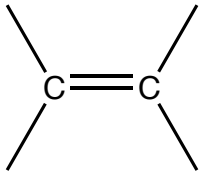
Lecture Outline 4: Alkenes, Alkynes

Alkene and Alkyne Nomenclature

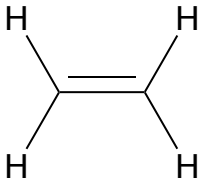
Alkene = double bond = olefin (oleum facere = to make oil)

Alkyne = triple bond = acetylene (as functional group, not compound)

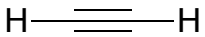


Alkene

Alkyne



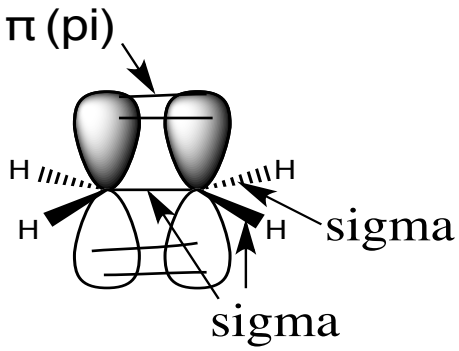
Ethylene

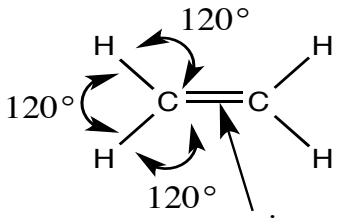


Acetylene

Simplest Alkene and Alkyne Possible

Recall:





ethylene = ethene

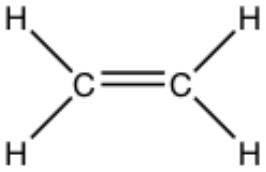
sigma + pi = double bond

sp^2+sp^2 p+p

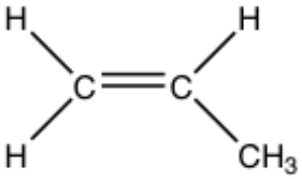
Alkene Nomenclature

Find longest chain, number from end to contain both ends of C=C and give lowest number to 1st C of C=C

Change "ane" to "ene" precede with number to indicate first double bond position



ethylene OR ethene

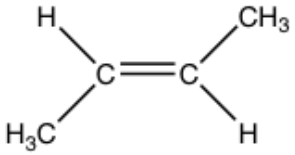


propylene OR 1-propene
prop-1-ene

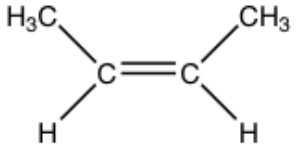
$CH_3CH_2CH=CH_2$

butylene OR 1-butene
but-1-ene

Below are two structural isomers of 1-butene



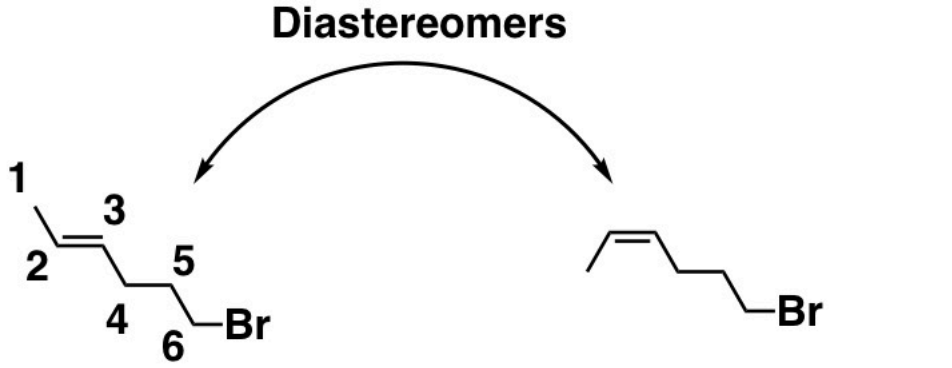
trans-2-butene



cis-2-butene

} diastereomers

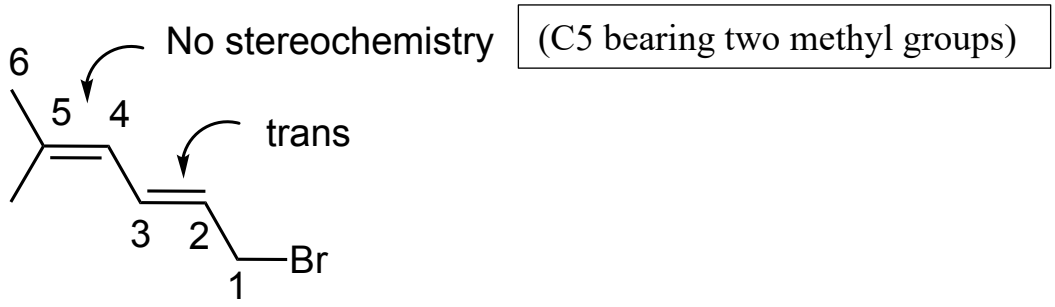
Example 1: 6-Bromo-2-hexene



trans-6-Bromo-2-hexene **cis-6-Bromo-2-hexene**

In the cis isomer, the two higher priority groups on either side of the carbon-carbon double bond are pointing in the same direction.

Example 2:



2-trans-1-bromo-5-methyl-hexa-2,4-diene

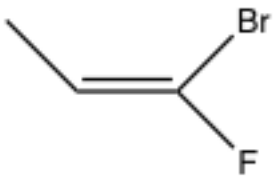
Alkene and Alkyne Nomenclature

E, Z - Nomenclature

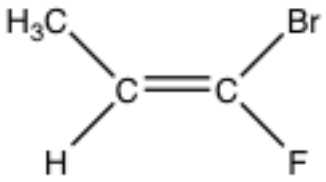
E - Entegegen - Opposite
Z - Zusammen - Together

Naming based on atomic number, similar process to identifying S/R stereochemistry

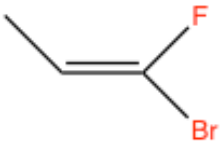
Example 2: 1-Bromo-1-fluoro-1-propene



means



1-bromo-1-fluoropropene



1-bromo-1-fluoropropene

Question: Are the compounds above the same?

Answer: No, they are diastereomers and we can differentiate them by using the E and Z nomenclature

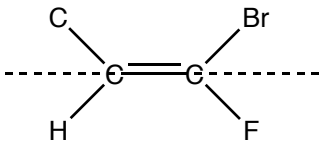
E, Z - Nomenclature

E - Entegegen - Opposite
Z - Zusammen – Together

Example 1: 1-bromo-1-fluoro-1-propene
- compare the atomic no. of the adjacent atoms.

Compare the left side of the C=C bond

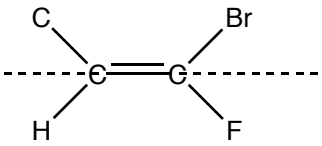
larger



smaller

Compare the right side of the C=C bond

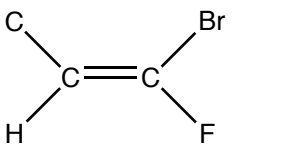
larger



smaller

same side = Z

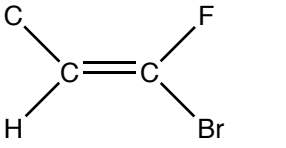
larger larger



smaller smaller

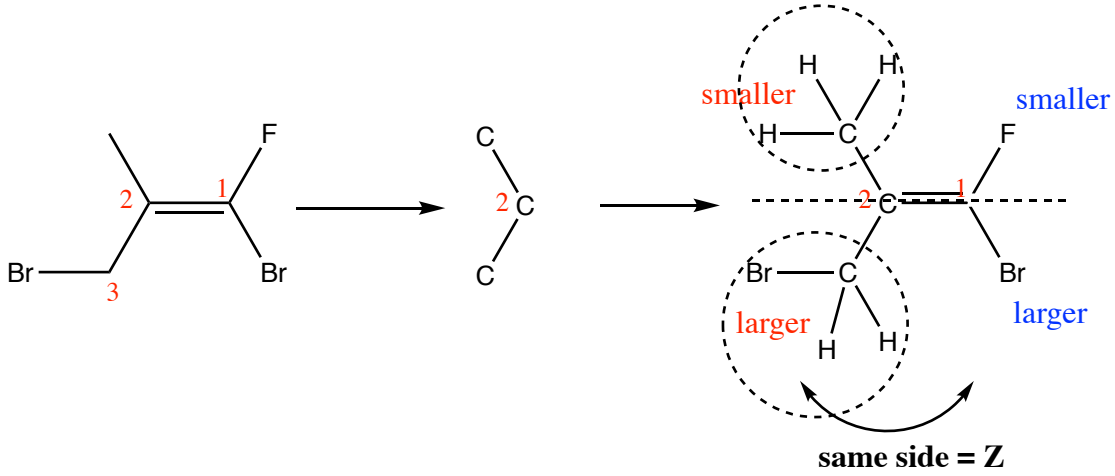
opposite = E

larger smaller



smaller larger

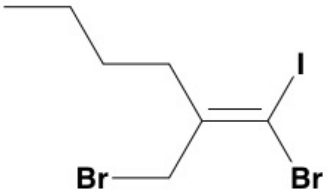
Example : 1,3-dibromo-1-fluoro-2-methyl-1-propene



Therefore the name is: (Z)-1,3-dibromo-1-fluoro-2-methyl-1-propene

If you cannot decide on basis of atomic number of atoms directly attached to double bond, go to the next set of atoms until a higher atomic number is found

Example 3:



E-1-Bromo- 2-bromomethyl-1-iodohex-1-ene

Iodine is on the opposite side to the bromomethyl (highest priority groups on either side of the alkene) and so the stereochemistry is deemed E.

Nomenclature of Cycloalkenes

Cyclopropene

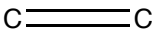
Cyclobutene

Cyclopentene

Cyclohexene

1,5,5-trimethyl-1-cyclohexene

Nomenclature of alkenes with multiple carbon-carbon double bonds (poly-enes):

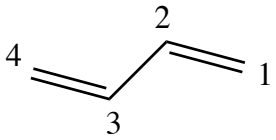
Multiple 

2 Diene

3 Triene

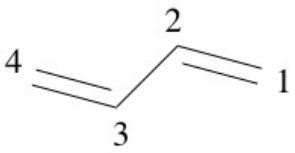
4 Tetraene

…etc



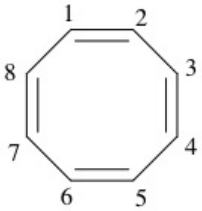
Buta-1,3-Diene
1,3-Butadiene

Drop -ne and add "diene", "triene", etc.

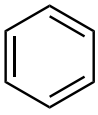


Buta-1,3-diene
1,3-Butadiene

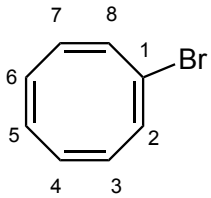
1,3-Cylcobutadiene



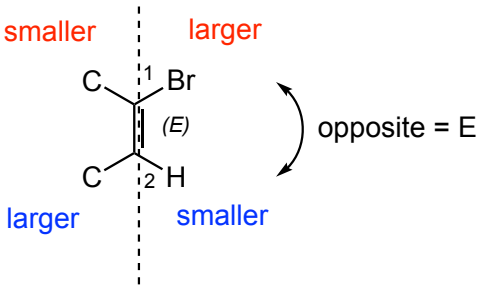
1,3,5,7-Cyclooctatetraene
COT

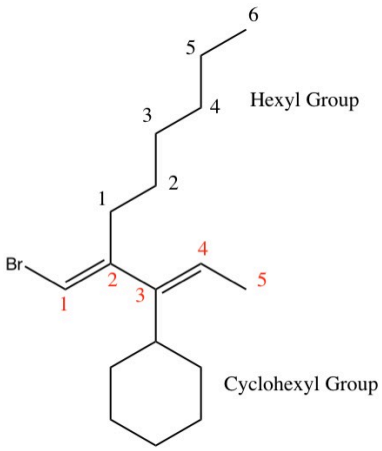


1,3,5-cyclohexatriene
Benzene

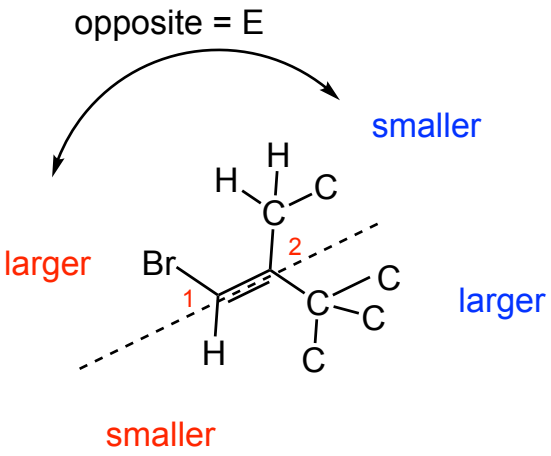


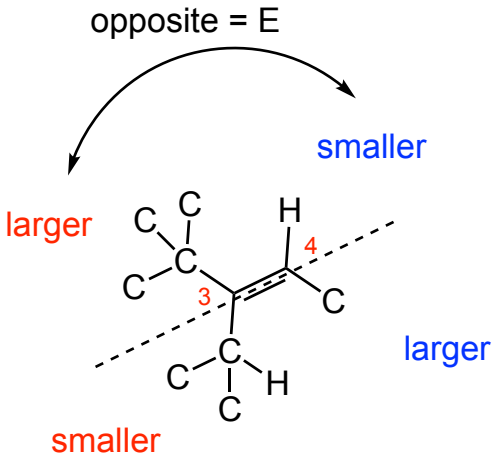
E-1-bromo-1,3,5,7-cyclooctatetraene



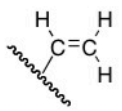


1E,3E-1-Bromo-3-cyclohexyl-2-hexyl-1,3-pentadiene



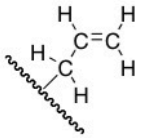


Special Nomenclature of Common Groups:

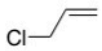


Vinyl group

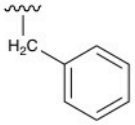
Vinyl chloride
1-chloroethene



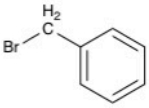
Allyl group



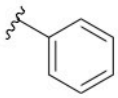
Allyl chloride
3-chloropropene



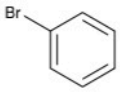
Benzyl group



Benzyl bromide



Phenyl group



Phenyl bromide

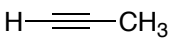
phenyl bromide is commonly called bromobenzene

Nomenclature of Alkynes

Rules:

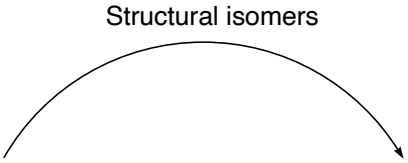
- Find longest chain with max number of multiple bonds
- Number from end to give 1st multiply bonded position the lowest number
- Drop "ane" and add "yne"
- For multiple triple bonds, drop "ne" and add "diyne"," triyne", etc.

ethyne
acetylene



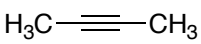
propyne

methylacetylene (common name)



1-butyne

ethylacetylene



2-butyne

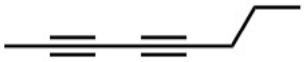
dimethylacetylene

Multiple alkynes end with:

2	C≡C	diyne
3	C≡C	triyne
4	C≡C	tetrayne

Mixed double and triple bond containing compounds are “eneynes”

Example 1:

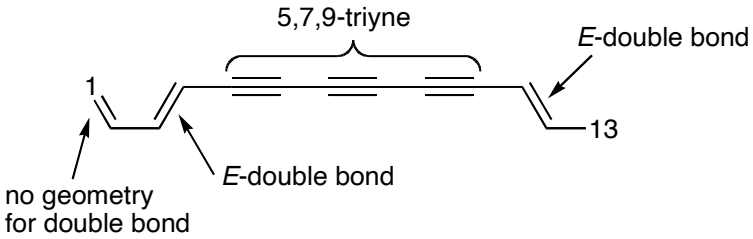


2,4 - Octadiyne

Example 2:

The below example is from canola – defense substance (anti-nematode)

Parent alkane of 13 carbons is tridecane – hence trideca



3*E*,11*E*-trideca-1,3,11-triene-5,7,9-triyne