or one ring in the structure.
- 2^o of unsaturation is equivalent to:
  - one triple bond
  - OR one double bond + one ring
  - OR two rings
  - OR two double bonds

Degree of Unsaturation with Other Elements

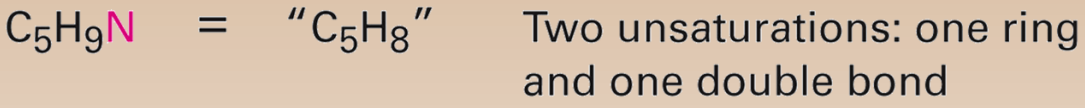
- Organohalogens (X: F, Cl, Br, I) Halogen replaces hydrogen
  - $C_4H_6Br_2$ and C_4H_8 have one degree of unsaturation



- Organoxygen compounds (C,H,O) – Oxygen forms 2 bonds and don't affect the formula of equivalent hydrocarbons. They can be ignored.



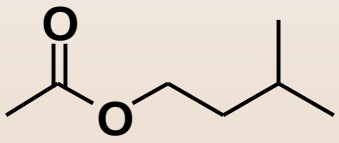
- Nitrogen compounds – subtract the N and one H– they have two connections.



Example: Degree of Unsaturation

Problem: isopentyl acetate has a molecular formula of $C_7H_{14}O_2$. Calculate its HDI.

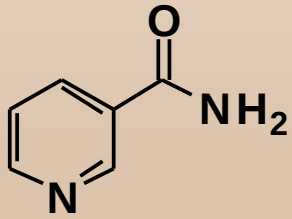
- Ignore the two oxygens
- New formula = C_7H_{14}
- C_nH_{2n+2} = C_7H_{16}
- (16-14)/2 = HDI of 1



Isopentyl acetate

Problem: calculate the HDI for niacin, molecular formula $C_6H_6N_2O$.

- Ignore the oxygen; for N – remove the two N and one H with each N so remove two H also
- New formula = C_6H_4
- C_nH_{2n+2} = C_6H_{14}
- (14-4)/2 = HDI of 5

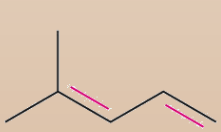


Niacin

Example: Degree of Unsaturation

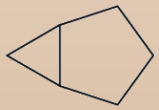
Calculate the degree of unsaturation for C_6H_{10} and propose the structures possible.

- Saturated is C_6H_{14}
  - therefore 4 H's are not present
- This has two degrees of unsaturation
  - Two double bonds?
  - or triple bond?
  - or two rings?
  - or ring and double bond?

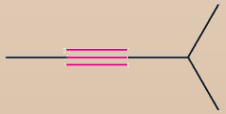


4-Methyl-1,3-pentadiene
(two double bonds)

Cyclohexene
(one ring, one double bond)



Bicyclo[3.1.0]hexane
(two rings)



4-Methyl-2-pentyne
(one triple bond)

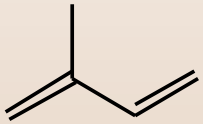
C_6H_{10}

Physical Properties of Alkenes

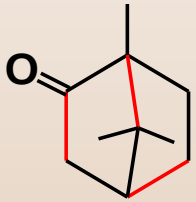
1. Boiling points – resemble alkanes; generally low bpts; IM force is primarily van der Waal's force and dispersion forces. Bpts increases with molecular weight.
2. Solubility in water – insoluble in water since water is polar and alkenes are non polar.
3. Density – less dense than water.
4. Odor – have unique odor.

Applications of Alkenes

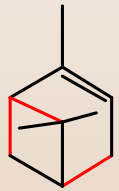
- Alkenes are found in a variety of compounds:
  - fragrances and flavors (***terpenes***) e.g. isoprene (the starting material for the rubber in tires; camphor, pinene



2-Methyl-1,3-butadiene (Isoprene)

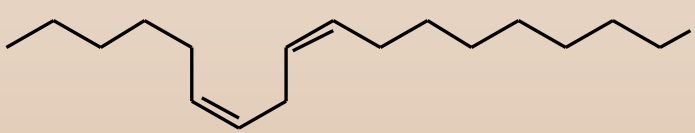


Camphor

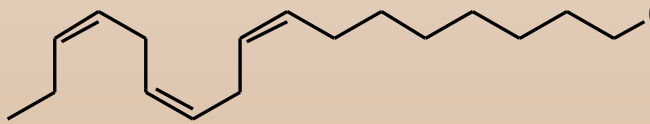


Pinene

  - ***fatty acids*** (oils)



Linoleic acid (18:2) (mp-5°C)



Linolenic acid (18:3) (mp -11°C)

  - vitamins (A and E)

- They are important in in the chemistry of vision (click this ***link*** to read more)
- We will talk more about alkenes after reactions of alkenes.

Key Words/Concepts

- Nomenclature
- Cis/trans isomerism
  - (geometric isomerism)
- E/Z nomenclature
- Stability of alkenes
- Hydrogen deficiency index
  - (degree of unsaturation)
- Properties of alkenes