BIO-ORGANIC CHEMISTRY
(Organic Chemistry for Biology Students)
(SQBS 1603)

Alkenes, Alkynes and Aromatic

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Functional groups

What is functional group?

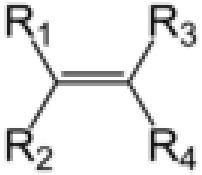
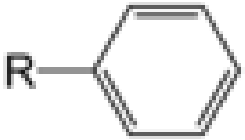
The chemical components that are added to the simple skeleton of an organic compound.

Molecules possessing the same functional group belong to the same family of organic compounds.

To generate chemical diversity and functionality.

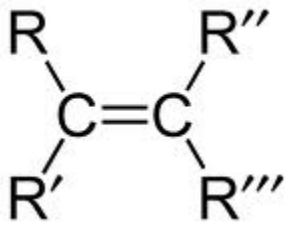
- Hydrocarbon
- Groups containing halogens
- Groups containing oxygen
- Groups containing nitrogen
- Groups containing phosphorus and sulfur

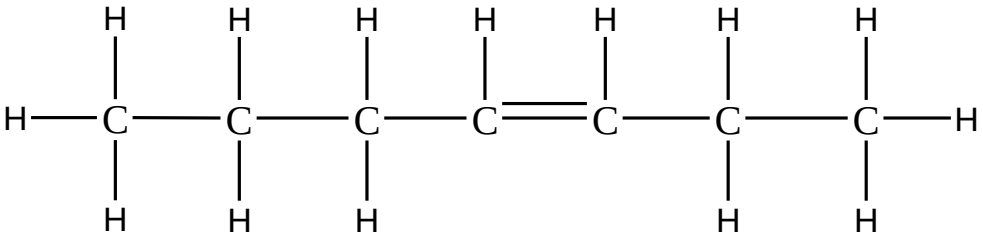
Functional groups

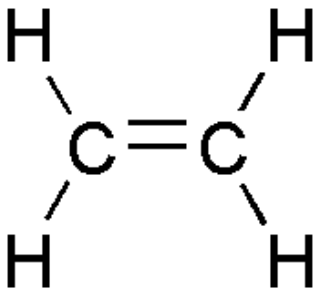
Chemical class	Group	Formula	Structural Formula	Prefix	Suffix
Alkane	Alkyl	RH		alkyl-	-ane
Alkene	Alkenyl	$R_2C=CR_2$		alkenyl-	-ene
Alkyne	Alkynyl	RC≡CR'		alkynyl-	-yne
Benzene derivative	Phenyl	RC_6H_5 RPh		phenyl-	-benzene
Toluene derivative	Benzyl	$RCH_2C_6H_5$ RBn		benzyl-	1-(*substituent*)toluene

Alkenes and alkynes

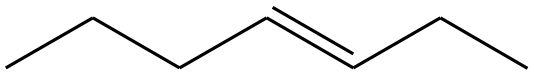
- Alkenes
  - Organic compounds that contain a carbon-carbon double bond







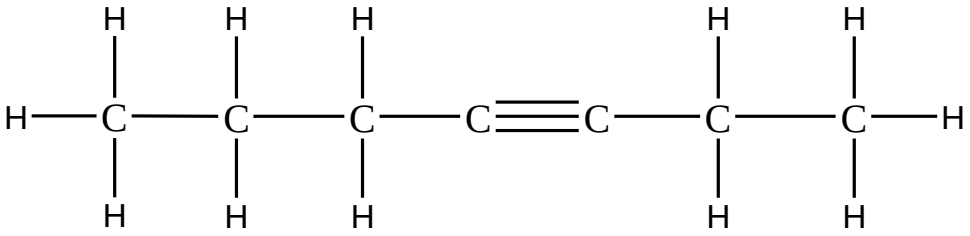
$CH_3CH_2CH_2CH{=}CHCH_2CH_2CH_3$



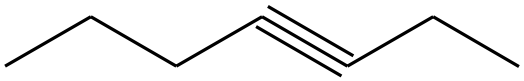
Hept-3-ene

Alkenes and alkynes

- Alkynes
  - Organic compounds that contain a carbon-carbon triple bond



$CH_3CH_2CH_2C{\equiv}CCH_2CH_2CH_3$

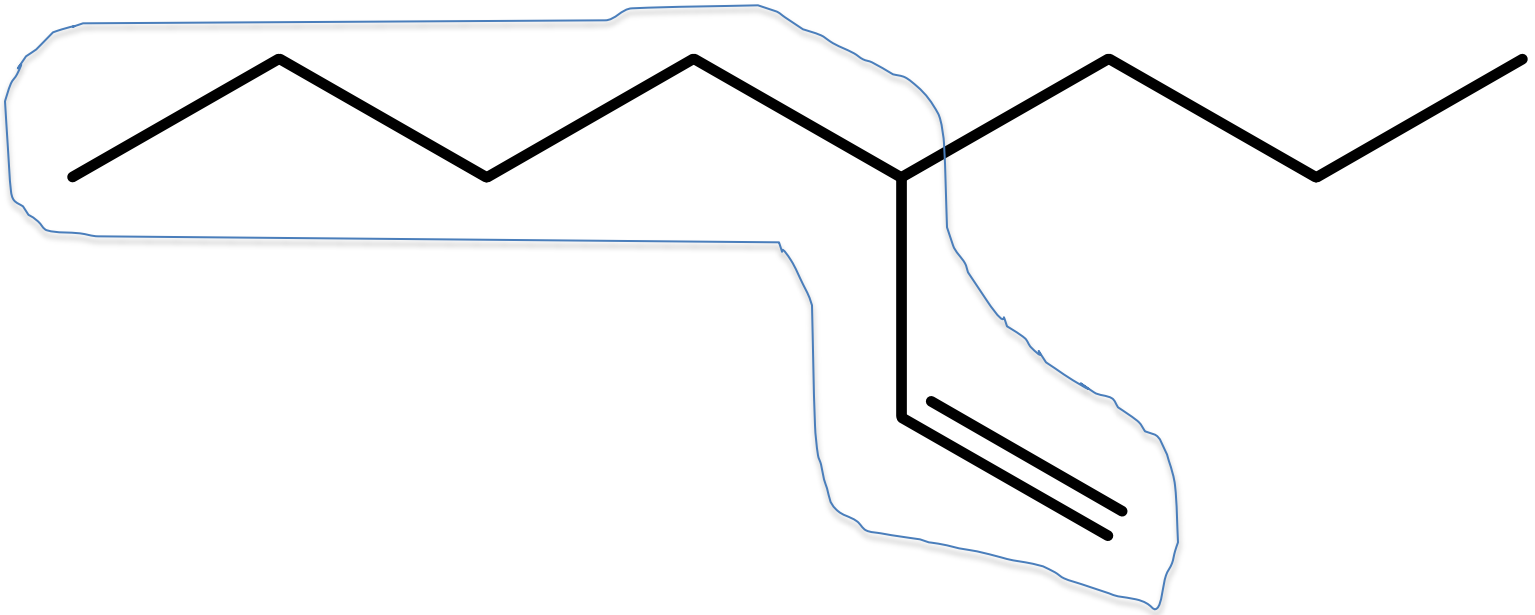


Hept-3-yne

Nomenclature (Alkenes)

Find the base structure → The longest chain that contains the largest possible number of double bonds.

Naming→ suffix = –*ene* (2 No. C=C:-diene, 3 No. C=C: -triene, 4 No. C=C: -tetraene and so on.

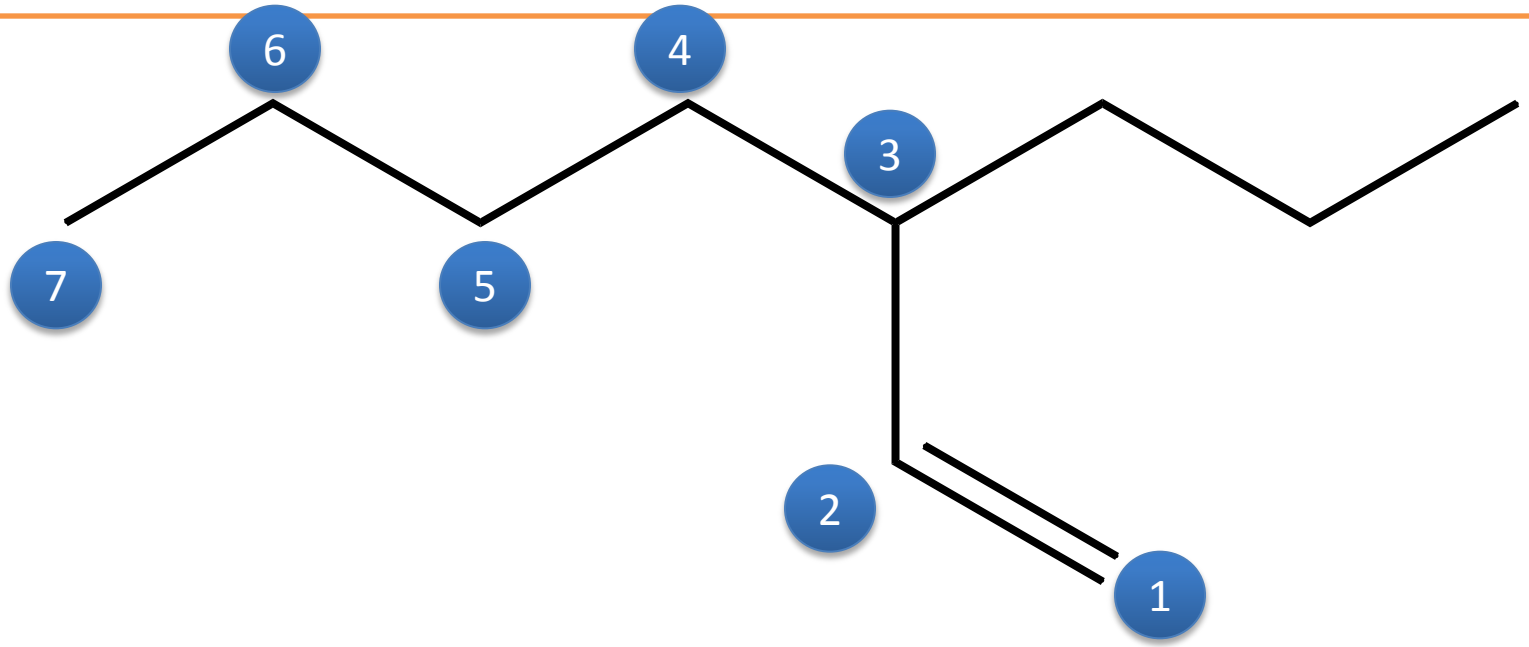


C: 7

heptene

Nomenclature (Alkenes)

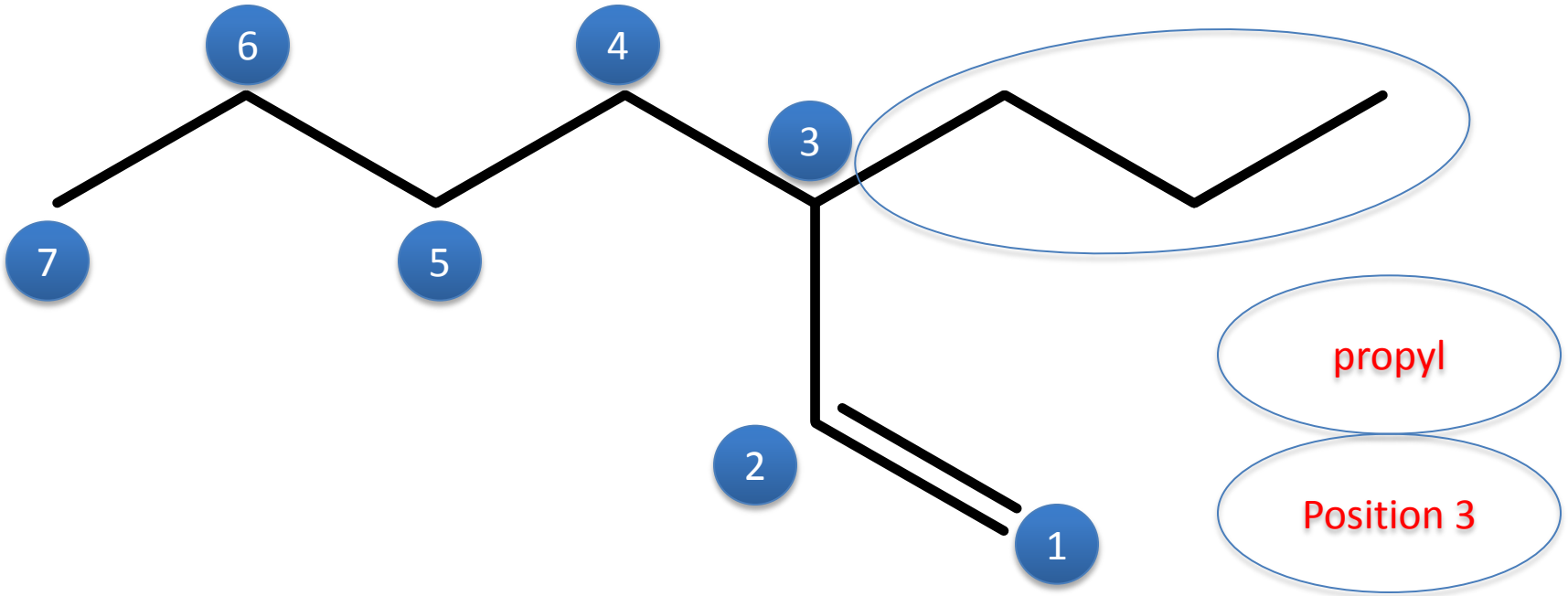
Numbering → start from the end closest to C=C.



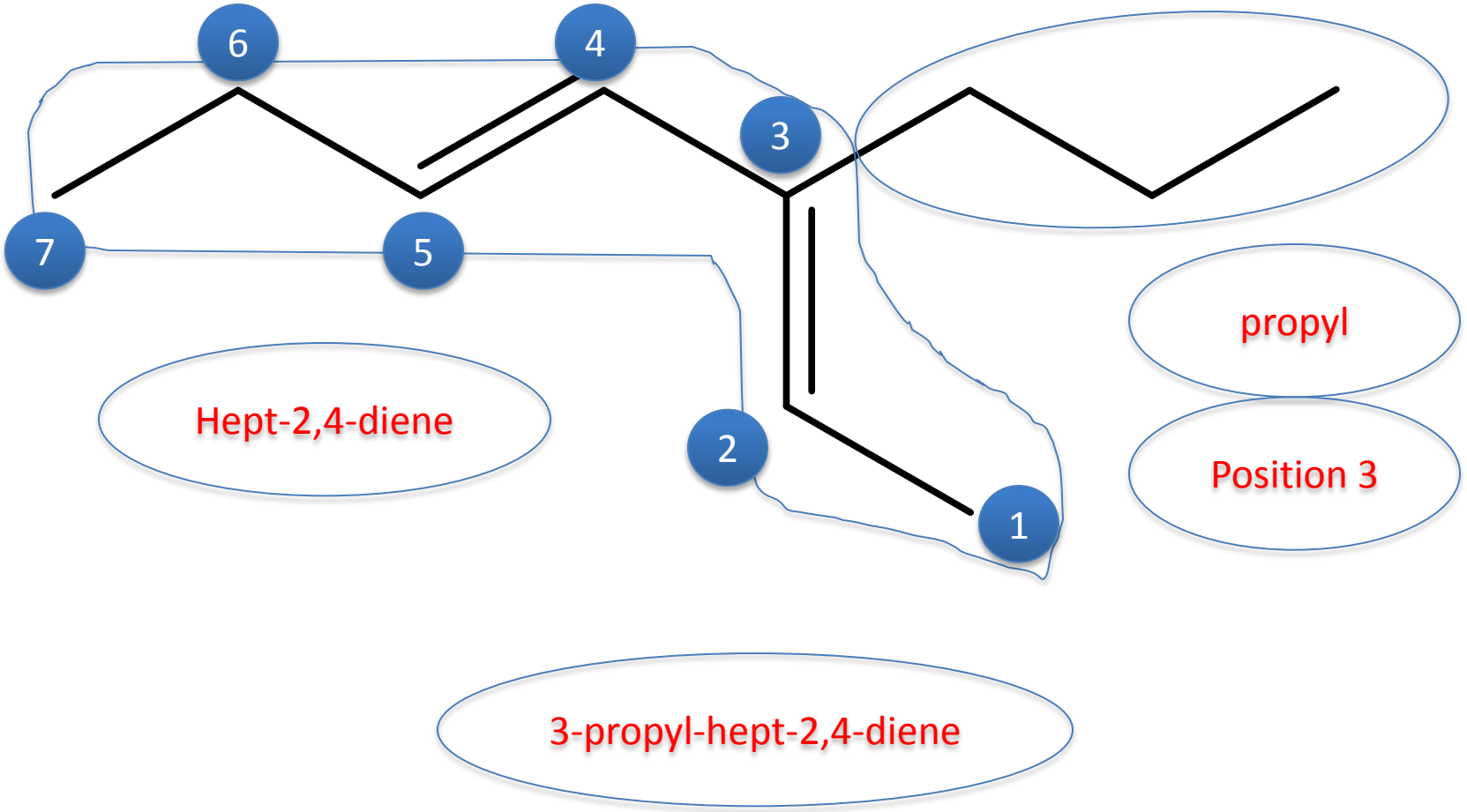
1-heptene

Nomenclature (Alkenes)

If there is substituent → insert number before its name.



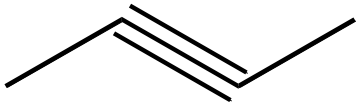
Nomenclature (Alkenes)



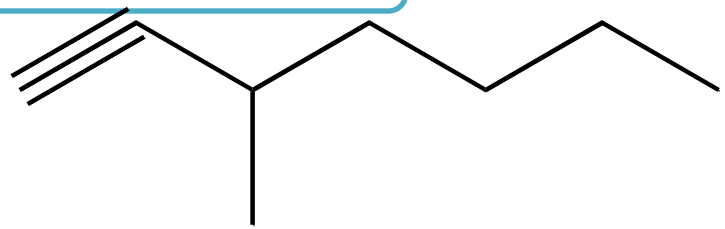
Nomenclature (Alkynes)

IUPAC or Systematic name

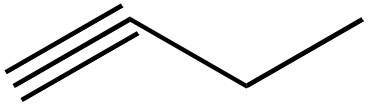
Similar to the naming of alkenes



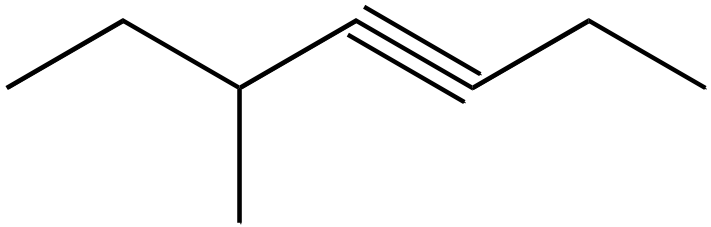
But-2-yne



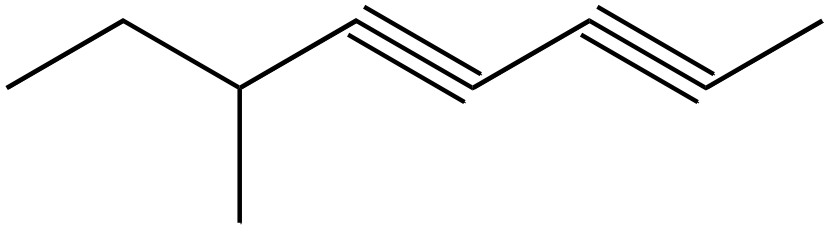
3-Methyl-hept-1-yne



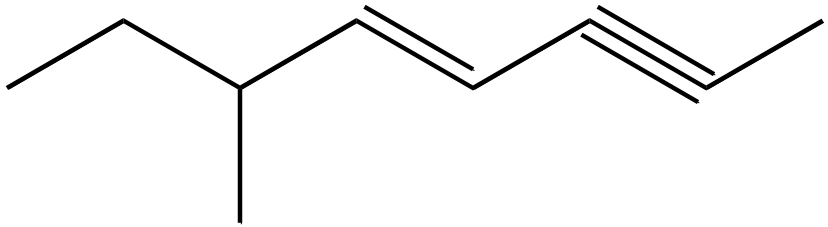
But-1-yne



5-Methyl-hept-3-yne

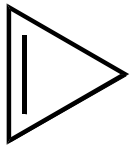


6-Methyl-octa-2,4-diyne

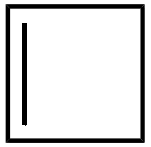


6-Methyl-oct-4-en-2-yne

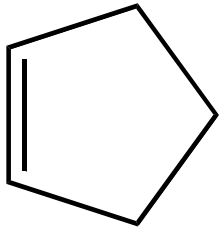
Cycloalkenes



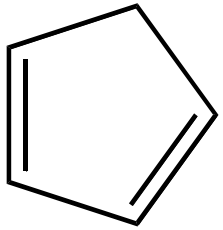
Cyclopropene



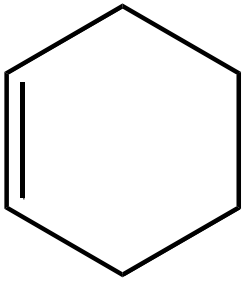
Cyclobutene



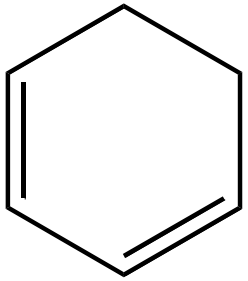
Cyclopentene



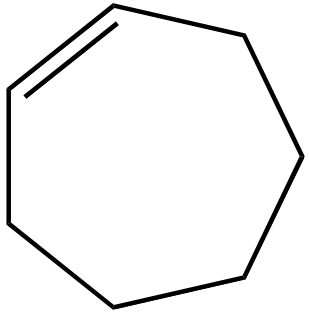
Cyclopenta-1,3-diene



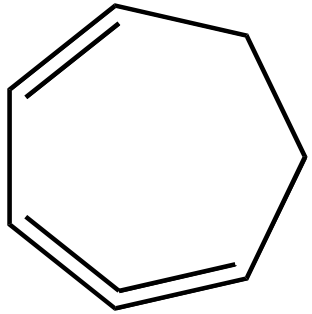
Cyclohexene



Cyclohexa-1,3-diene



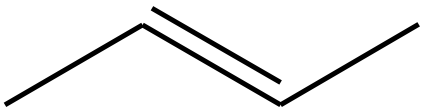
Cycloheptene



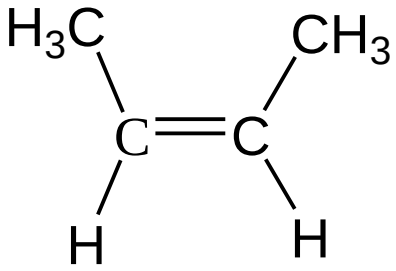
Cyclohepta-1,2,4-triene

Stereoisomers

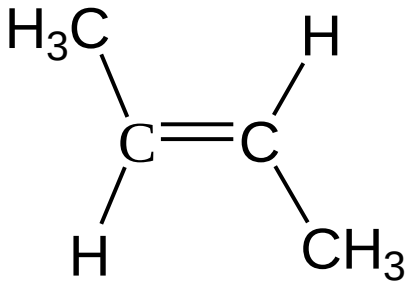
- Stereoisomers posses the same atoms, which exhibits the same connectivity but the composite atoms are oriented differently in space.
  - Different configuration.
  - Differ only in the 3-dimensional arrangement of atoms.
- Two classes
  1. Geometric (cis-trans) isomers.
  2. Enantiomers.



But-2-ene

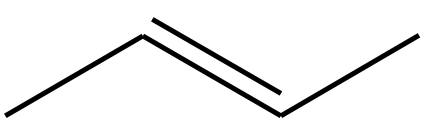


But-2-ene

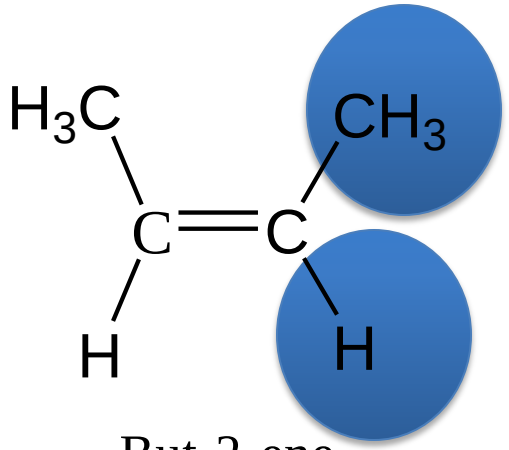


But-2-ene

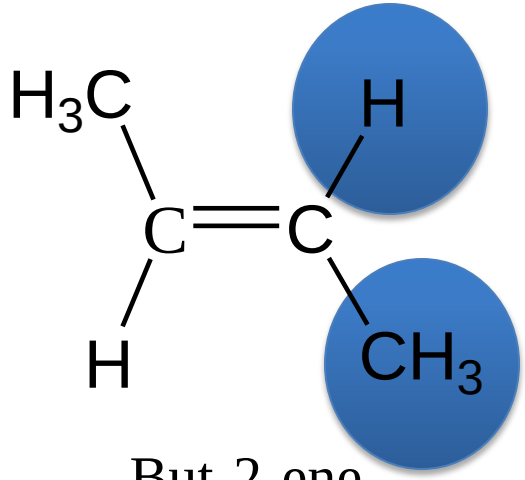
Geometric (cis-trans) isomers



But-2-ene

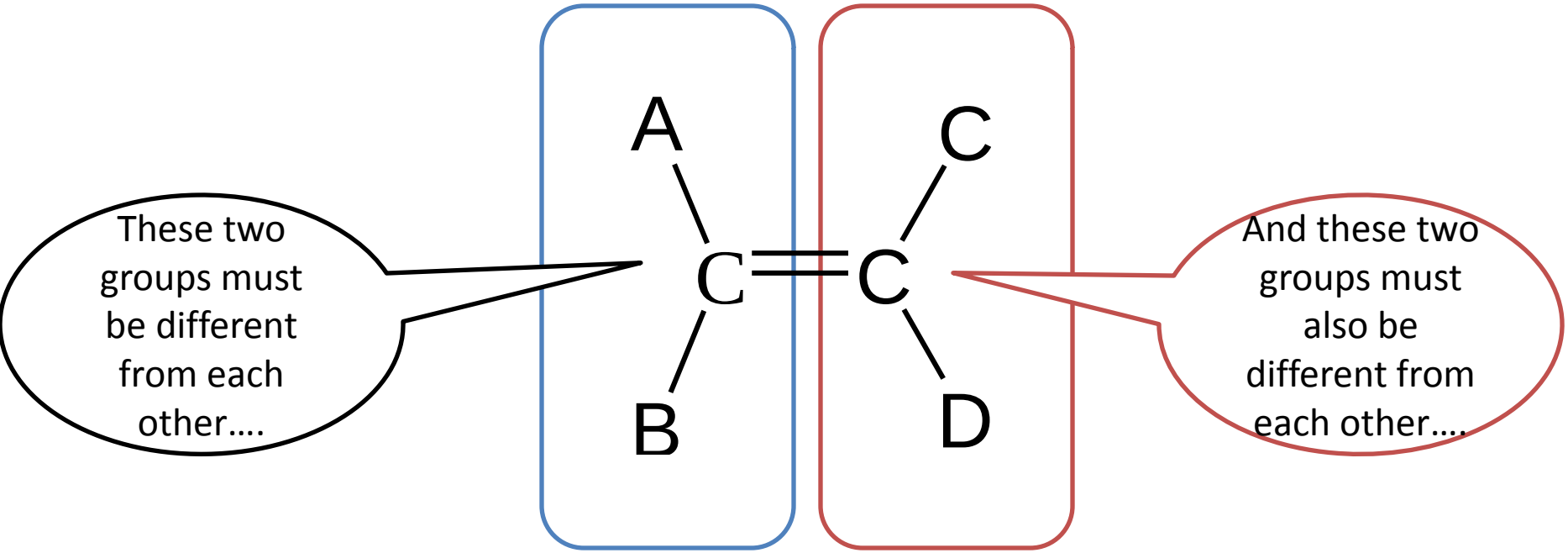


But-2-ene



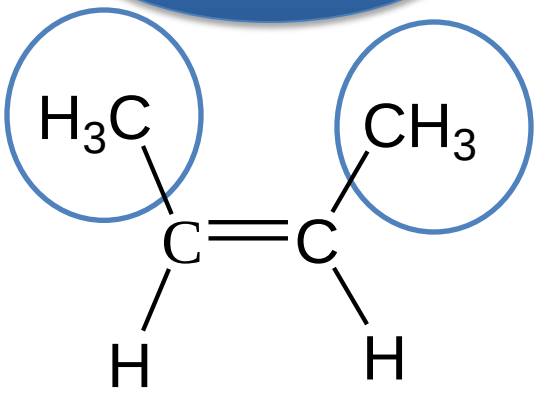
But-2-ene

Geometric (cis-trans) isomers



Geometric (cis-trans) isomers

Methyl groups on the same side

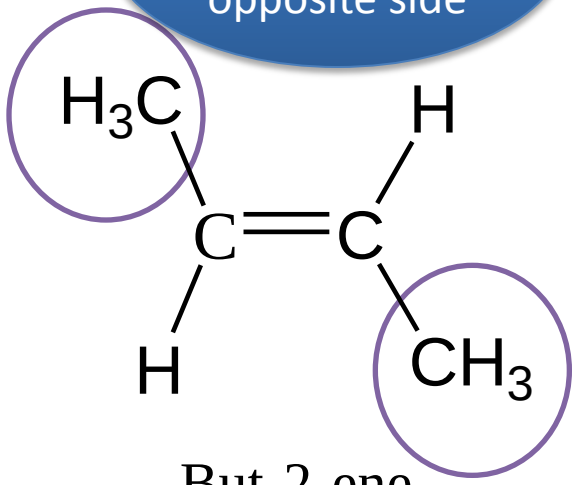


But-2-ene

Cis-2-butene

Cis isomers

Methyl groups on the opposite side



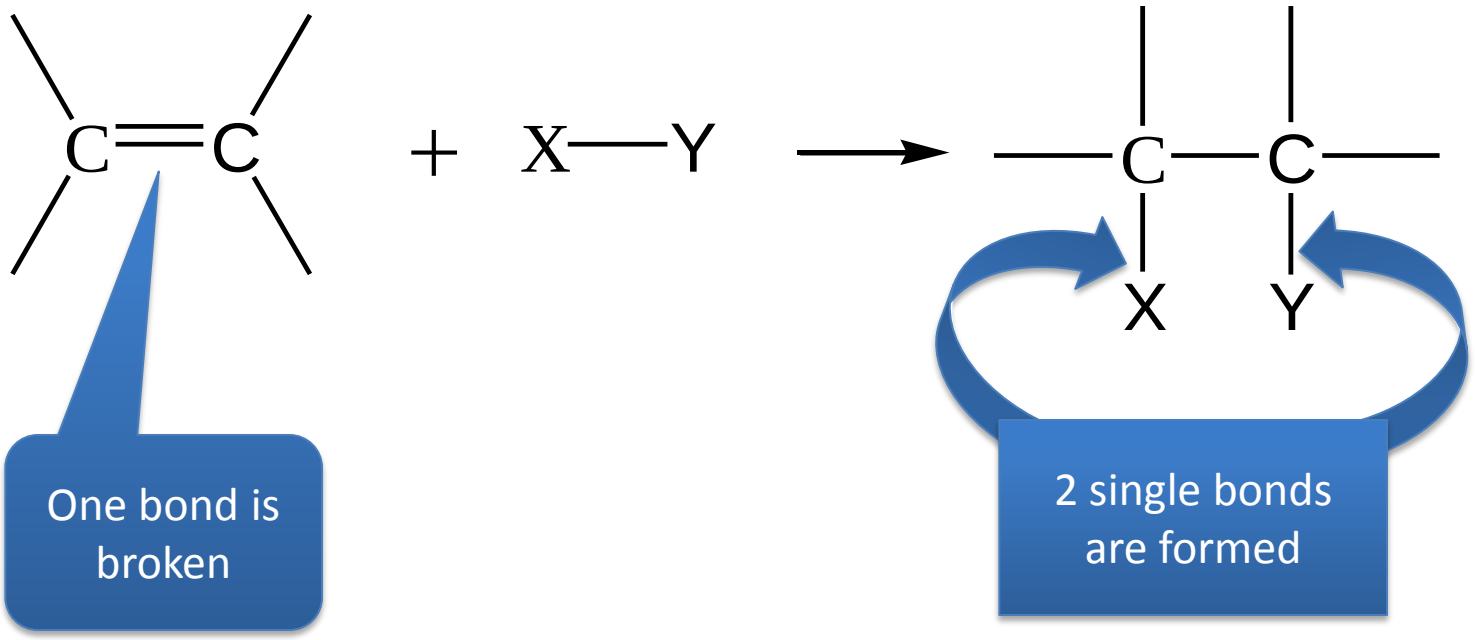
But-2-ene

Trans-2-butene

Trans isomers

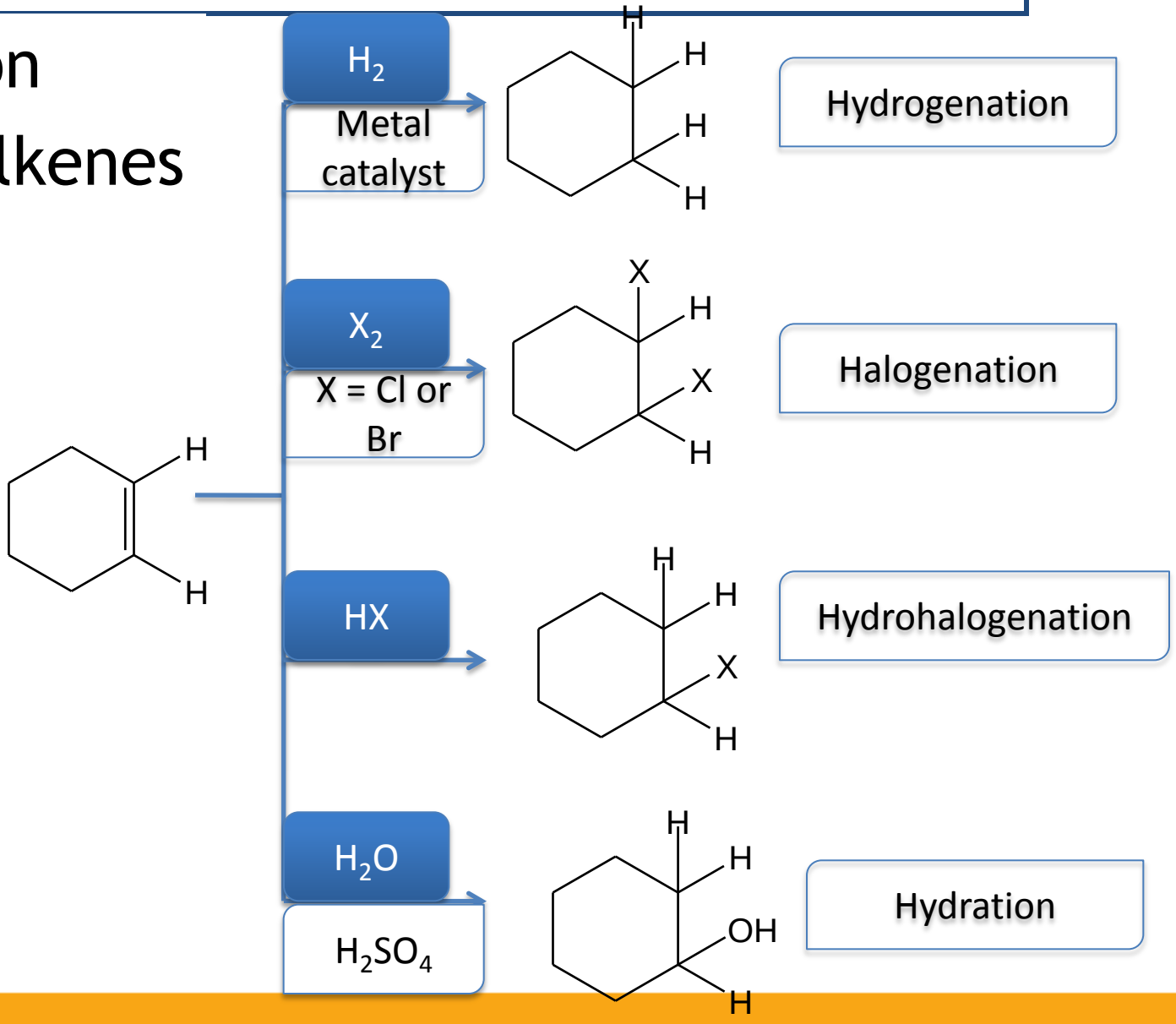
Reactions of Alkenes

- Addition reaction
  - Reaction in which elements are added to a compound



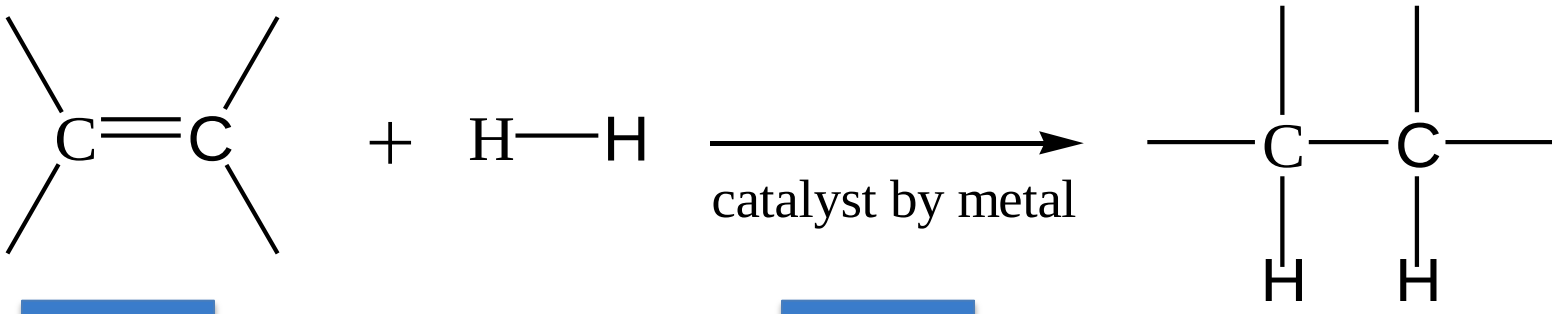
Reactions of Alkenes

- Four addition reactions of alkenes



Hydrogenation

- Addition of hydrogen



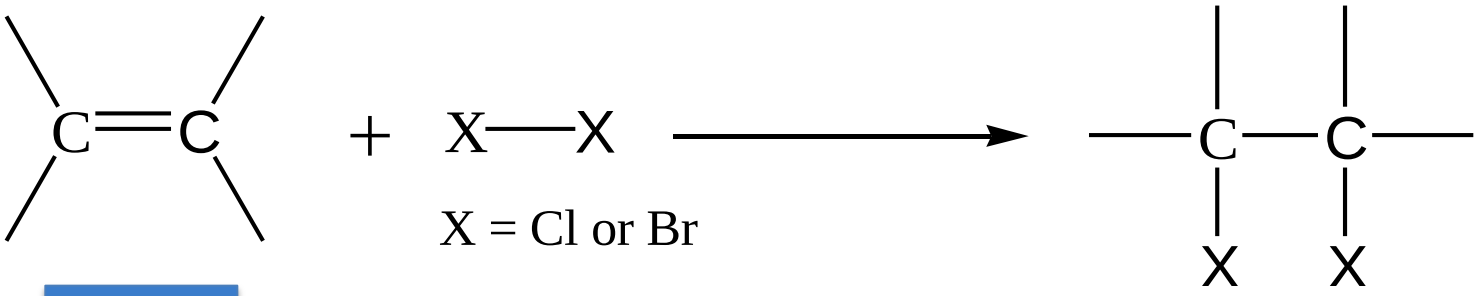
Alkene

E.g. Pd

Alkane

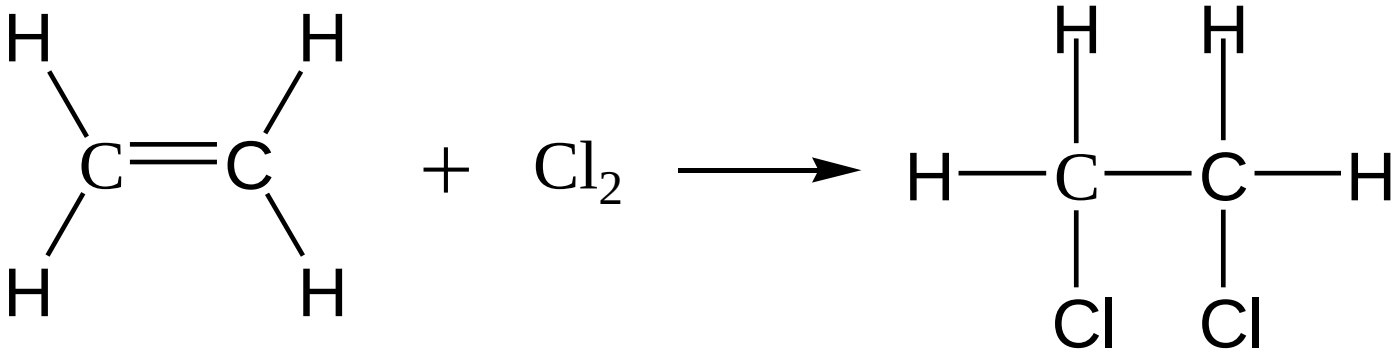
Halogenation

- The addition of halogen (X_2) to an alkene



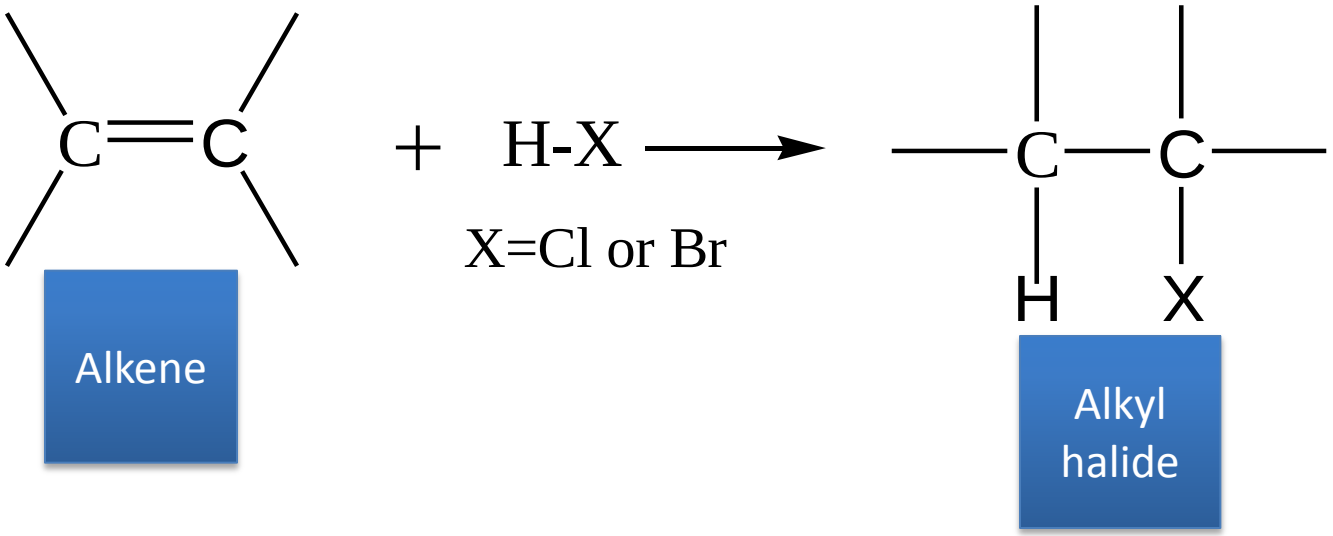
Alkene

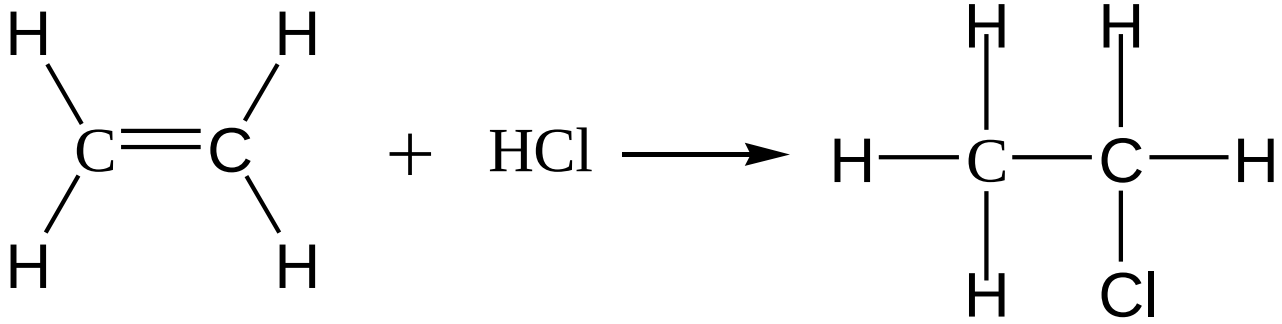
Alkyl dihalide



Hydrohalogenation

- The addition of HX (X = Cl or Br) to an alkene



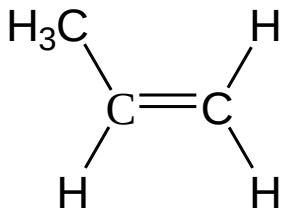


Hydrohalogenation

- Markovnikov's rule
  - In the addition of HX to an unsymmetrical alkene, the H atom bonds to the less substituted carbon atom

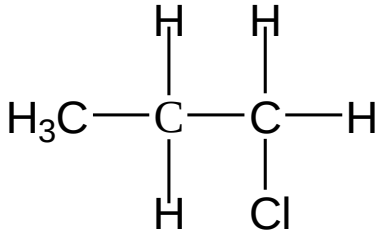
  → The carbon that has more H's to begin with.

Hydrohalogenation



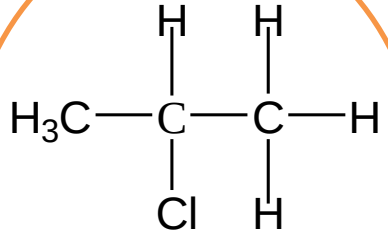
Propene

+ HCl ⟶



1-Chloro-propane

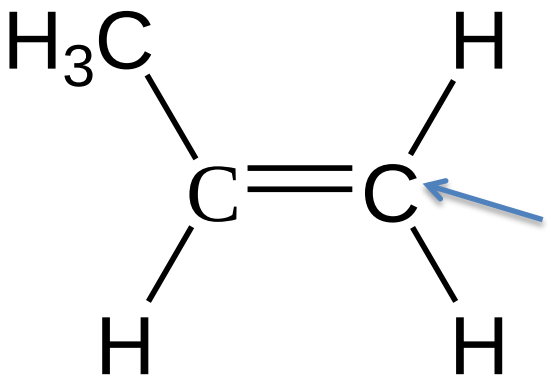
or



2-Chloro-propane

Only product

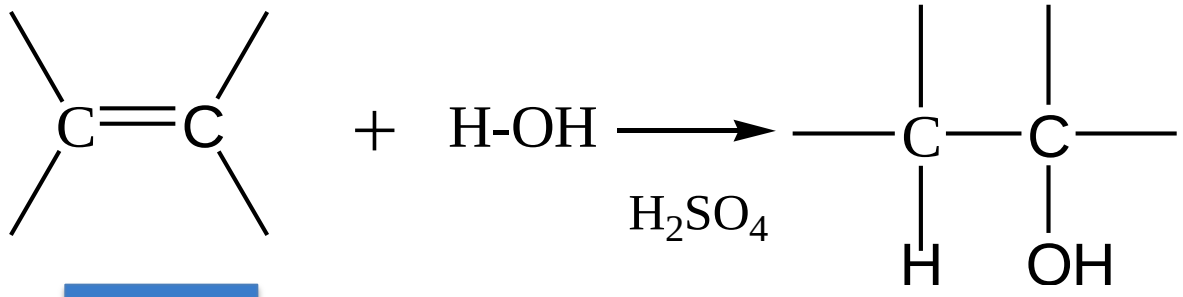
According to Markovnikov's rule



the H atom bonds to the less substituted carbon atom (has more H's)

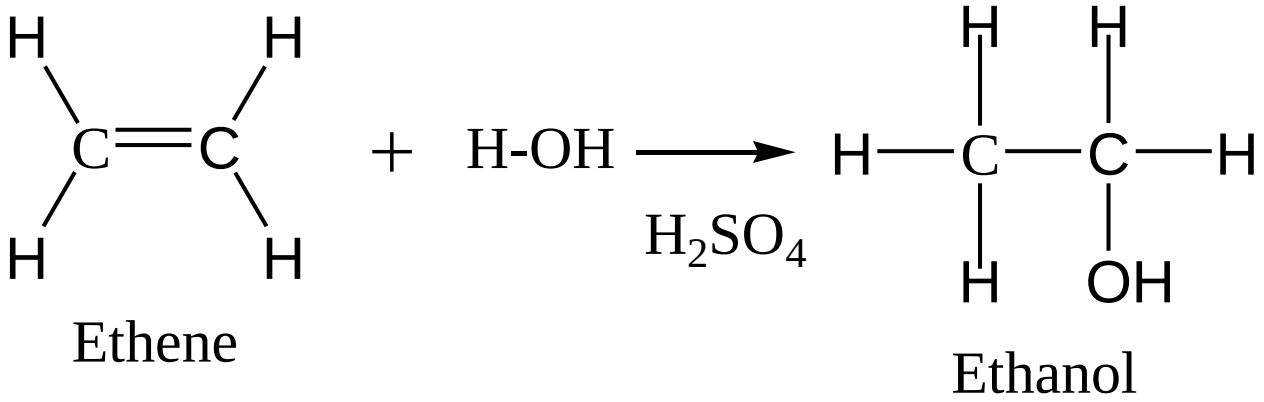
Hydration

- The addition of water (H_2O) to an alkene



Alkene

Alcohol

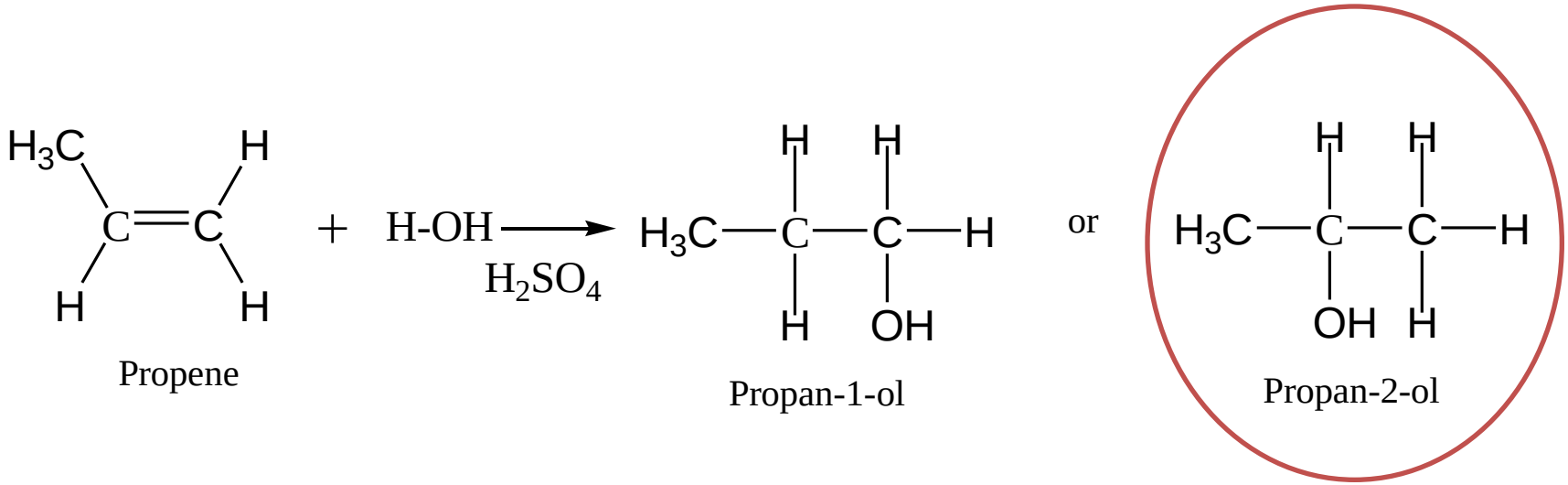


Ethene

Ethanol

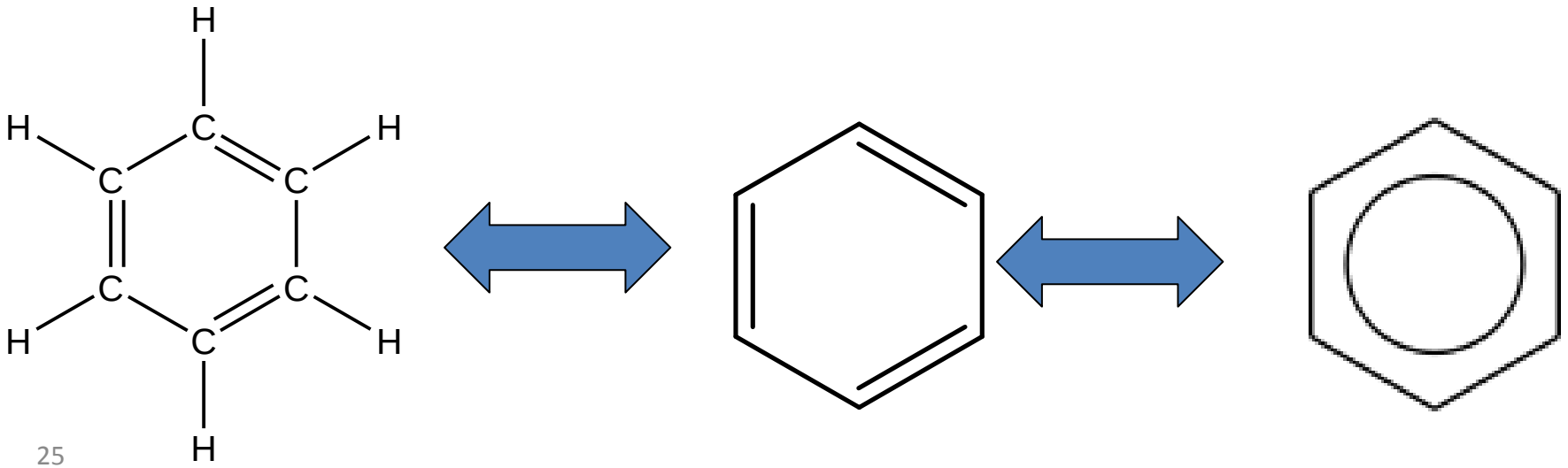
Hydration

- The hydration of unsymmetrical alkene follows markovnikov's rule



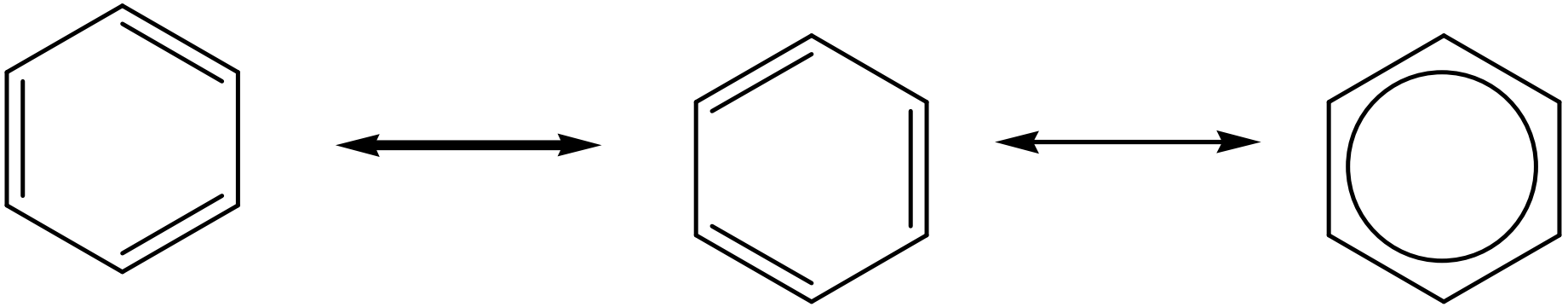
Benzene and aromatic compounds

- Unsaturated hydrocarbons
- Benzene
  - The simplest and widely known aromatic compound
  - Six-membered ring and 3 double bonds.
  - Molecular formula: C_6H_6

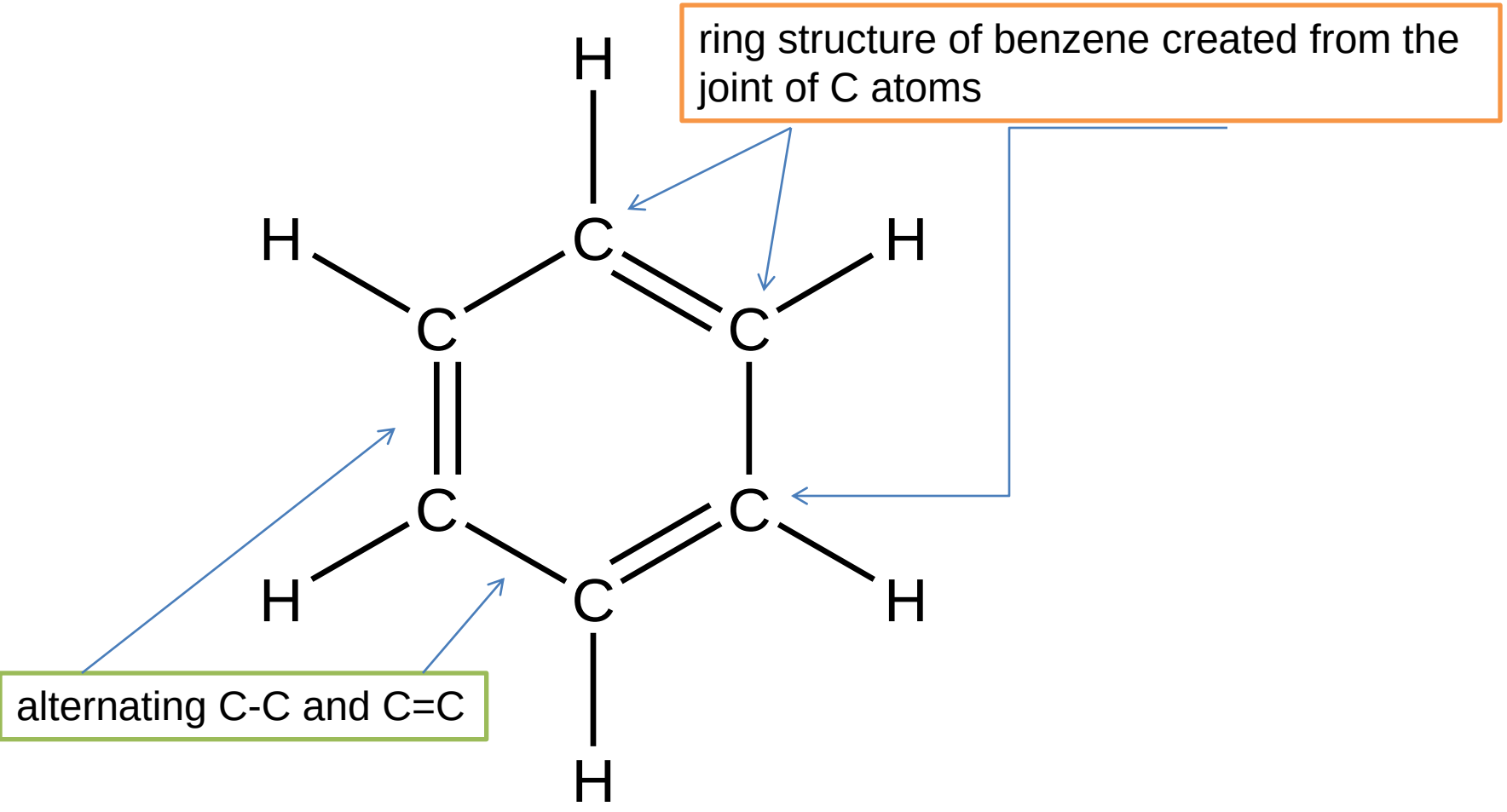


Benzene

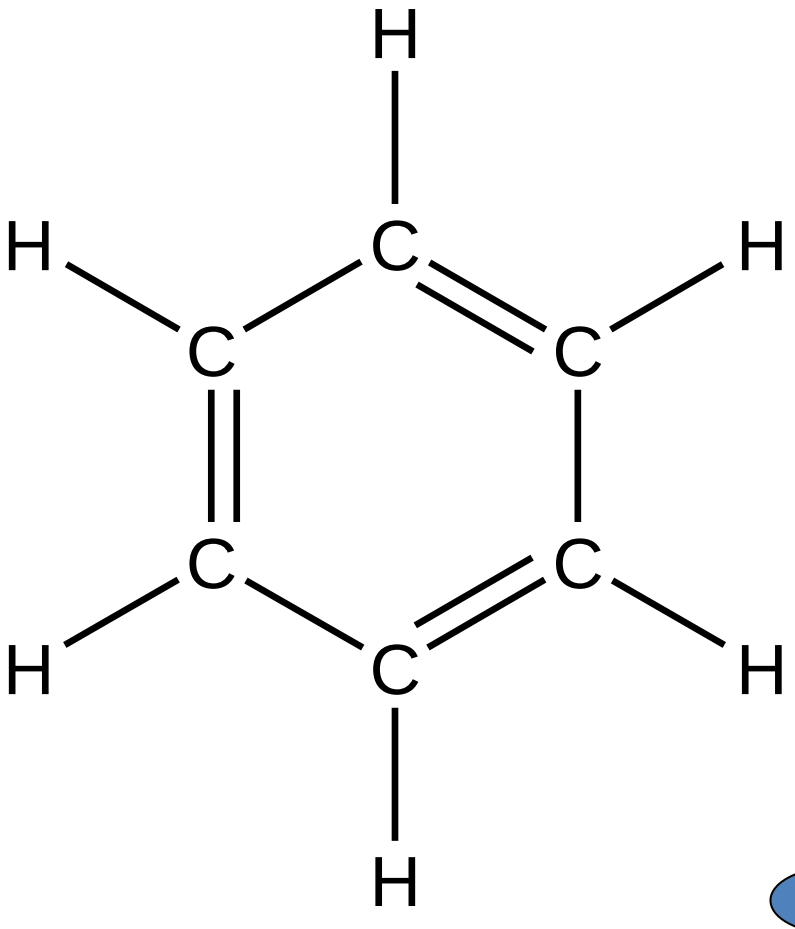
- Resonance structures
  - Lewis structure with the same arrangement of atoms but a different arrangement of electrons



Aromatic compounds and conjugated bonds



Aromatic compounds and conjugated bonds



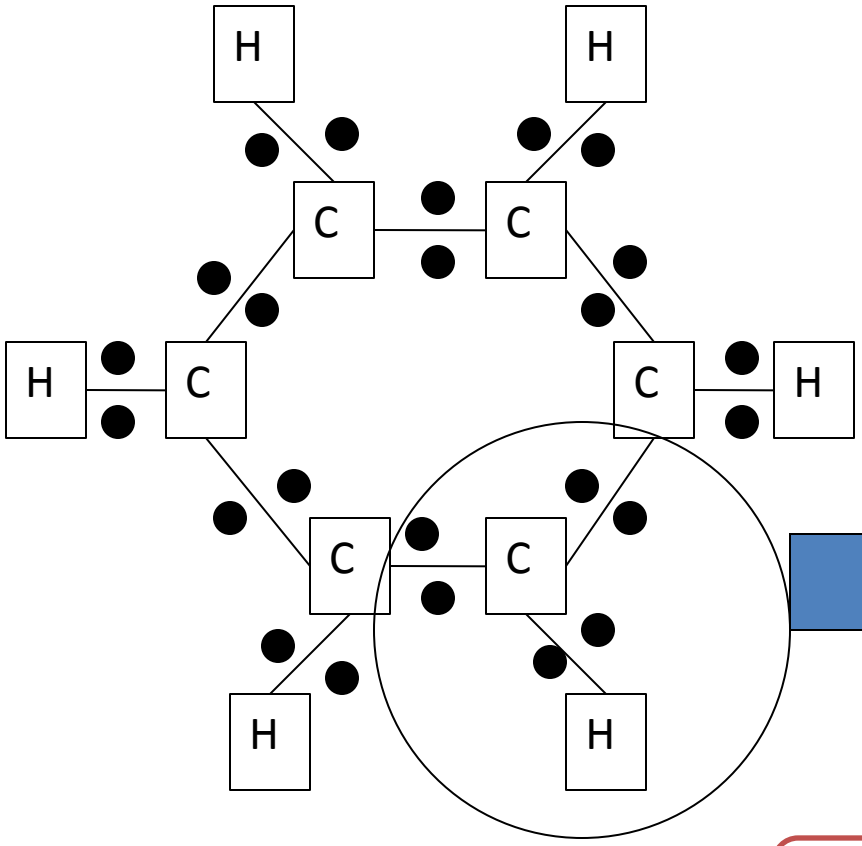
Actually

- C atoms are not joined by alternating C-C and C=C:
- But, by a network of bonds that fall halfway between single and double.

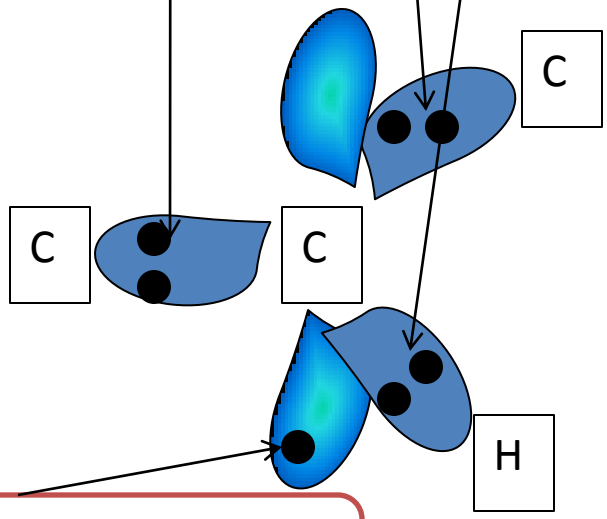
So what is happening here?

How can there be this 'special' bond network?

Aromatic compounds and conjugated bonds



3 σ bonds containing 3 valence electrons from the central C atom

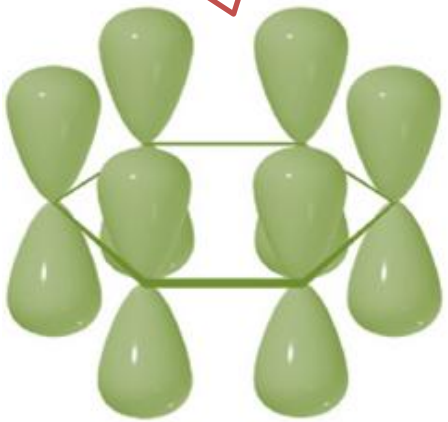


Each C atom contributes 3 valence electrons to 3 single covalent bonds

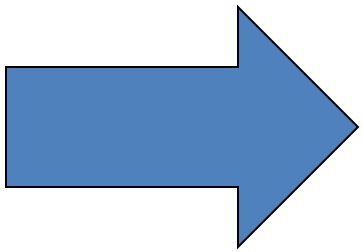
The fourth valence electron occupies a *p* orbital

Aromatic compounds and conjugated bonds

The p orbital on adjacent C atoms overlap



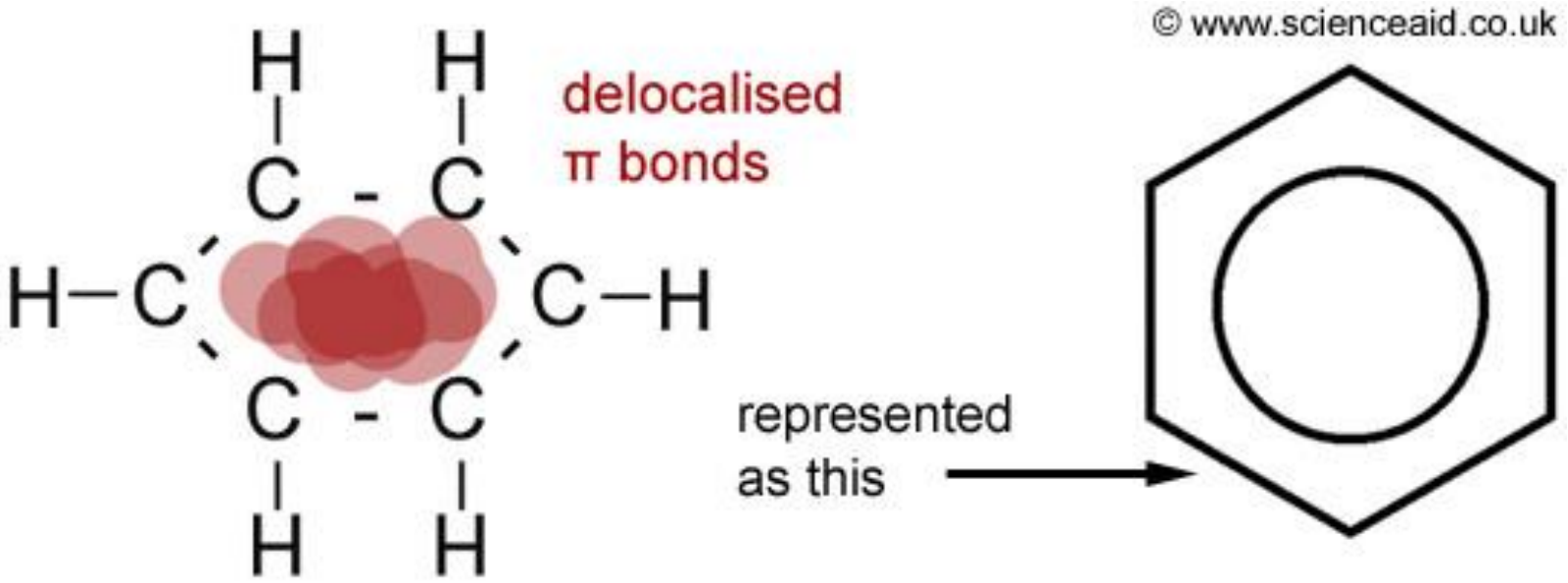
Two doughnut-shaped rings form a unique π-bond above and below the benzene ring



The p orbitals of 6 C atoms that form a benzene ring overlap to form an unusual pi (π) orbital, which takes the form of two doughnut-shaped rings.

Aromatic compounds and conjugated bonds

The valence electrons occupying the overlapping π orbitals are not restricted to being associated with one or two specific C atoms
→ **free to move** anywhere within the doughnut-shaped π bond



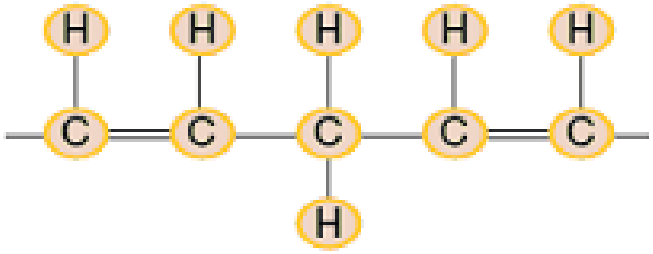
Aromatic compounds and conjugated bonds

Conjugated system → Overlap of p-orbitals

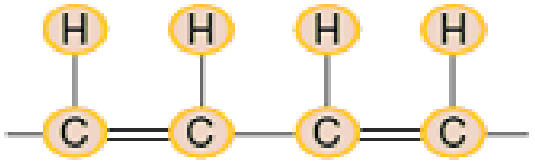
→

Conjugation of bonds (to form a network of delocalized electrons) can occur wherever **2 double bonds are separated by one single bond**.

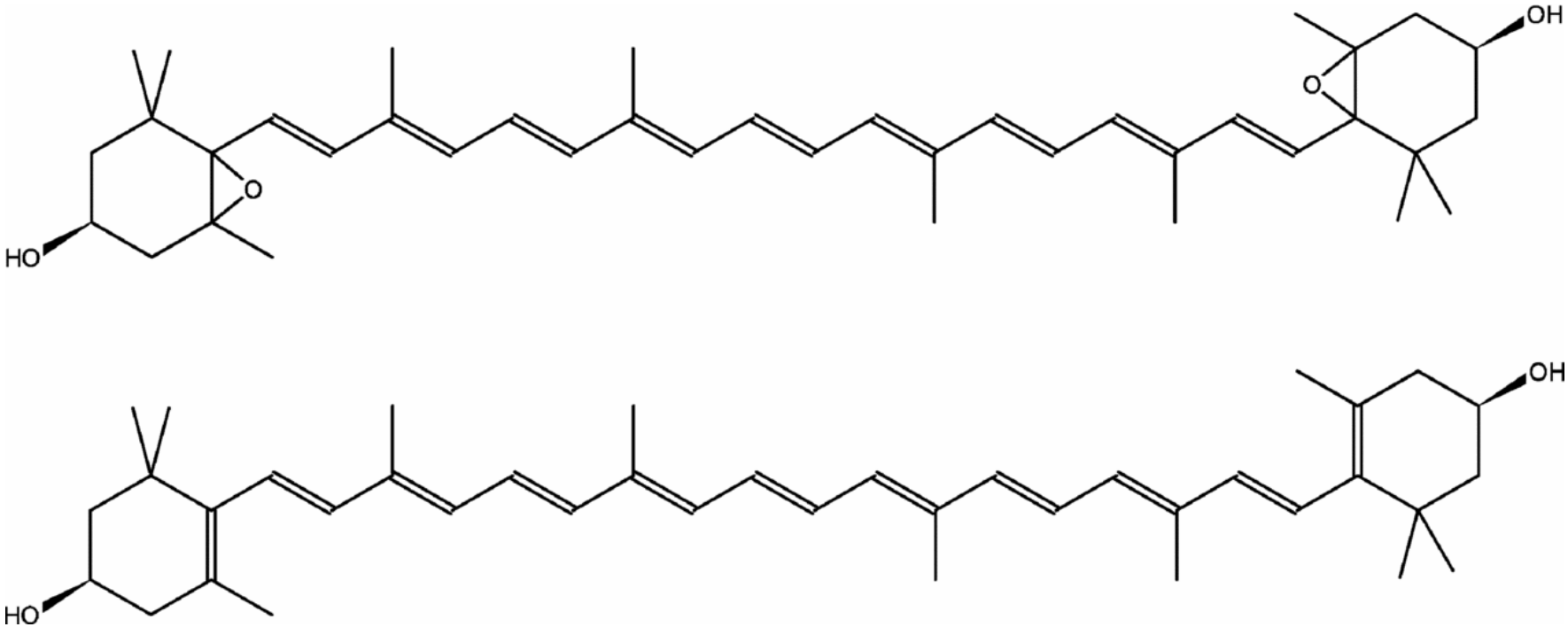
non-conjugated



conjugated

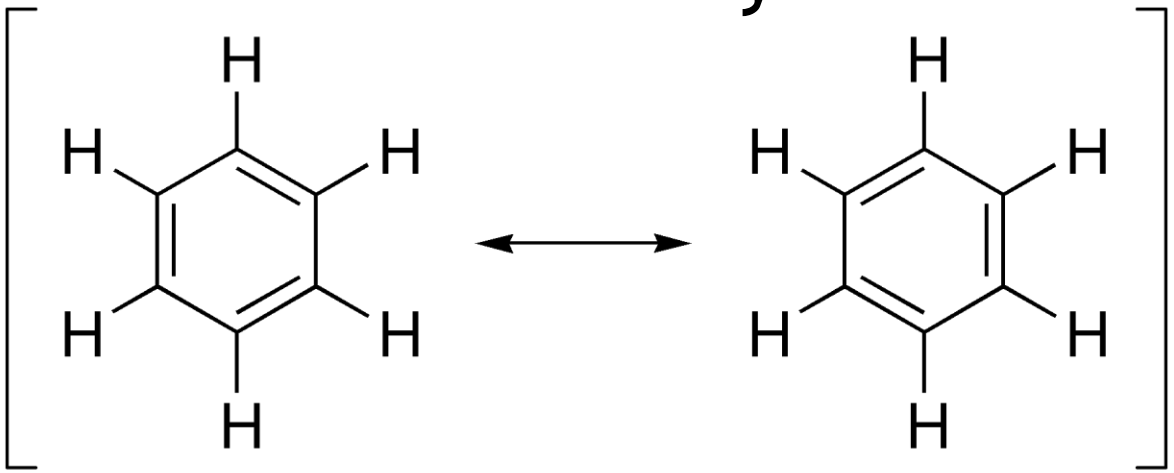


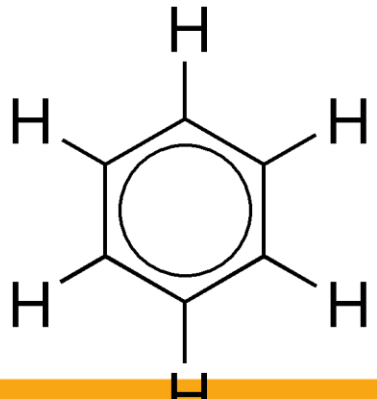
Aromatic compounds and conjugated bonds



Aromatic compounds and conjugated bonds

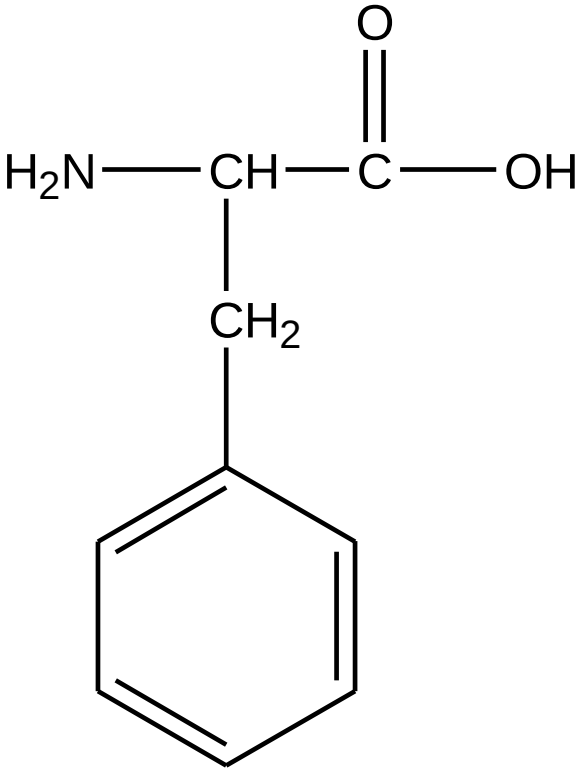
Resonance Hybrid



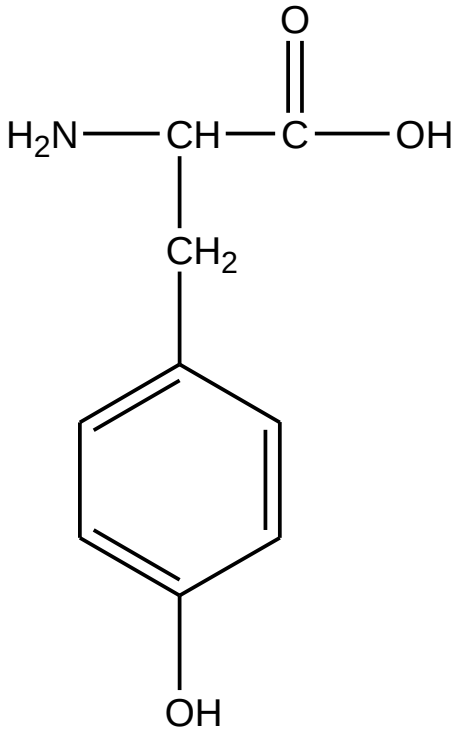


Aromatic compounds and conjugated bonds

- Aromatic compounds in biological systems



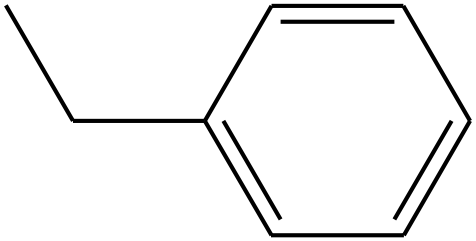
Phenylalanine (amino acid)



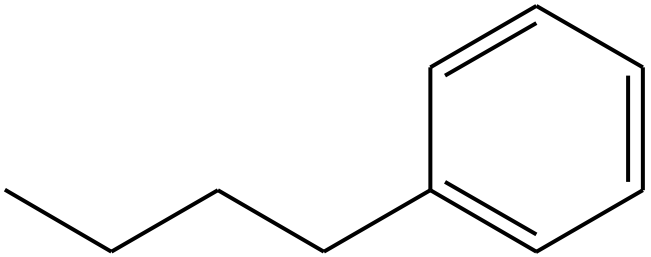
tyrosine (amino acid)

Nomenclature

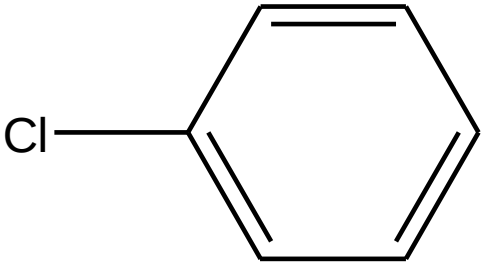
- **Monosubstituted** benzenes
  - Name of substituents + benzene.



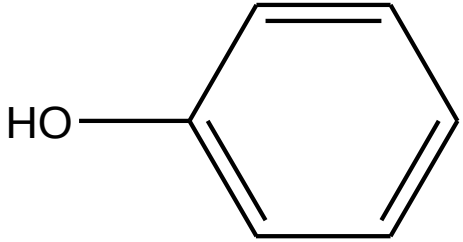
ethylbenzene



butylbenzene

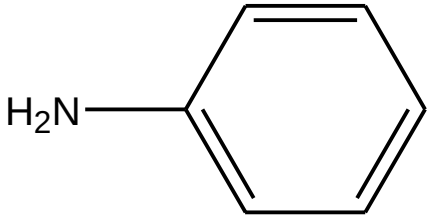


chlorobenzene



phenol

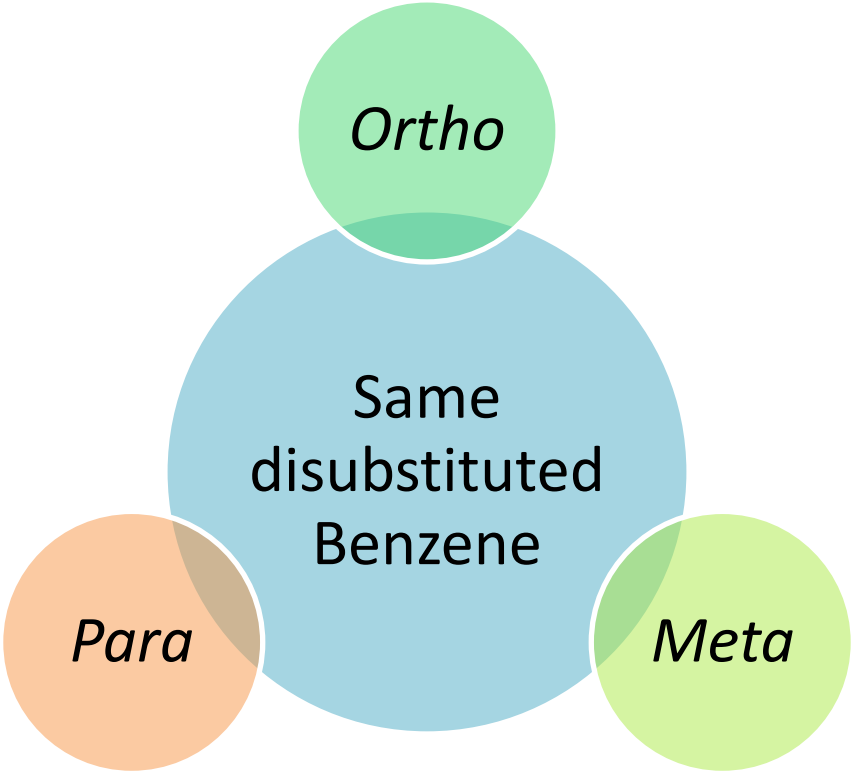
IUPAC name: hydroxybenzene



aniline

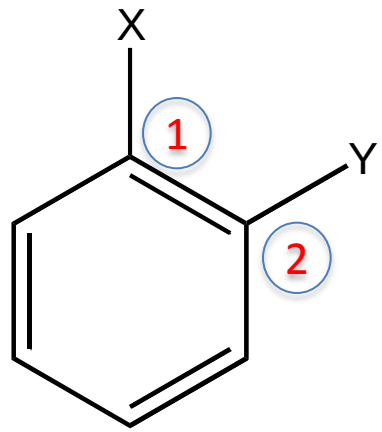
IUPAC name: aminobenzene

Nomenclature

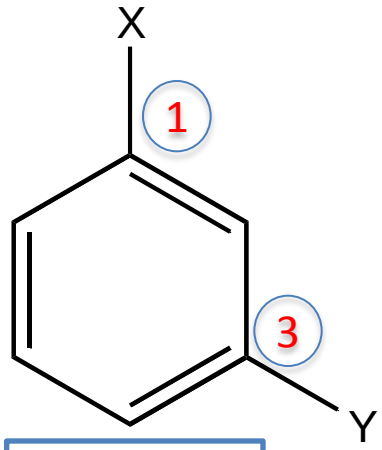


Nomenclature

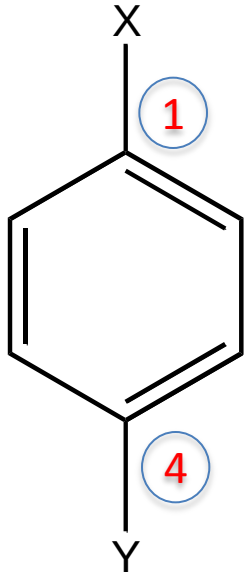
- Disubstituted benzene



1,2- or
ortho- (***o***)



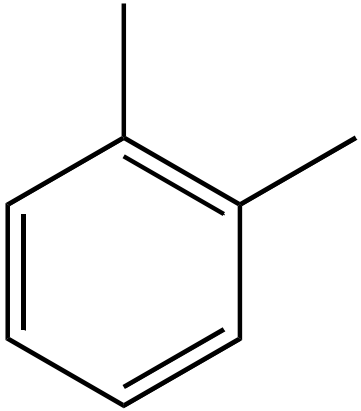
1,3- or
meta- (***m***)



1,4- or
para- (***p***)

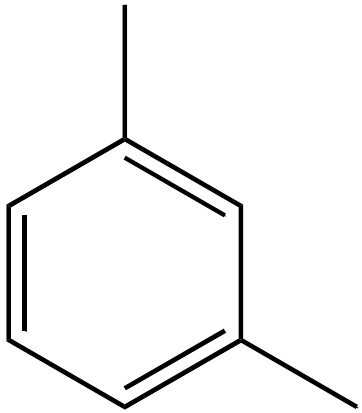
Nomenclature

- Disubstituted benzene
  - Example



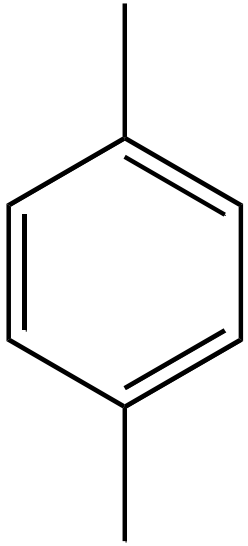
o-Xylene

1,2-dimethylbenzene (IUPAC)



m-Xylene

1,3-dimethylbenzene (IUPAC)

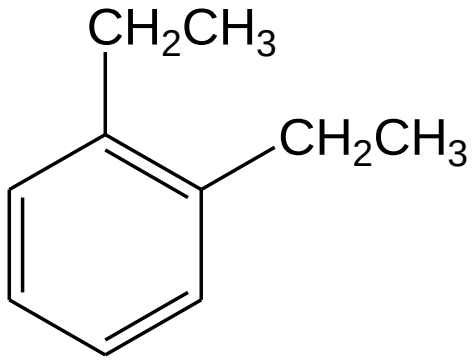


p-Xylene

1,4-dimethylbenzene (IUPAC)

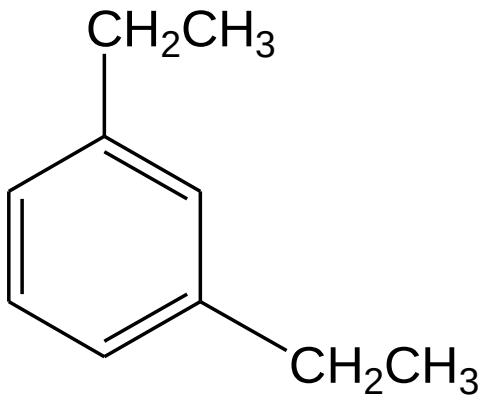
Nomenclature

- Disubstituted benzene
  - Example



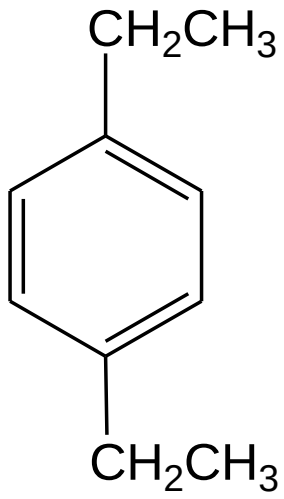
1,2-Diethyl-benzene

ortho-diethyl-benzene
or
o-diethyl-benzene



1,3-Diethyl-benzene

meta-diethyl-benzene
or
m-diethyl-benzene

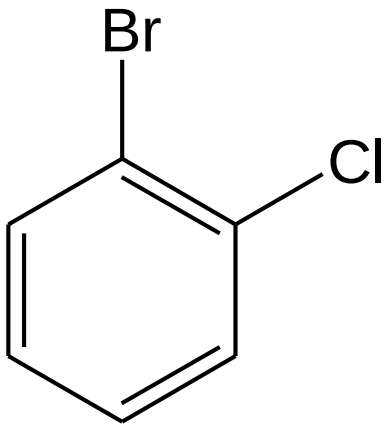


1,4-Diethyl-benzene

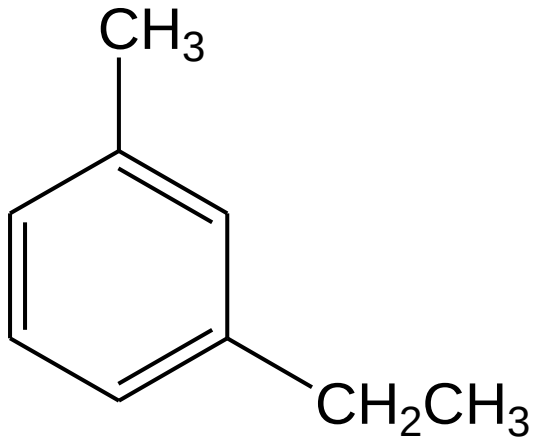
para-diethyl-benzene
or
p-diethyl-benzene

Nomenclature

- Disubstituted benzene
  - Different substituents → alphabetize the name of the substituents.



1-Bromo-2-chloro-benzene



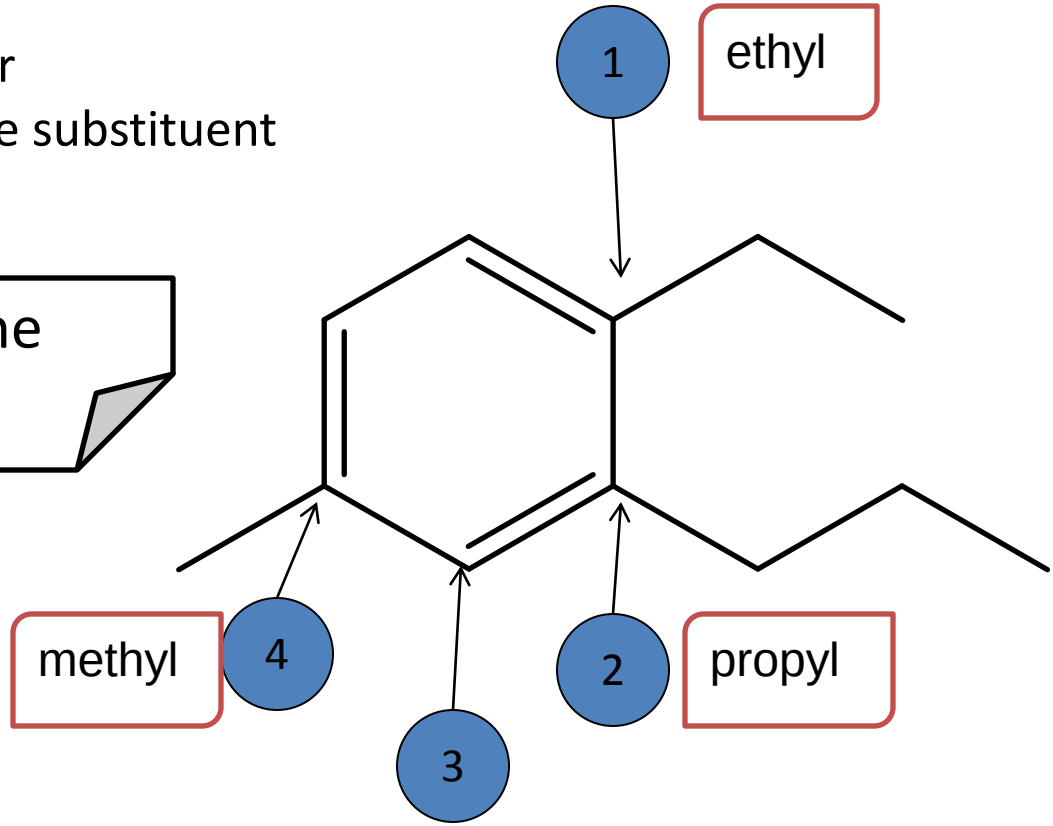
1-Ethyl-3-methyl-benzene

Nomenclature

- **Polysubstituted** (Three or more substituents) benzenes

1. Assign the lowest set of number
2. Alphabetize the names of all the substituent

1-ethyl-4-methyl-2-propylbenzene

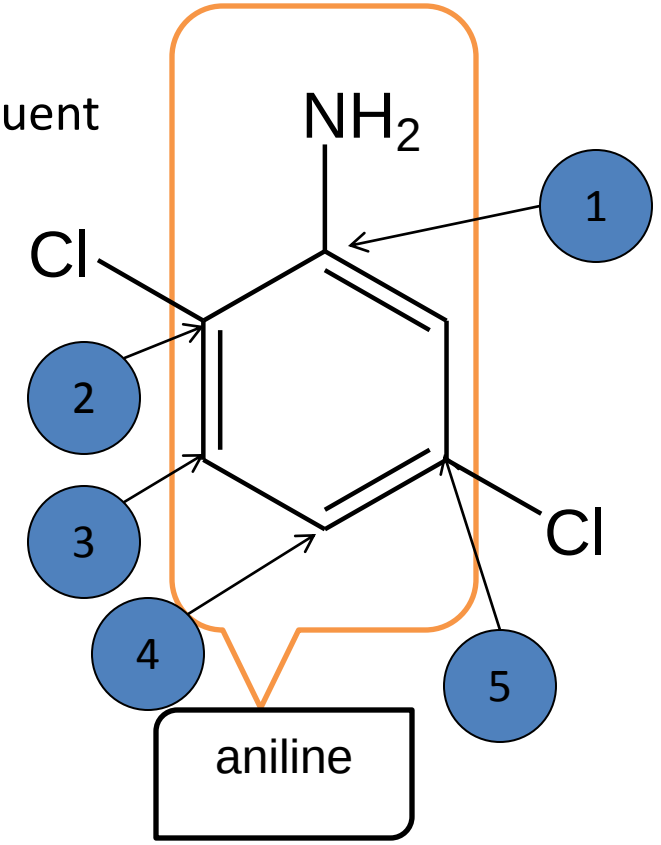


Nomenclature

- **Polysubstituted** (Three or more substituents) benzenes

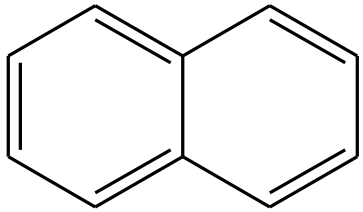
1. The common root = aniline
2. Alphabetize the names of all the substituent

2,5-dichloroaniline

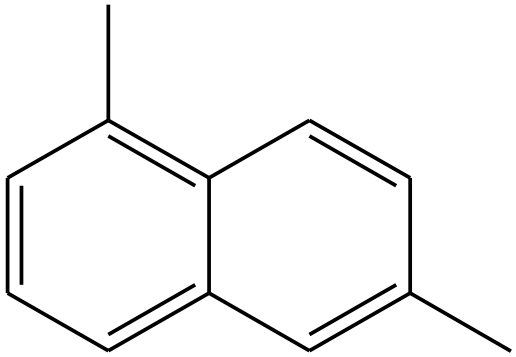


Nomenclature

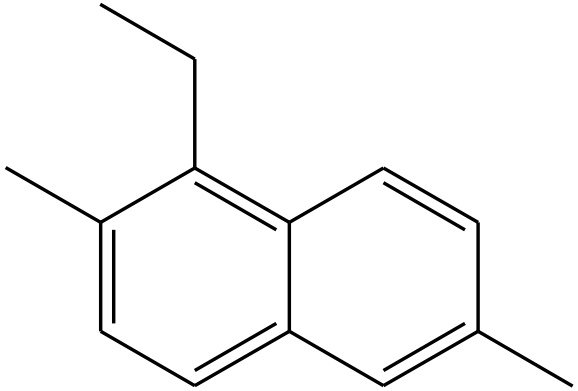
- Aromatic compounds with more than one ring



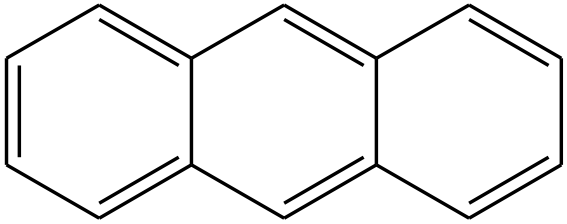
Naphthalene



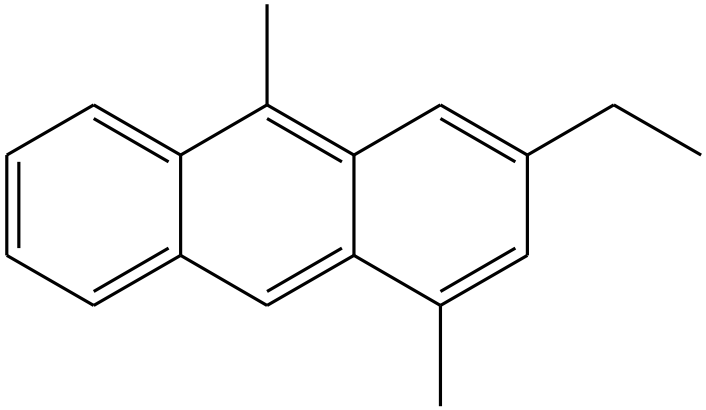
1,6-Dimethyl-naphthalene



1-Ethyl-2,6-dimethyl-naphthalene



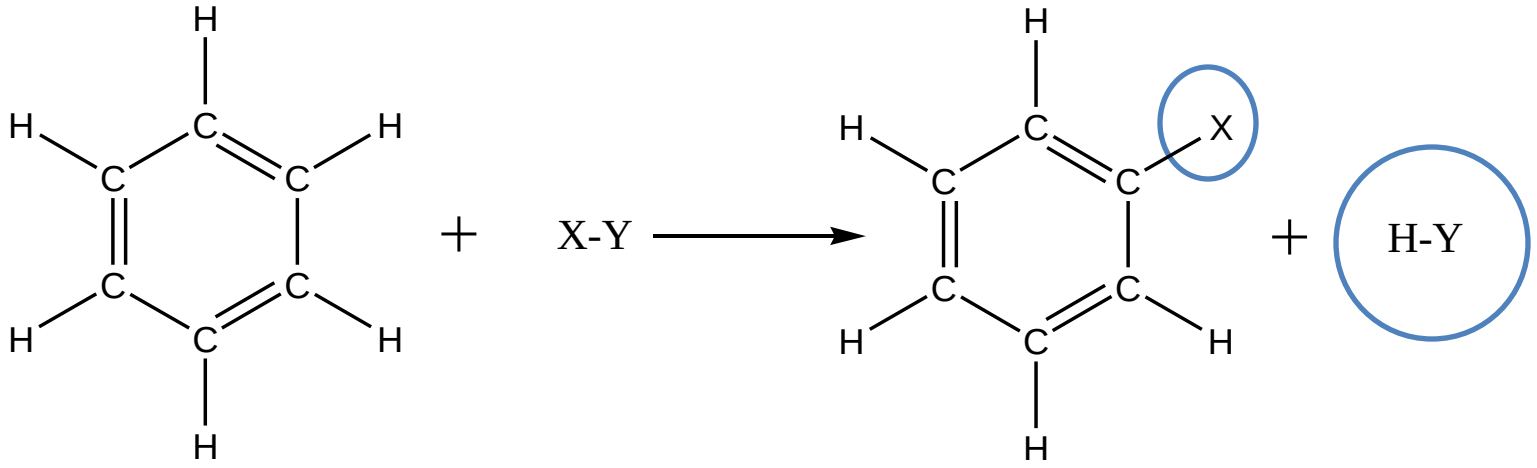
Anthracene



3-Ethyl-1,10-dimethyl-anthracene

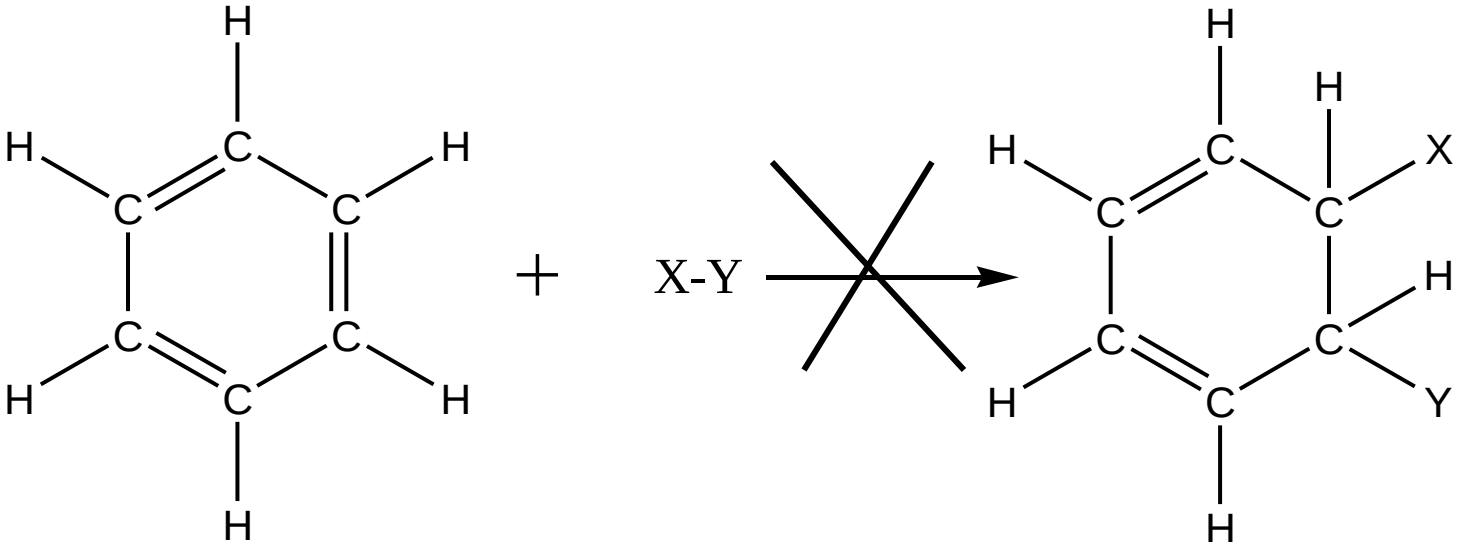
Reaction of aromatic compounds

- Aromatic compounds undergo substitution not addition
- Substitution
  - A reaction in which an atom is replaced by another atom or a group of atoms.



Reaction of aromatic compounds

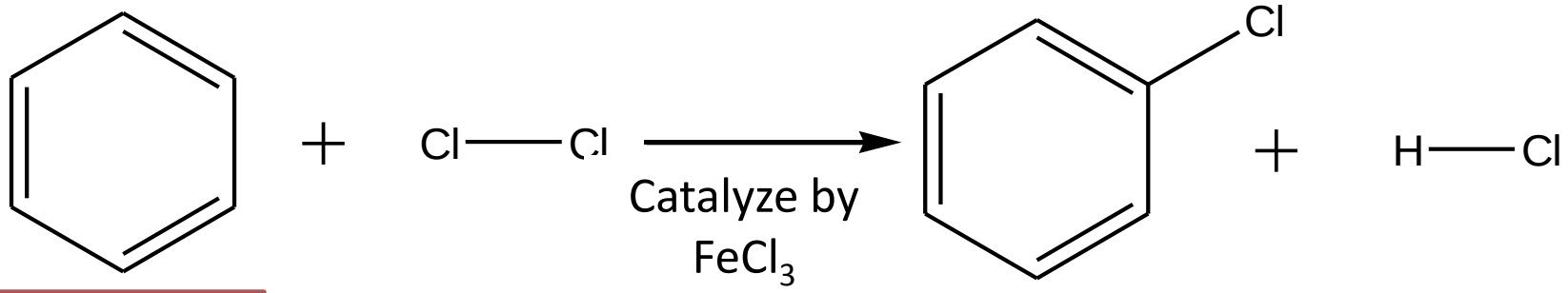
- No addition reaction for benzene
- C=C in Benzene ≠ C=C in alkene



Reaction of aromatic compounds

- Three specific reactions
  - Chlorination → -Cl
  - Nitration → $-NO_2$
  - Sulfonation → $-SO_3H$

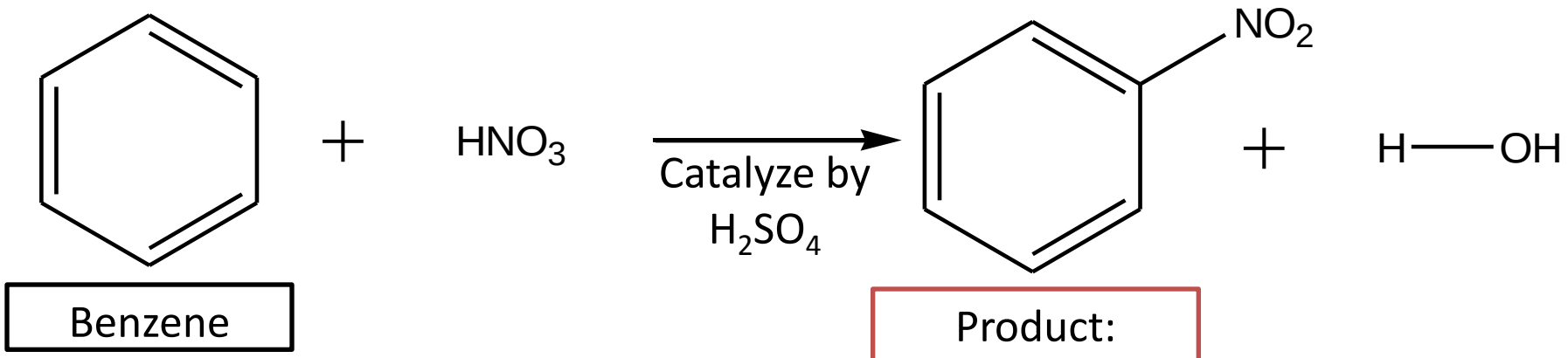
Reaction of aromatic compounds



Benzene

Product: aryl halide

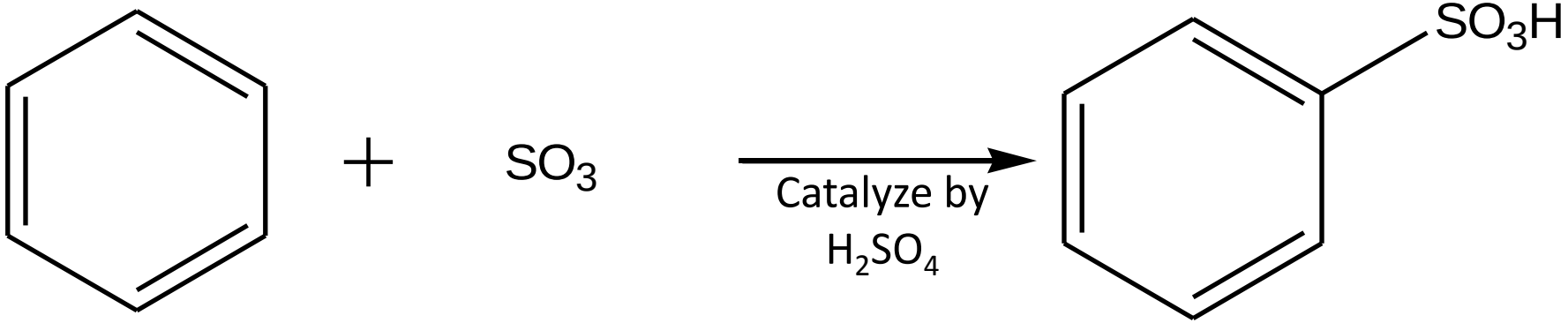
Nitration



Benzene

Product: nitrobenzene

Sulfonation



Benzene

Product:
benzenesulfonic acid

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