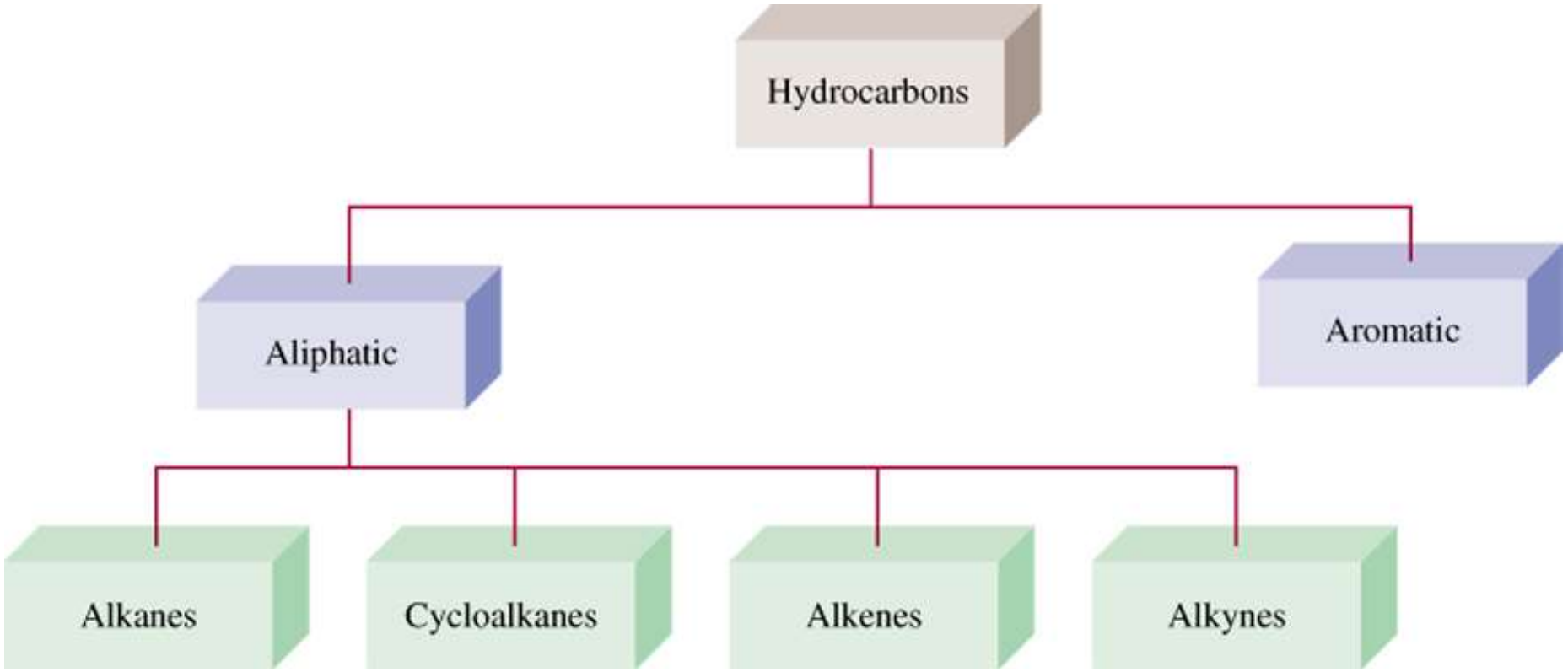
Chapter 2: Hydrocarbon

- The **simplest** organic compounds are **hydrocarbons**, compounds containing only carbon and hydrogen

- There are three main groups:
  - **Saturated hydrocarbons**, hydrocarbons with only single bonds between the carbon atoms.
  - **Unsaturated hydrocarbons**, hydrocarbons that contain double or triple bonds between carbon atoms.
  - **aromatic hydrocarbons**, hydrocarbons that contain a benzene ring (a six-membered ring of carbon atoms with alternating single and double carbon-carbon bonds described by resonance formulas).

Chapter 2: Hydrocarbon

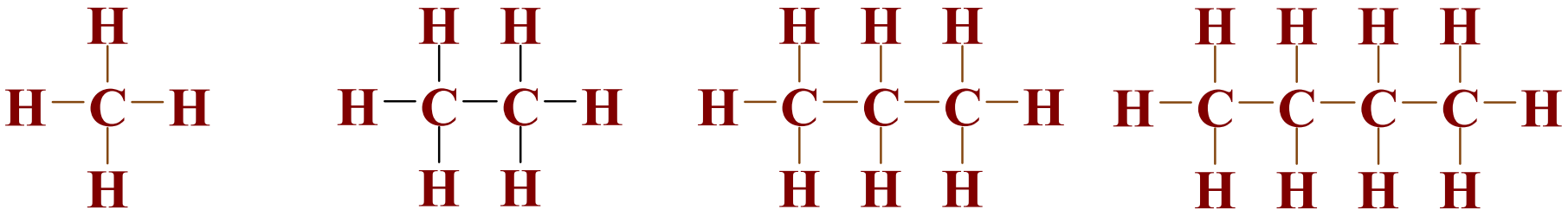


Alkanes

- The alkanes are acyclic, saturated hydrocarbons that form a homologous series of compounds, with the general formula C_nH_{2n+2}.

- Examples: CH_4 ; C_2H_6; C_3H_8; C_4H_{10} ; etc.

- Draw **Lewis** Structures



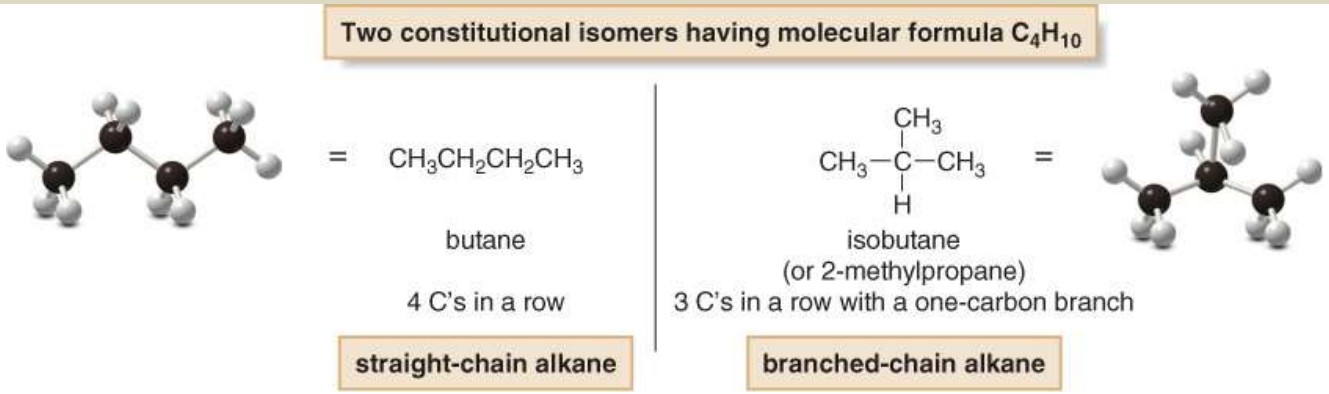
methane CH_4

ethane $CH_3{-}CH_3$

propane $CH_3{-}CH_2{-}CH_3$

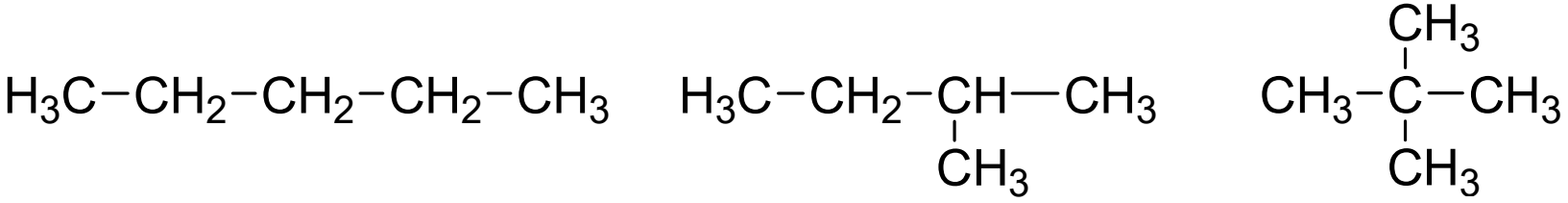
butane $CH_3{-}CH_2{-}CH_2{-}CH_3$

Isomerism



- **Constitutional Isomers (Structural Isomers)** are different compounds of the same formula.
- **Example**: How many isomers are there of an **alkane** containing five carbons (C_5H_{12})?

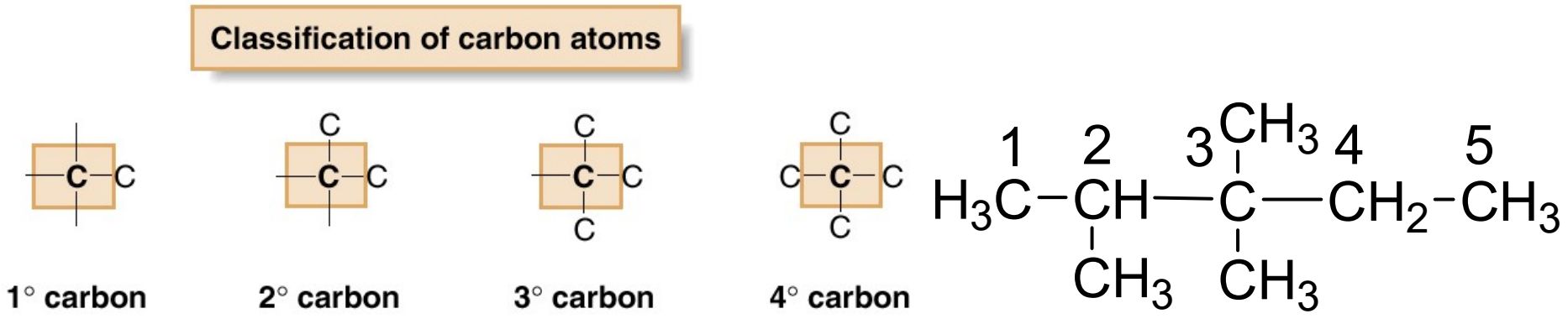
Isomer Strategy – Draw Lewis possible different length chains of carbons atoms connected with a covalent bond



- **Example**: How many isomers are there of an **alkane** containing six carbons (C_6H_{14})?

Types of carbon

- Carbon atoms in alkanes and other organic compounds are classified by the number of other carbons directly bonded to them.
  - **Primary** (1°) Carbon connected to one carbon atoms.
  - **Secondary** (2°) Carbon connected to two carbon atoms.
  - **Tertiary** (3°) Carbon connected to three carbon atoms.
  - **Quaternary** (4°) Carbon connected to four carbon atoms.



Nomenclature (danh pháp) : **Common Name**

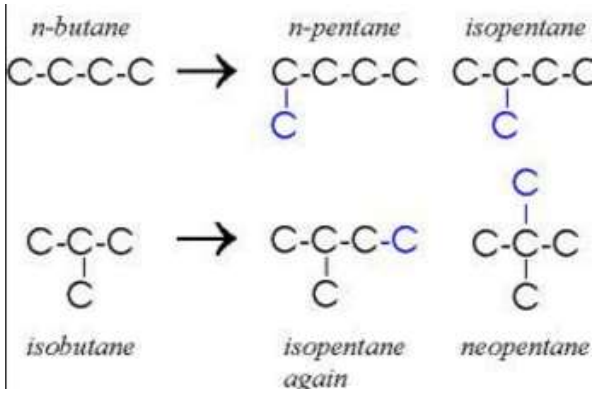
There are **two types**: **Common** and **Systematic** name

1. Common Name: Works best for **low** molecular weight hydrocarbons

❑ Steps to give a hydrocarbon with a common name:

- **Count** the total number of carbon atoms in the molecule.
- Use the **Latin root** from the following slide that corresponds to the number of carbon atoms followed by the **suffix** "**ane**"
- **Unbranced** hydrocarbons use the **prefix** *normal, or n-,*
- **Branched** hydrocarbons use specific **prefixes**, iso- and neo-

Name = Prefix + Latin root + suffix



Nomenclature (danh pháp) : Common Name

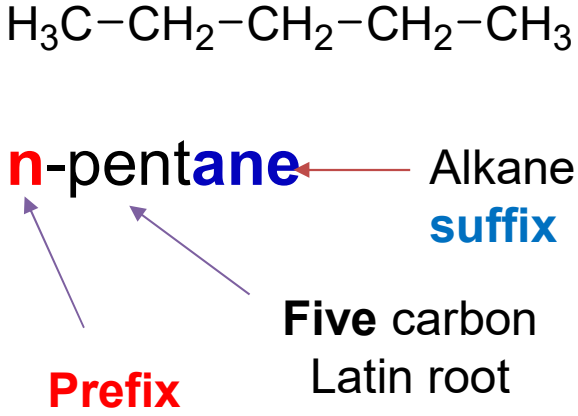
Latin Hydrocarbon Roots

Number of Carbons	Latin Root
1	meth
2	eth
3	prop
4	but
5	pent
6	hex
7	hept
8	oct
9	non
10	dec
11	undec

Latin Hydrocarbon Roots

Number of Carbons	Latin Root
12	dodec
13	tridec
14	tetradec
15	pentadec
16	hexadec
17	heptadec
18	octadec
19	nonadec
20	eicos
21	unicos
22	doicos

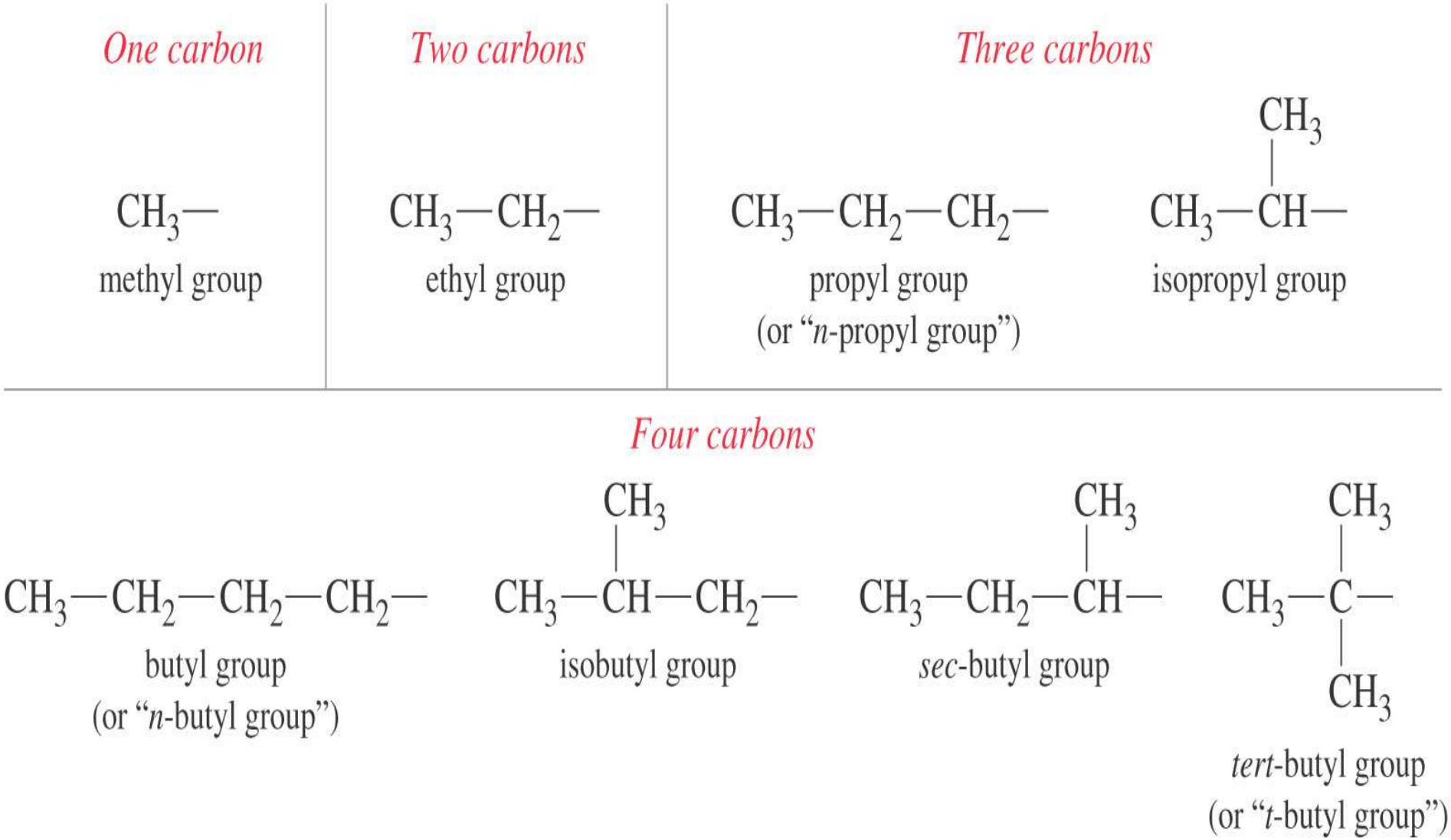
Example: Give a name for the following compound?



Nomenclature: 2. Systematic Name

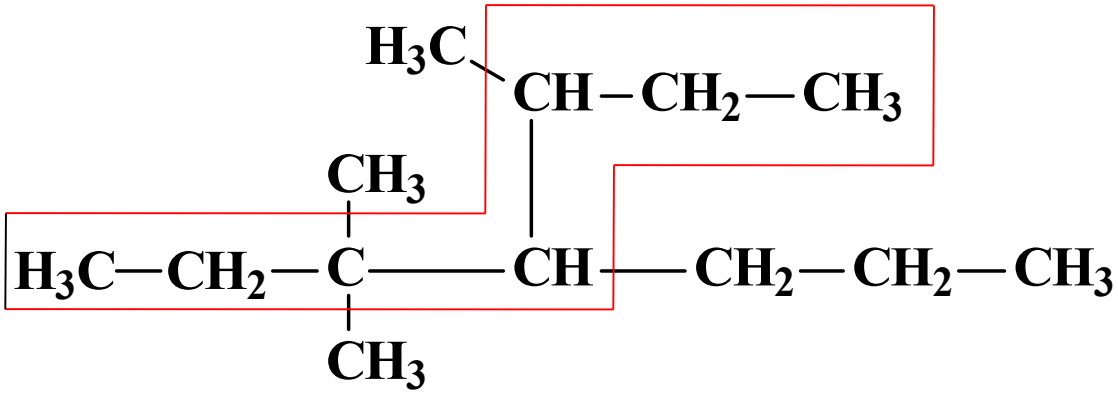
- Steps to give a hydrocarbon a systematic name:
  - Find the **longest** continuous chain of carbon atoms.
  - Use a **Latin root** corresponding to the number of carbons in the longest chain of carbons.
  - Follow the root with the **suffix** of "**ane**" for alkanes
  - Carbon atoms not included in the chain are named as **substituents** preceding the root name with **Latin root** followed by "**yl**" suffix.
  - Number the carbons, **starting closest** to the first branch.
  - Name the **substituent's** attached to the chain, using the carbon number as the locator in alphabetical order.
  - Use di-, tri-, etc., for **multiples** of same substituent.
  - If there are **two possible chains** with the same number of carbons, use the chain with the **most substituent's**.

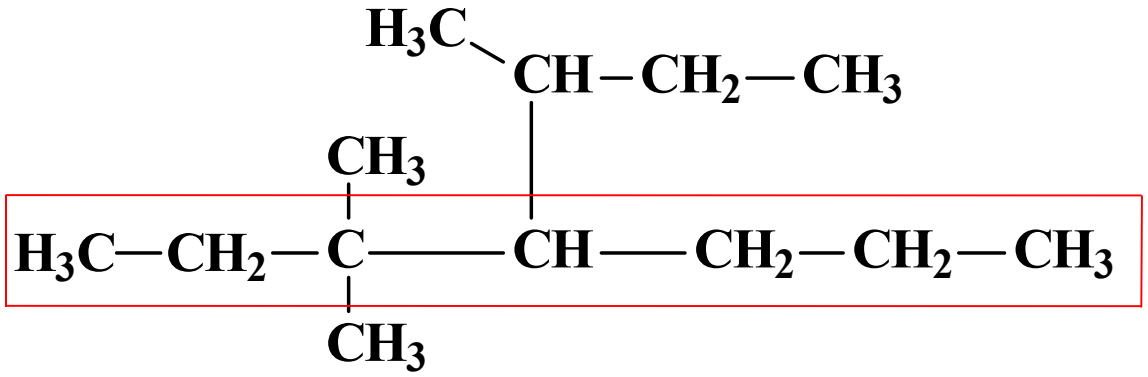
Substituent Names (Alkyl groups)



Nomenclature: Example

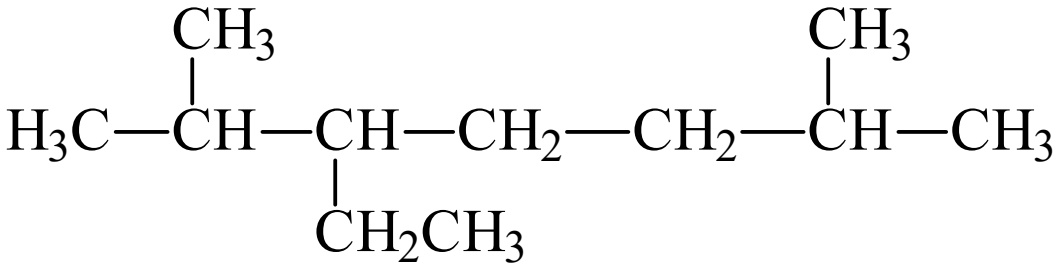
There are two possible chains:





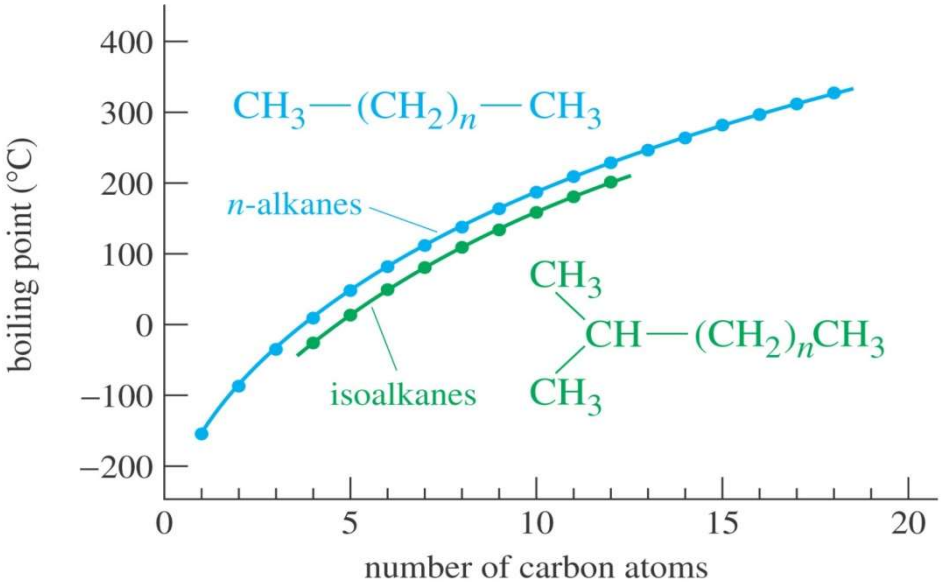
Which one is correct? And what is name?

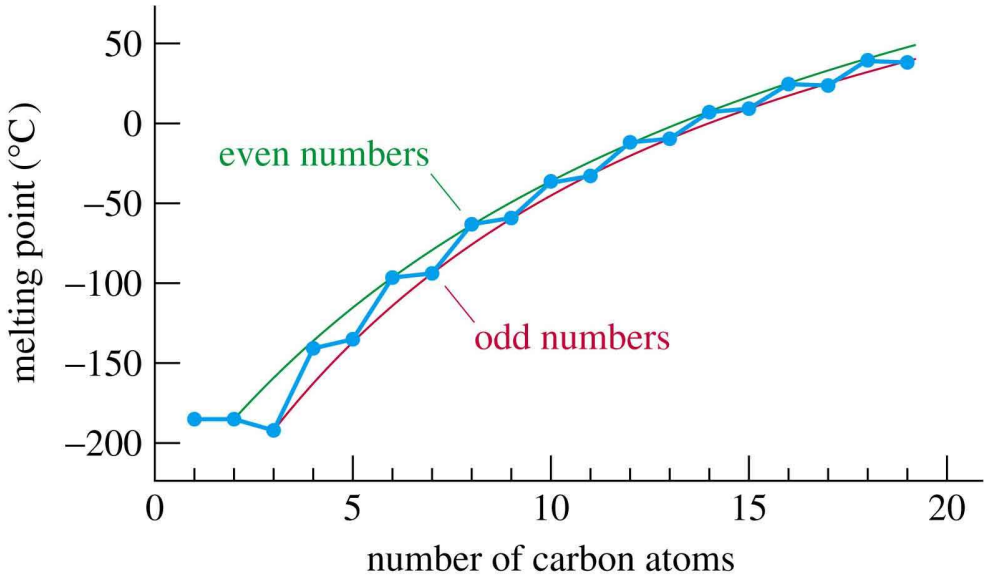
What is its name?



Physical Properties

- **Solubility**: **hydrophobic** (not water soluble)
- **Density**: **less** than 1 g/mL
- **Boiling points increase** with **increasing** carbons (little less for branched chains) due to dispersion forces being larger.
- **Melting points increase** with **increasing** carbons (less for odd-number of carbons).

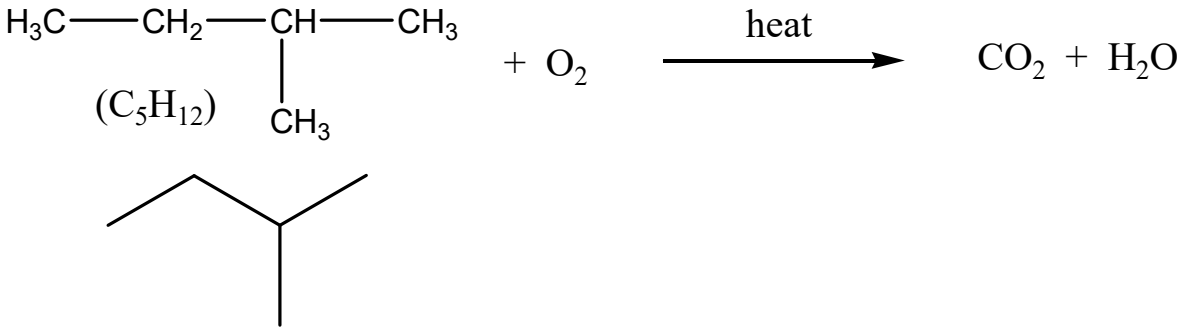




Chemical Properties

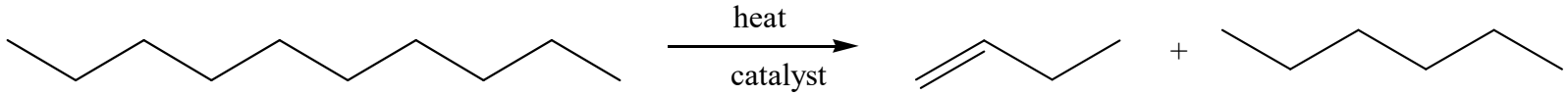
❑ Combustion reaction

$$CH_4 + O_2 \xrightarrow{\text{heat}} CO_2 + H_2O$$

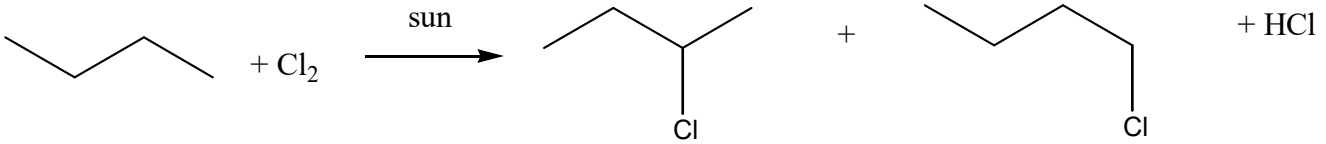


$$+ O_2 \xrightarrow{\text{heat}} CO_2 + H_2O$$

❑ Cracking reaction



❑ Halogenation reaction (substitution reaction)



Butane | 2-chlorobutane | 1-chlorobutane

Example

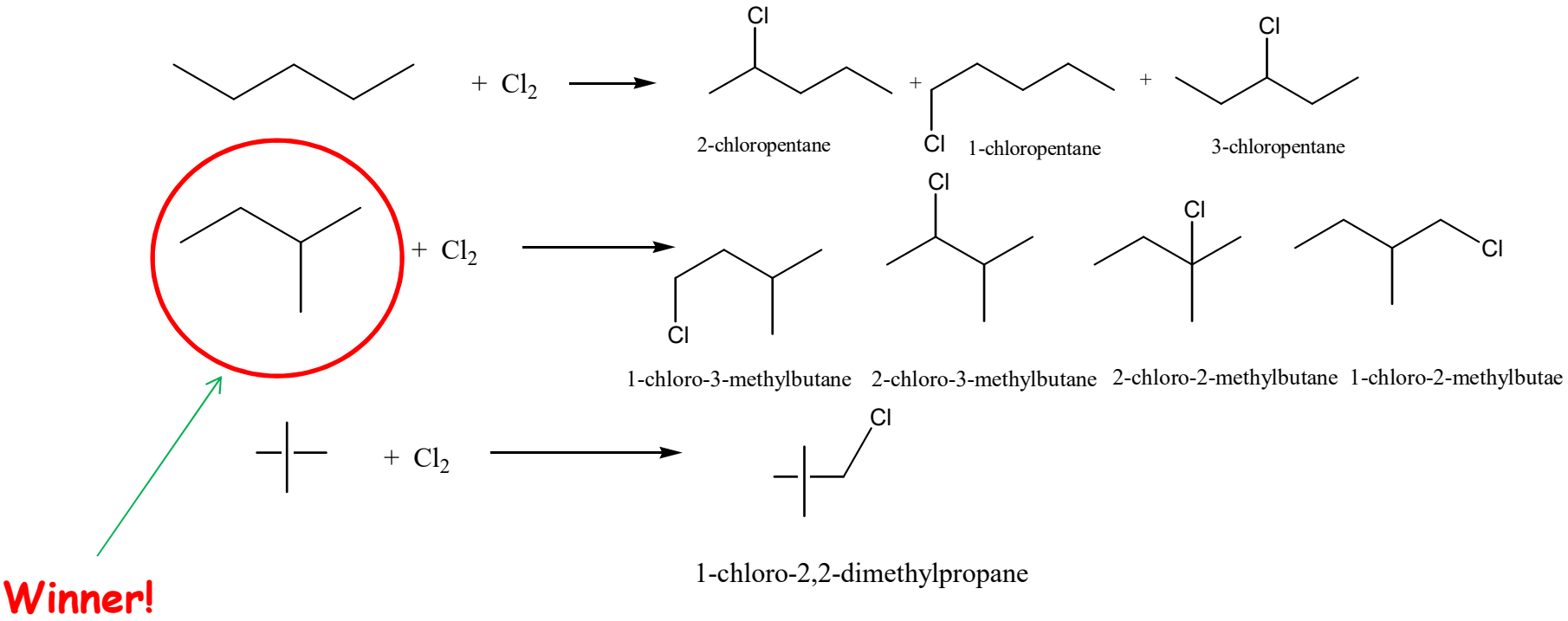
Which **isomer** of C_5H_{12} has the **most** monochloro isomers?

Problem solving process:

Step 1 draw the isomers of C_5H_{10}

Step 2 react each isomer with chlorine

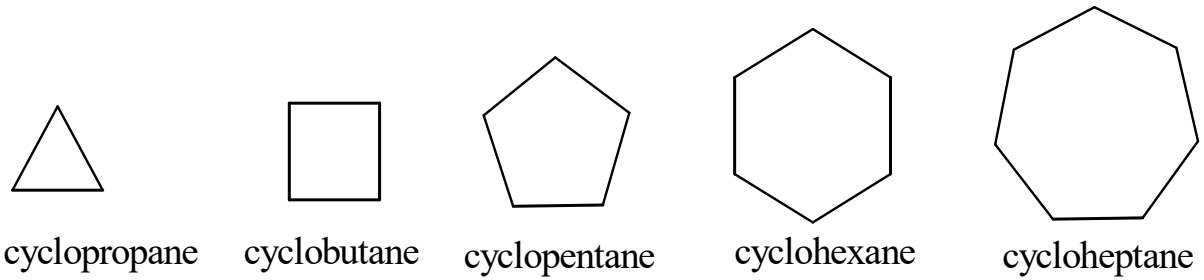
Step 3 count the products



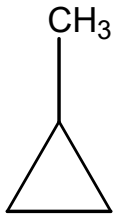
Cycloalkane

- The **cycloalkanes** are **cyclic**, **saturated** hydrocarbons that form another homologous series with the general formula C_nH_{2n} $(n \geq 3)$
- Nomenclature: Simple cycloalkanes are named by adding the **prefix** ***cyclo-*** to the name of the acyclic alkane having the **same** number of carbons

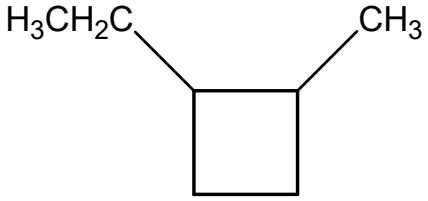
Name = Prefix (Cyclo-) + Latin root + suffix (ane)



cyclopropane cyclobutane cyclopentane cyclohexane cycloheptane



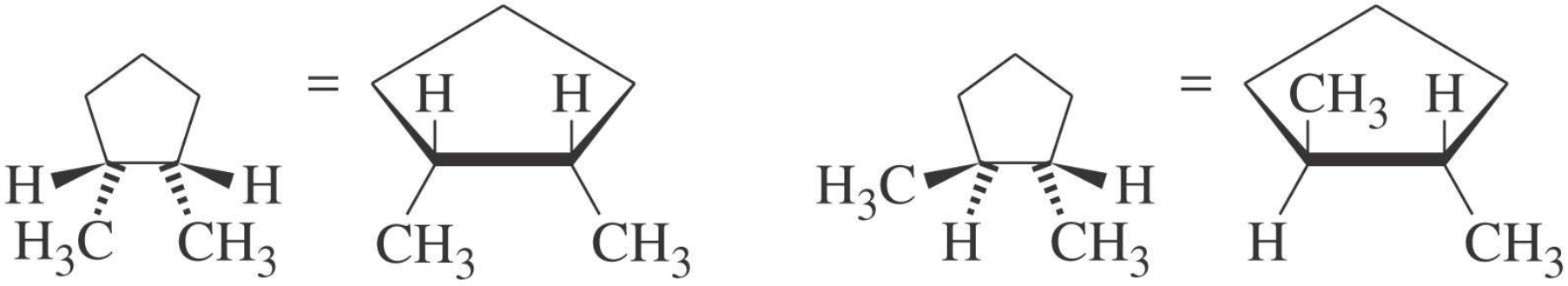
mehtylcyclopropane



1-ethyl-2-methylcyclobutane

Cis-Trans Isomerism of Cycloalkane

Cis-Trans Isomerism requested cycloalkanes contain at least **two substituent groups** at the different carbons.



cis-1,2-dimethylcyclopentane

trans-1,2-dimethylcyclopentane

- **Cis isomer**: like groups on **same sides** of ring
- **Trans isomer**: like groups on **opposite sides** of ring

Example: How many cycloalkane isomers of compound C_5H_{10} ?

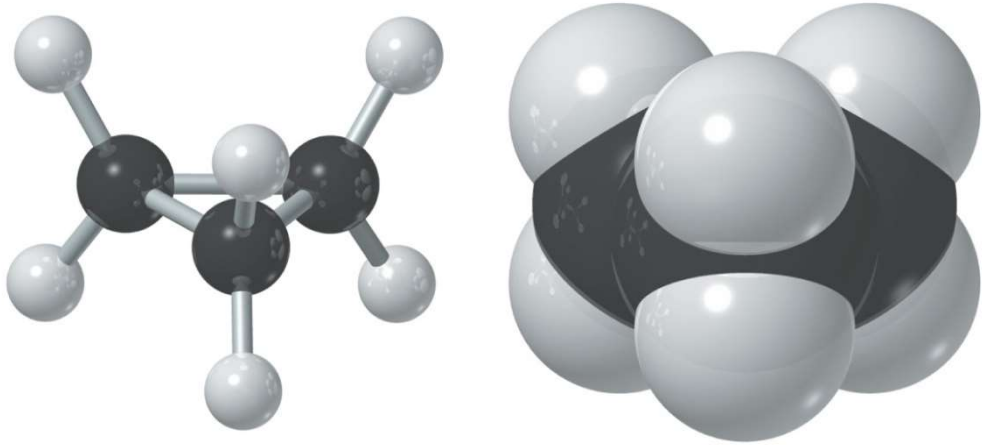
Physical properties and stability

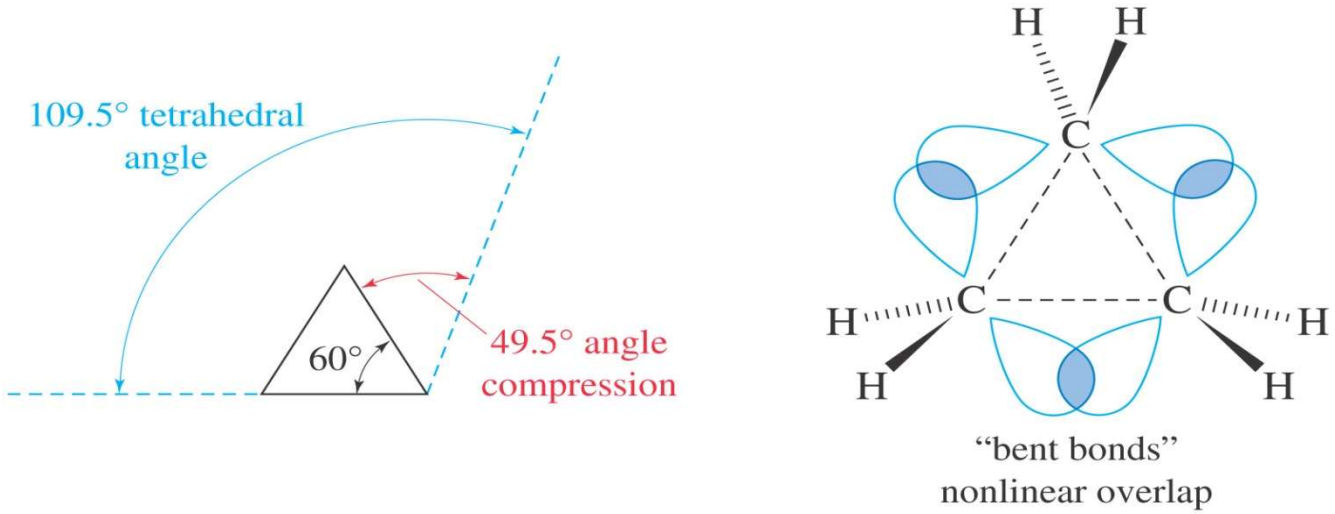
- Nonpolar, insoluble in water
- **Melting** and **boiling points** similar to **branched** alkanes with same number of carbons
- Slightly unsaturated compared to alkanes

  ⇒ Lightly **less stable** in compared to alkanes

- **6-membered** rings (cyclohexane) is **most** stable because Bond angle closest to 109.5°
- **Stability**: $C_3 < C_4 < C_5 < C_6 > C_7 > C_8$

Cyclopropane (C_3H_6)



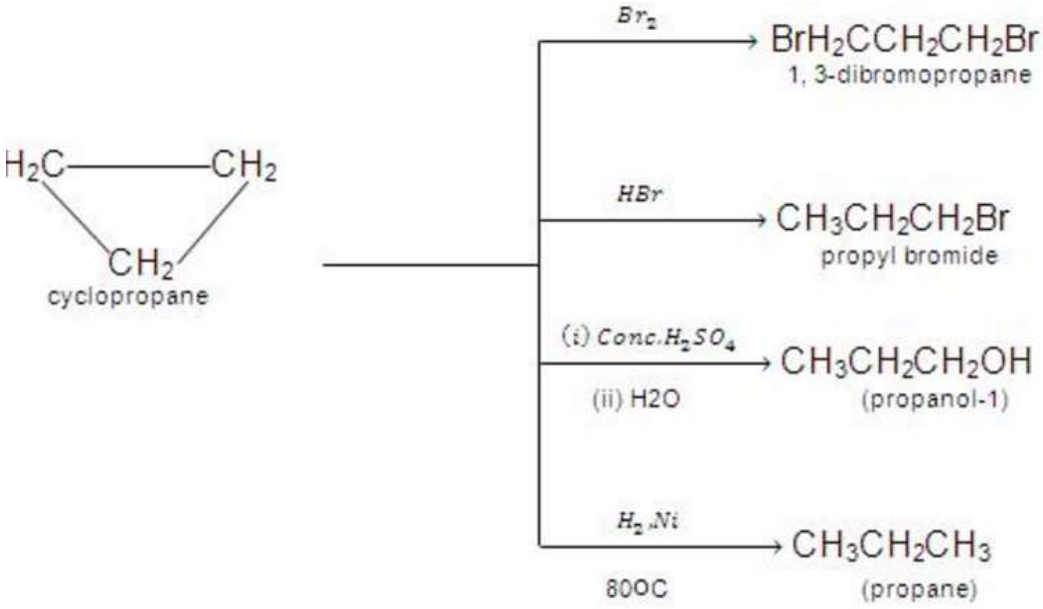


- Large ring strain due to angle compression
- **Very reactive, weak bonds**

Chemical properties of cyclopropane

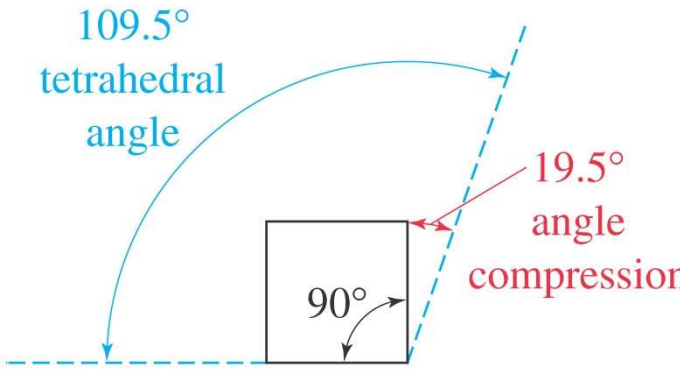
- least stable, Very reactive, weak bonds

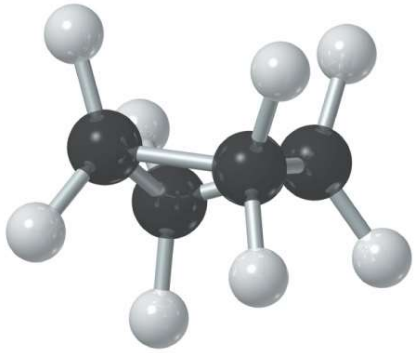
→ **Addition** Reaction: **Open** the cyclic



Other cycloalkanes

Cyclobutane (C_4H_8)

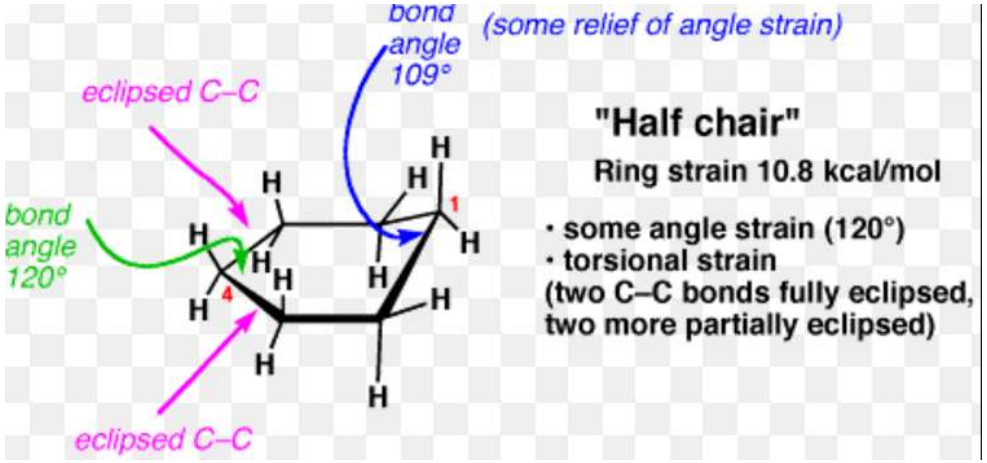




More stable than cyclopropane

Cyclopentane (C_5H_{10})

Corrected

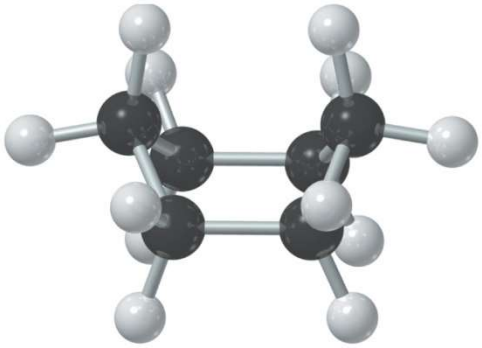


Stable

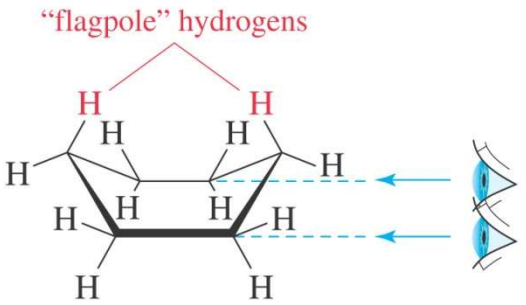
Other cycloalkanes

Cyclohenxane (C_6H_{12})

- **Boat Conformation**

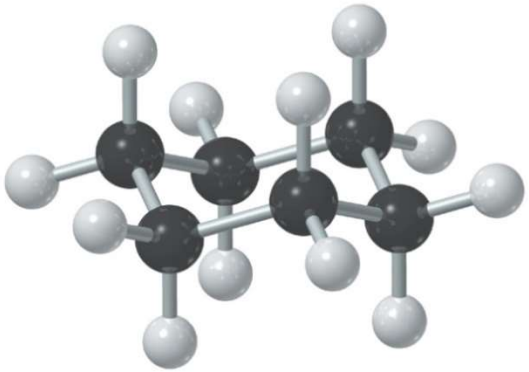


boat conformation

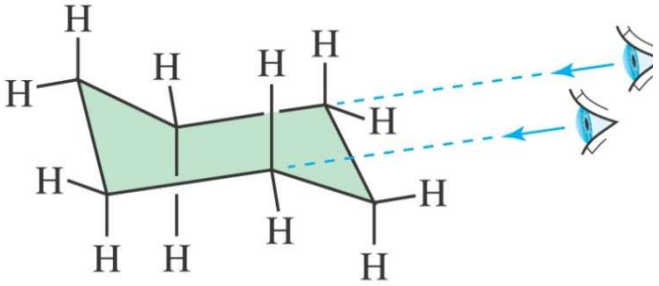


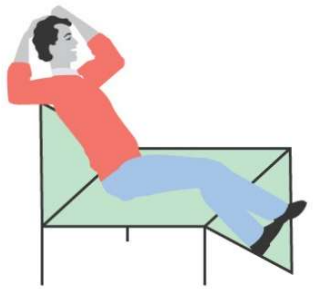
symmetrical boat

- **Chair Conformation**



chair conformation





viewed along the "seat" bonds

The chair conformer has **109.5° bond angles** and all hydrogen's are **staggered** ➡ **most stable**

Alkenes

The **alkenes** (also called **olefins**) are **unsaturated** hydrocarbons (cyclic or acyclic) that contain carbon-carbon double bonds with the general formula C_nH_{2n} ($n \geq 2$).

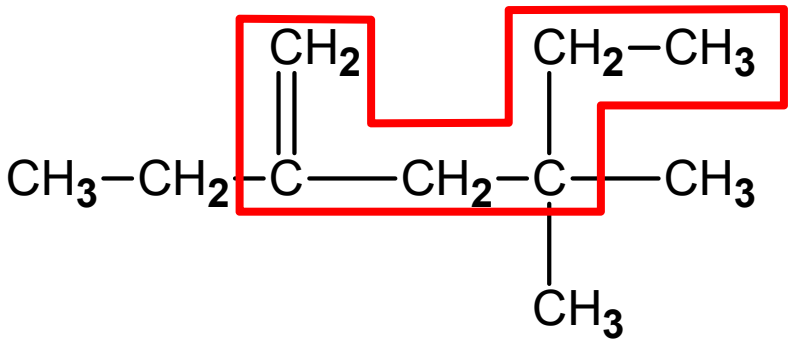
- Nomenclature: Simple alkenes are named by adding the **number of double bonds** to the name of alkane having the **same** number of carbons and suffix **ene**

Name = Number of C=C + Latin root + suffix (ene)

$CH_3– CH = CH – CH_3$ $CH_3– CH_2 – CH = CH_2$

2-butene **1-butene**

Note: Always give double bond the **lowest** number

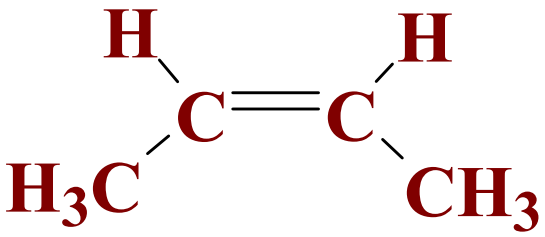


2-ethyl-4,4-dimethyl-1-hexene

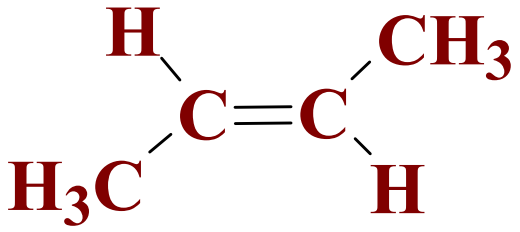
Geometric Isomers (Configurational isomers)

- Because double bonds of alkenes **cannot rotate**, it forms two isomers when containing two substituent groups at double bonds. On the other words, **Geometric isomers** containing some atoms **occupy** different relative positions in space.

- **Example**: 2-butene has two geometric isomers



cis-2-butene



trans-2-butene

  - **Cis isomer**: like groups on same side of double bond
  - **Trans isomer**: like groups on opposite sides of double bond

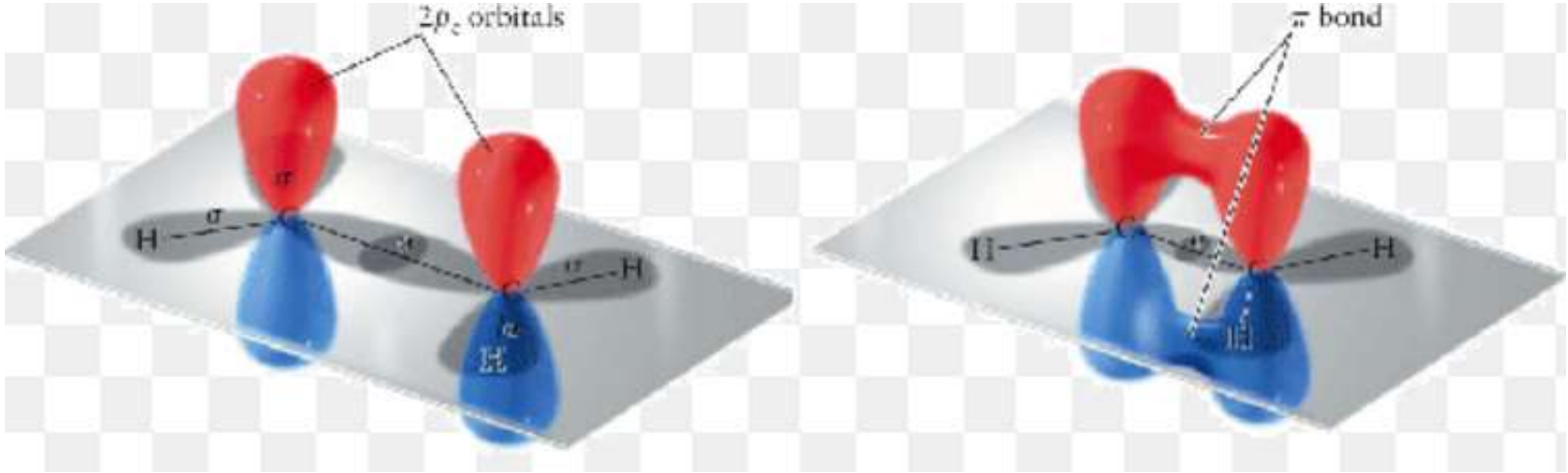
- **Example**: Write all isomers of C_5H_{10}?

Physical Properties

- The physical properties of alkenes and alkanes are **similar**.
- They are **colourless**, nonpolar, combustable, and almost **odorless**
- The physical state depends on **molecular mass**: like the corresponding saturated hydrocarbons, the simplest alkenes, ethene, propene, and butene are gases at room temperature. Linear alkenes of approximately five to sixteen carbons are **liquids**, and **higher** alkenes are waxy **solids**.
- **Configurational** isomers have different physical properties (boiling point, melting point)

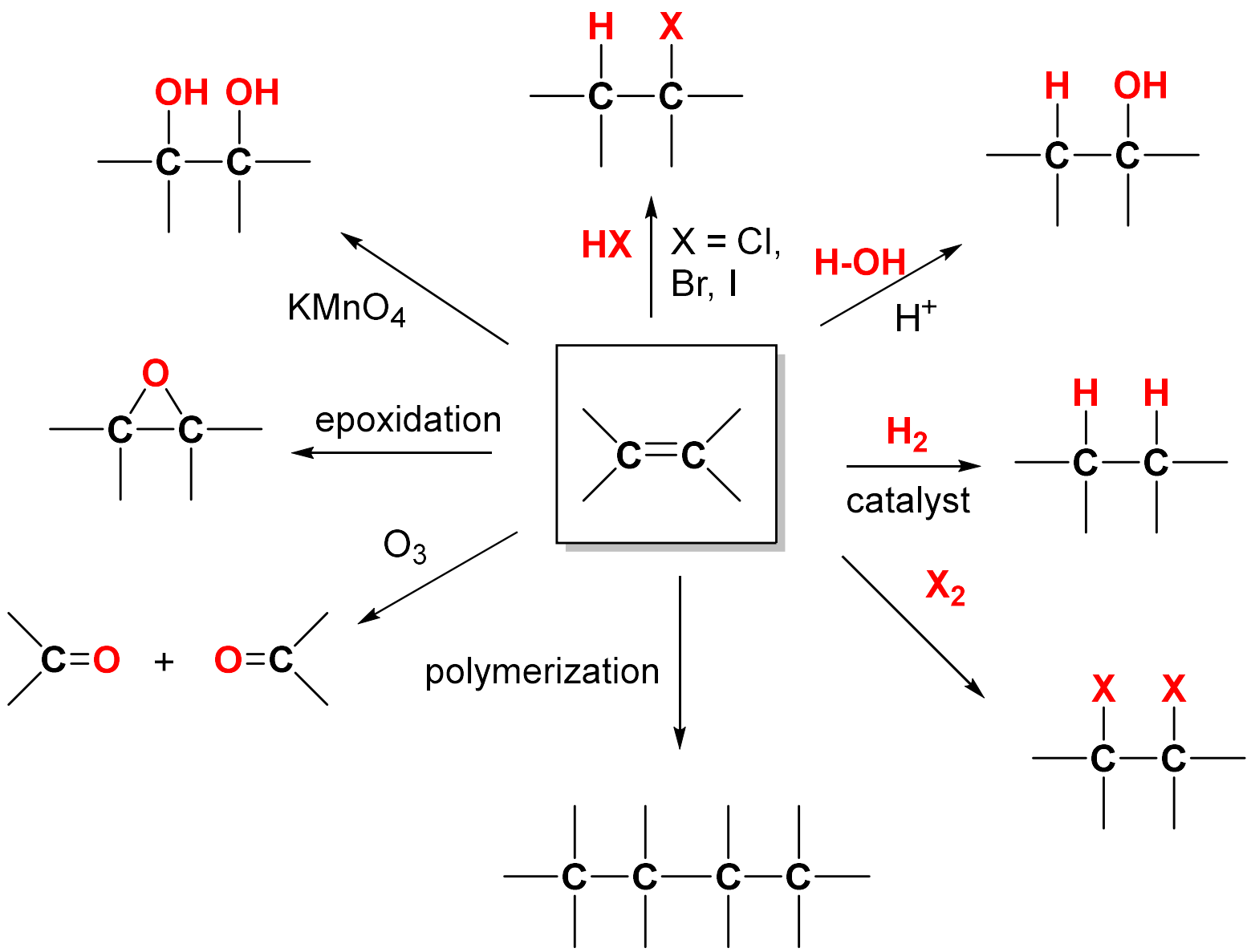
Chemical Properties

- A carbon–carbon double bond consists of one **σ bond** and one **π bond.** The π bond is very **less stable**. As a result, π bond in alkenes is **easy to break.**

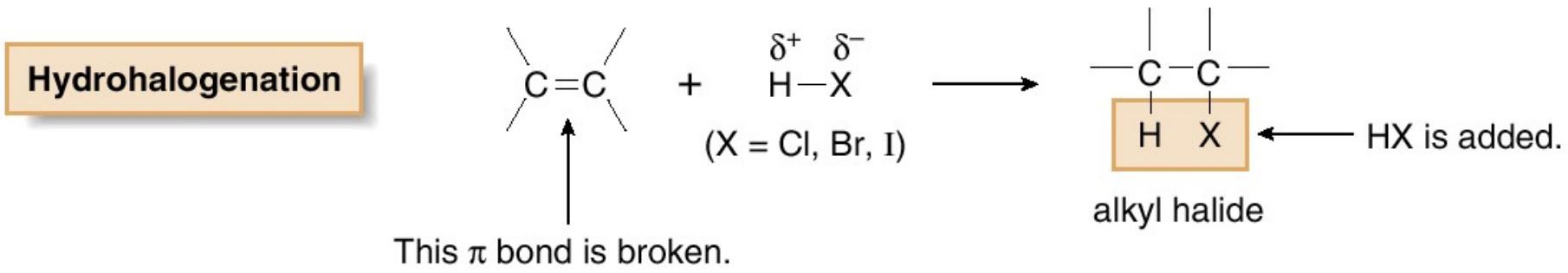


Addition reaction and **oxidation** reaction

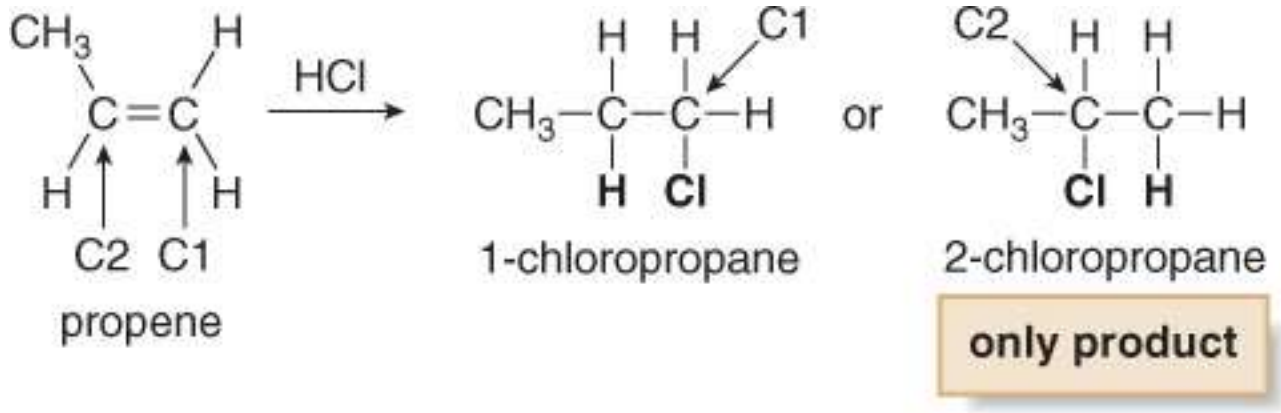
Chemical Properties



Addition reactions of HX

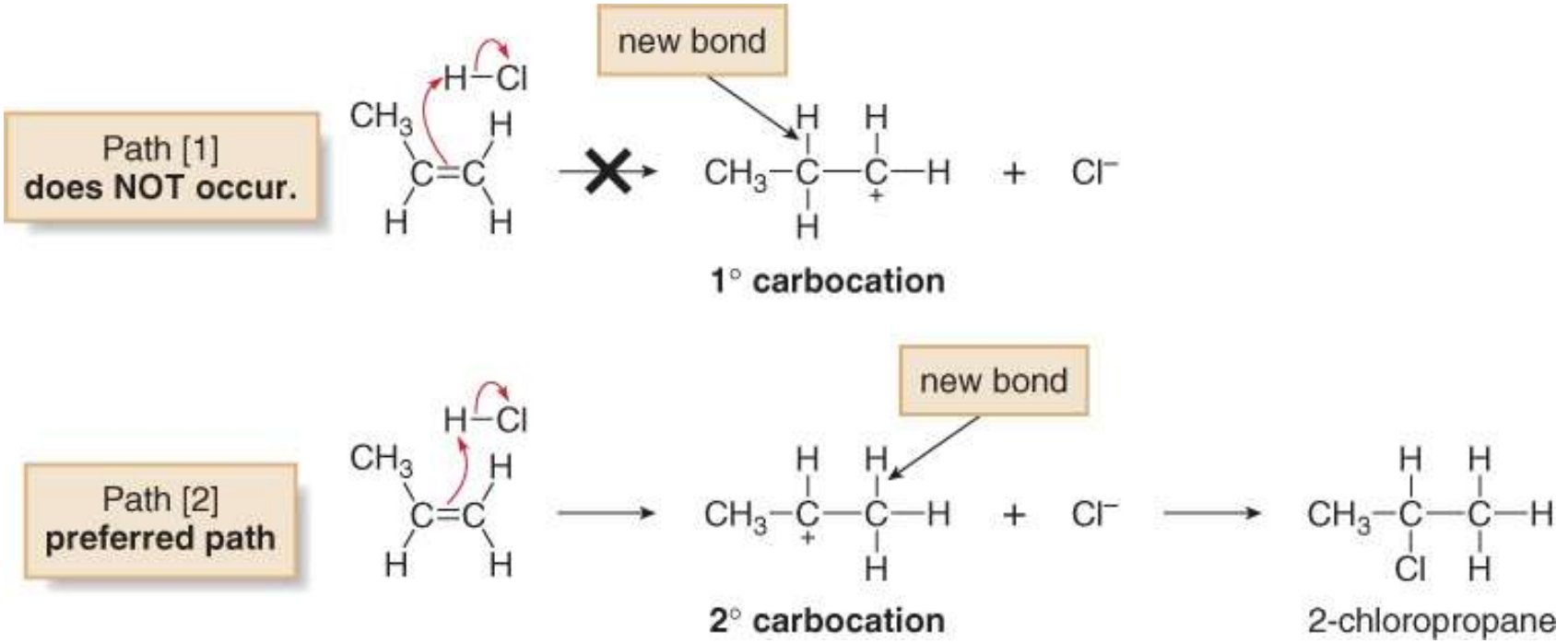


Markovnikov's rule

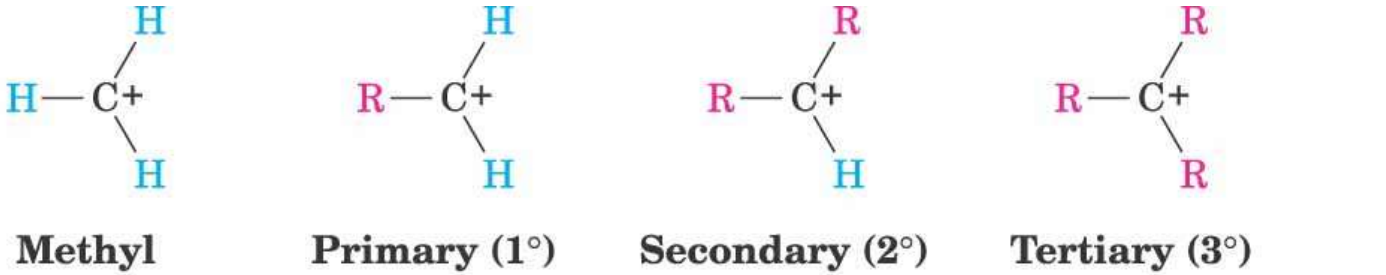


In additions of HX, H adds to the carbon with the greater number of hydrogens

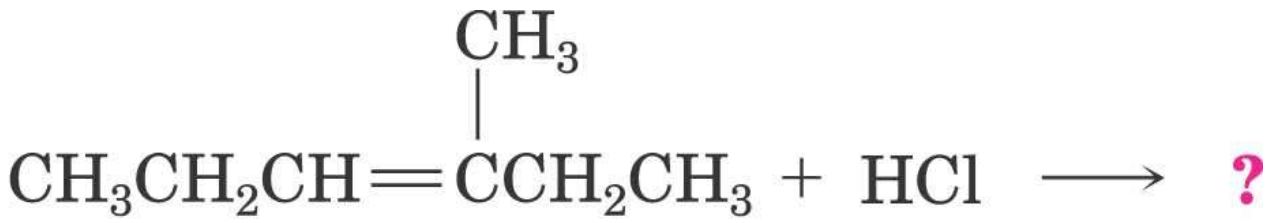
WHY?



Stability of Carbocations



Examples

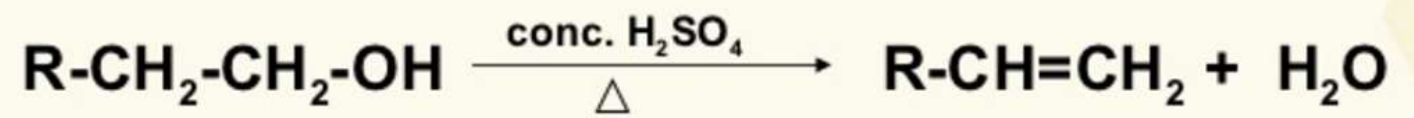


1-Ethylcyclopentene + HBr ⟶ ?

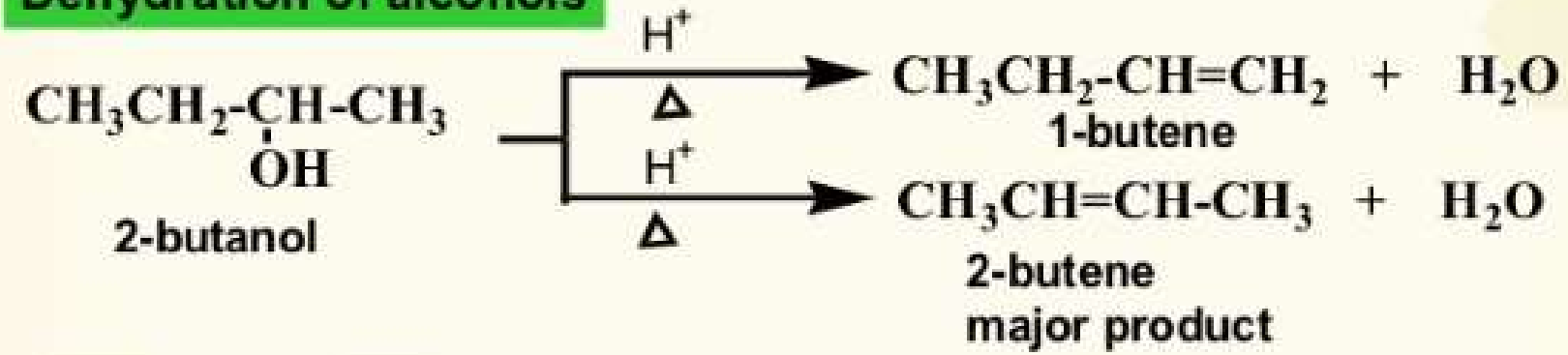
2,2,4-Trimethyl-3-hexene + HI ⟶ ?

Preparation of alkenes

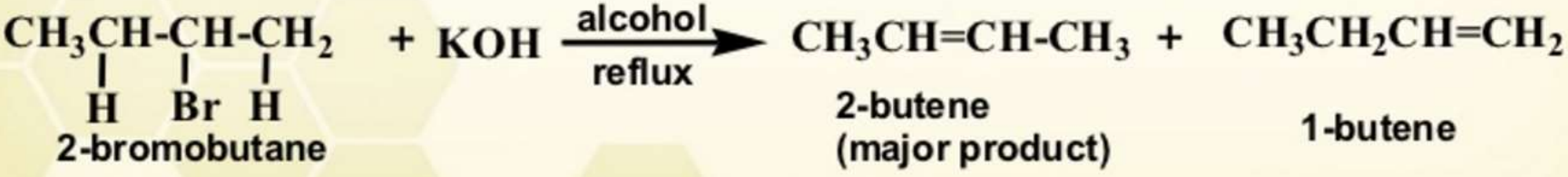
Dehydration of alcohols



Dehydration of alcohols



Dehydrohalogenation of haloalkanes



<u>Zaixep's Rule</u>: The alkene formed in the **greatest** amount (major product) is the one that corresponds to removal of the hydrogen from the **β-carbon** having the **fewest** hydrogen substituents

Alkynes

- **Alkynes** are unsaturated hydrocarbons containing a carbon-carbon **triple bond** with the general formula C_nH_{2n-2} ($n \geq 2$).

- Nomenclature: Simple alkynes are named by adding the **number of triple bonds** to the name of alkane having the **same** number of carbons and suffix **yne**

Name = Number of C ≡ C + Latin root + suffix (yne)

$CH_3– C \equiv C – CH_3$ — **2-butyne**

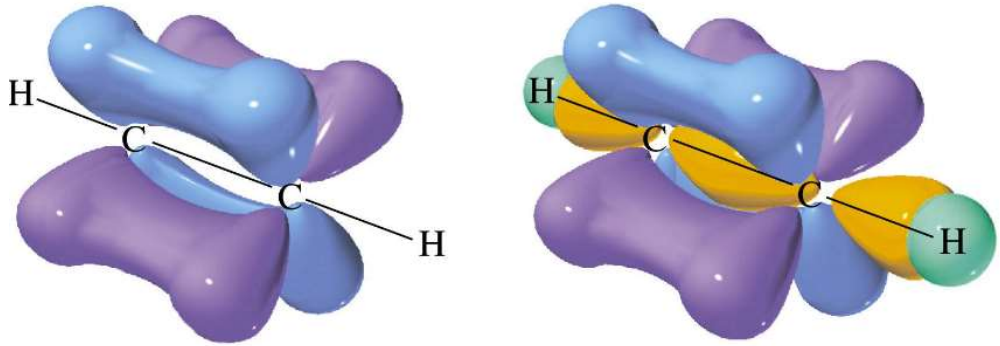
$CH_3– CH_2 – C \equiv CH$ — **1-butyne**

Note: Always give triple bond the **lowest** number

Physical Properties and Structure

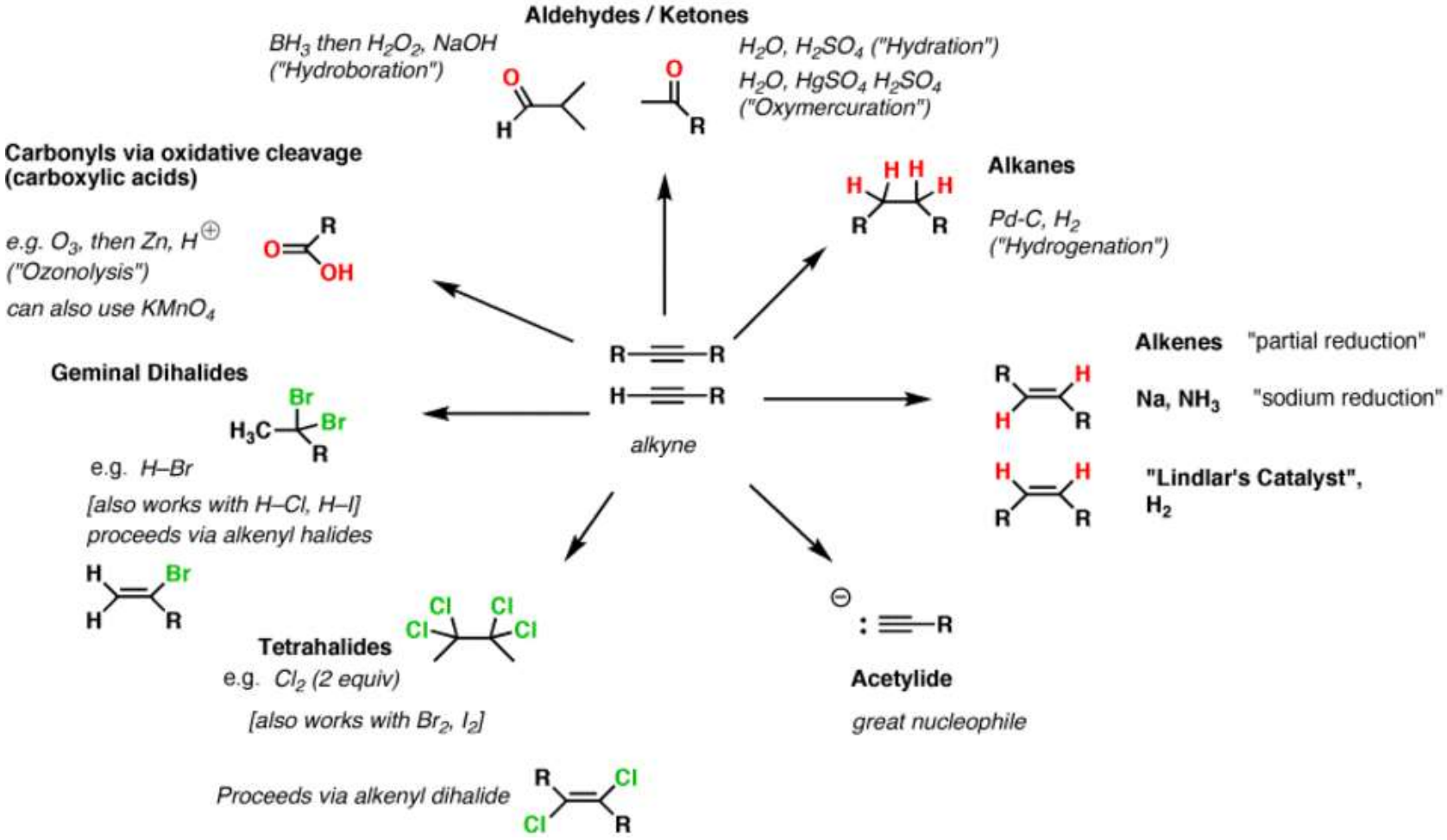
- The physical properties of alkynes are similar to alkanes and alkenes.

- A carbon–carbon triple bond consists of one **σ bond** and two **π bond.** The π bond is very **less stable**. As a result, two π-bonds in alkynes are **easy to break.**

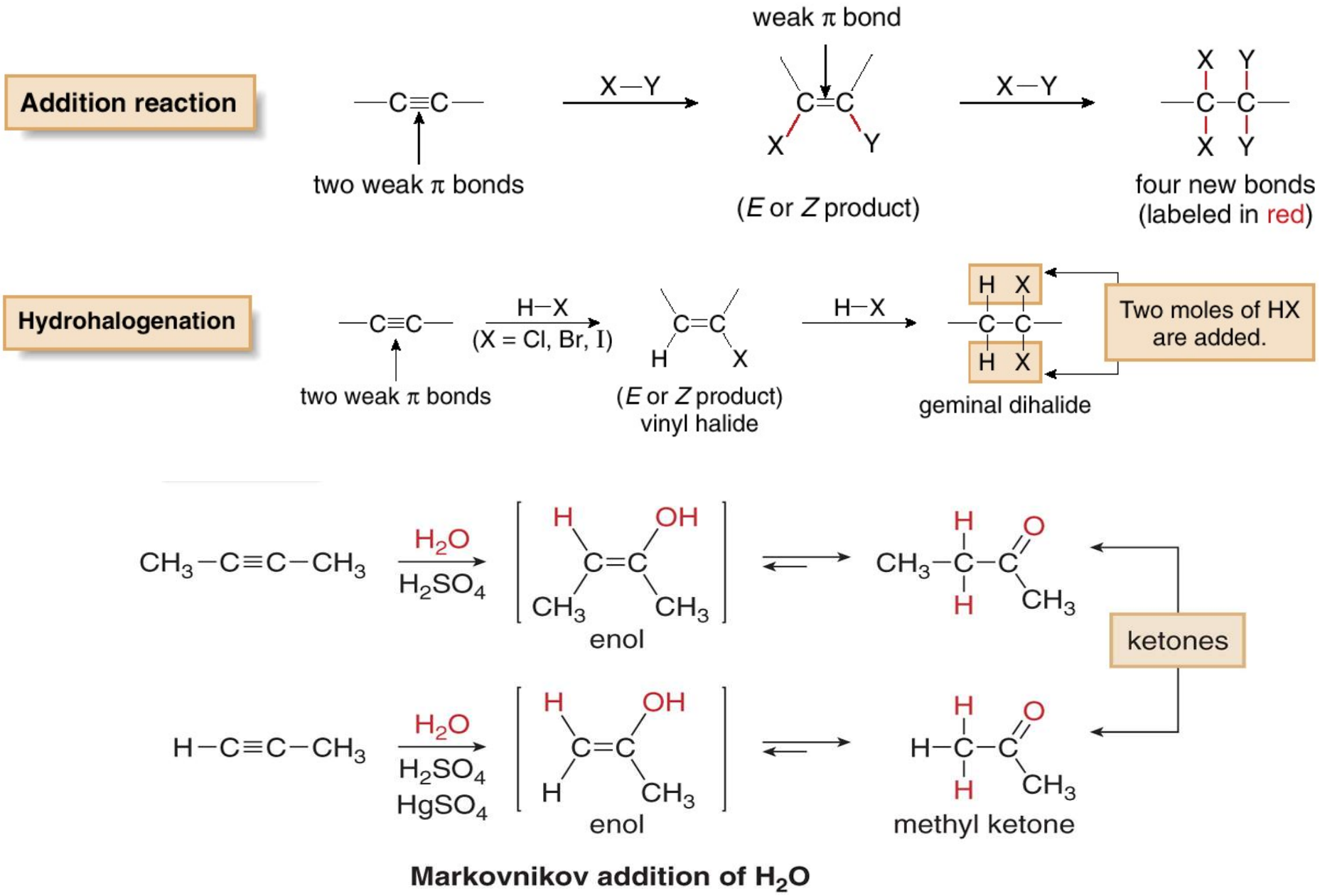


- **Terminal and internal alkynes**
  - **Internal** alkynes feature carbon **substituents** on each acetylenic carbon. **Symmetrical** examples include diphenylacetylene and 3-hexyne.
  - **Terminal** alkynes have the formula **RC≡CH**. Terminal alkynes, like acetylene itself, are **mildly acidic**, with pK_a values of around 25.

Chemical properties of Alkynes

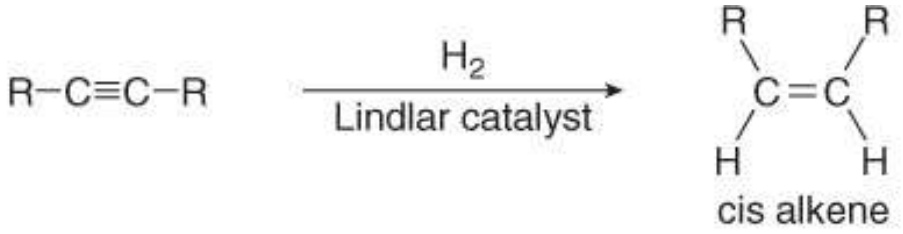


Chemical properties of Alkynes

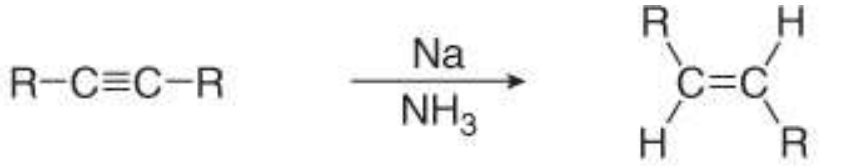


Adding Hydrogens to Alkynes

General reaction



General reaction

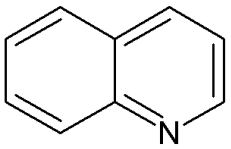


5% $Pd\text{-}CaCO_3$

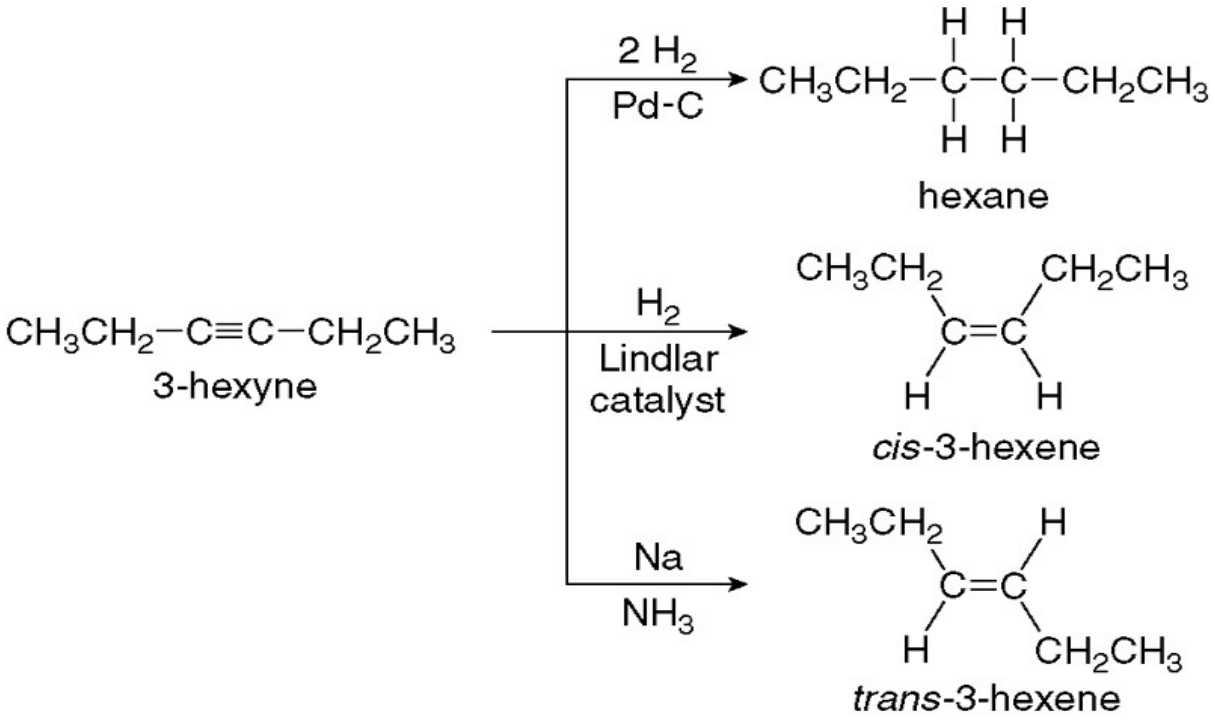
+

$Pb(OCOCH_3)_2$

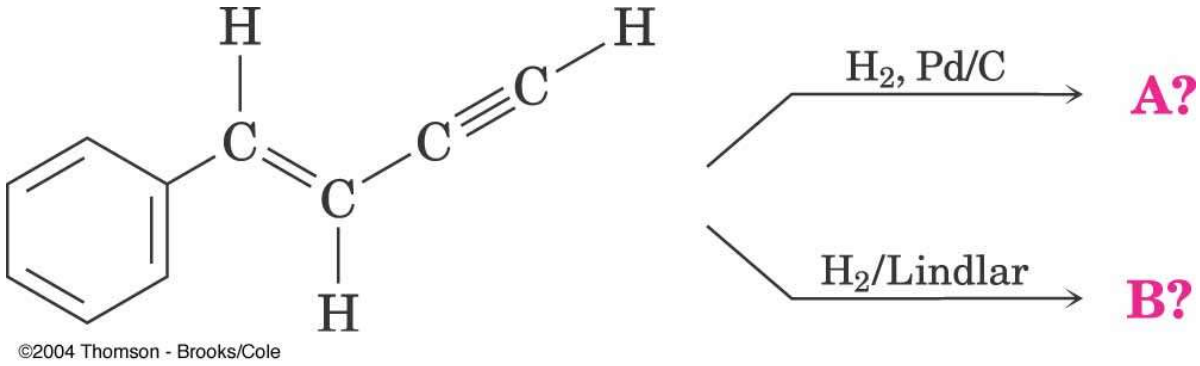
+

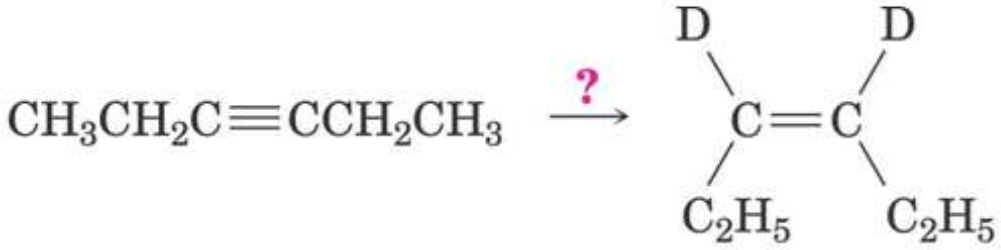


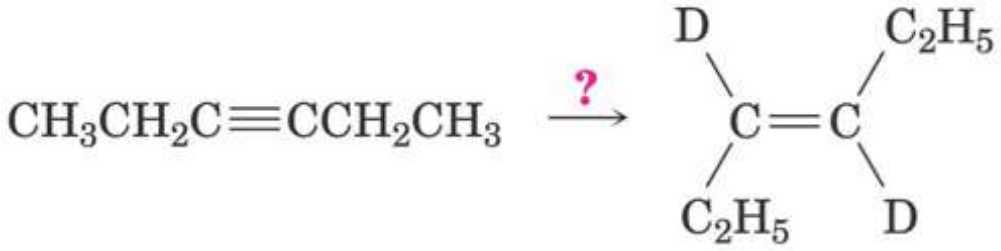
Lindlar cat.

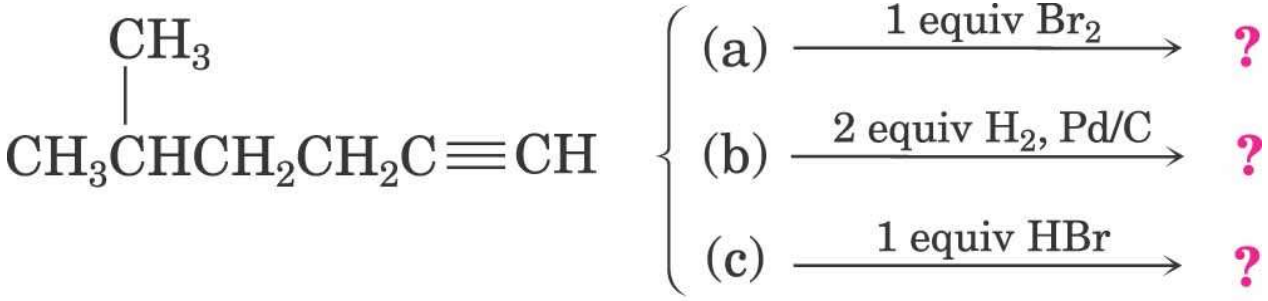


Examples









Reactions of terminal Alkynes

- terminal alkynes are reactive as **weak acids**

$$RC{\equiv}CH + MX \rightarrow RC{\equiv}CM + HX$$

(MX= $NaNH_2$, LiBu, RMgX)

$$RC{\equiv}CH + Ag(NH_3)_2OH \rightarrow RC{\equiv}CAg\downarrow + NH_3 + H_2O$$

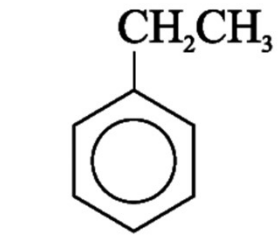
(Yellow precipitate)

➡ **Use to detect terminal alkynes**

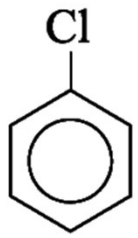
Aromatic Hydrocarbons

- **Aromatic hydrocarbons** usually contain benzene rings- six membered rings of carbon atoms with alternating C-C single and C=C double bonds with the general formula C_nH_{2n-6} (n ≥ 6)

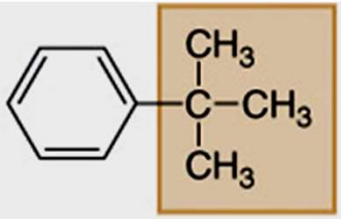
- Nomenclature:
  - Monosubstituted benzenes: For certain compounds, benzene is the parent name and the substituent is simply indicated by a prefix.



Ethylbenzene



Chlorobenzene



tert-butyl group

tert-butylbenzene

Aromatic Hydrocarbons

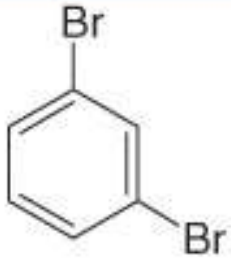
❑ Nomenclature:

•**Disubstituted benzenes:** There are three different ways that two groups can be attached to a benzene ring, so a prefix—ortho, meta, or para—can be used to designate the relative position of the two substituents.

1,2-disubstituted benzene
ortho isomer

ortho-dibromobenzene
or
o-dibromobenzene
or 1,2-dibromobenzene

1,3-disubstituted benzene
meta isomer



meta-dibromobenzene
or
m-dibromobenzene
or 1,3-dibromobenzene

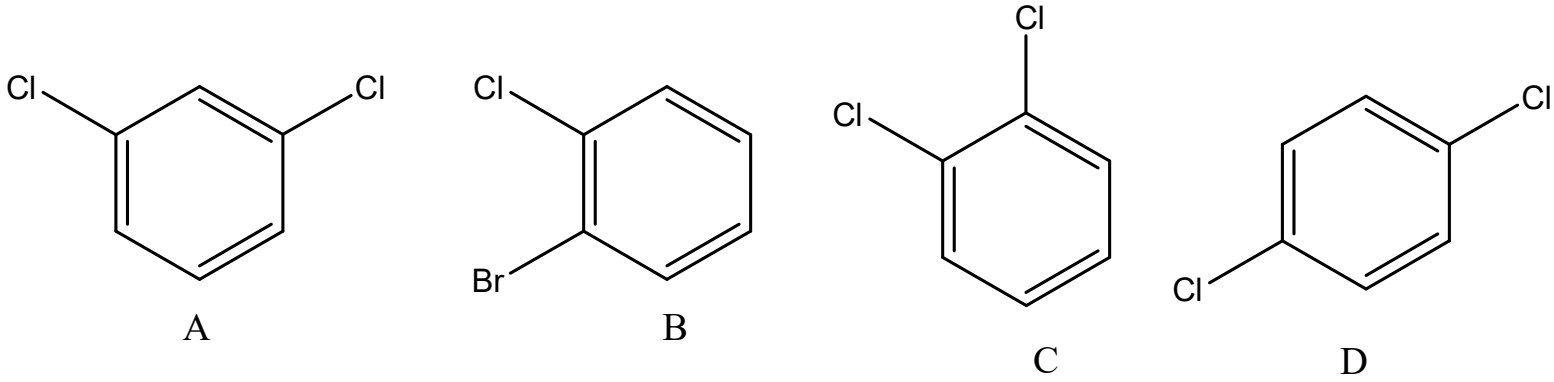
1,4-disubstituted benzene
para isomer

para-dibromobenzene
or
p-dibromobenzene
or 1,4-dibromobenzene

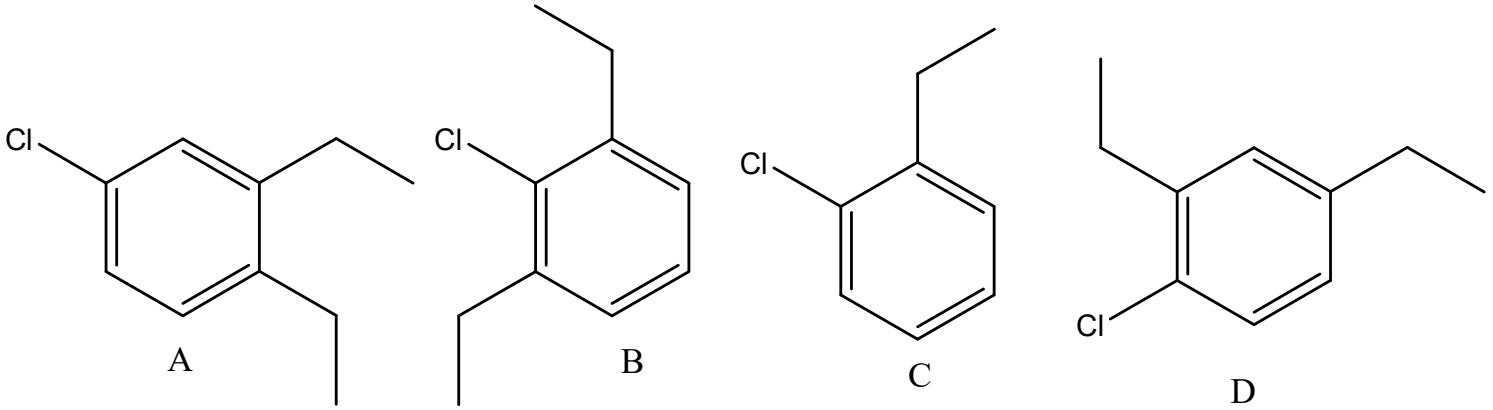
Examples

Which structure matches the given name?

o-dichlorobenzene



4-chloro-1,2-diethylbenzene

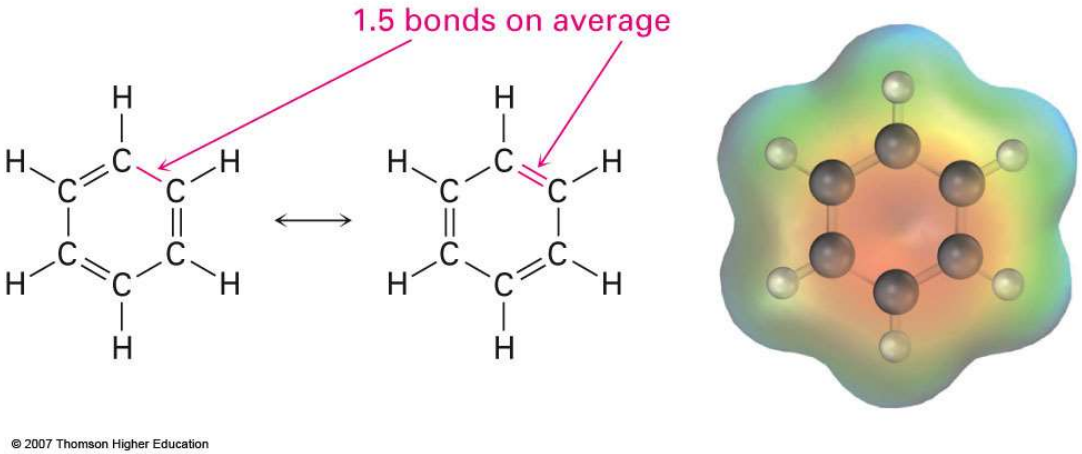


Physical properties

- have a **fragrant** smell
- generally **less dense than water** at 20°C
- usually **immiscible with water**
- **soluble in organic solvents**

Structure and Stability of Benzene

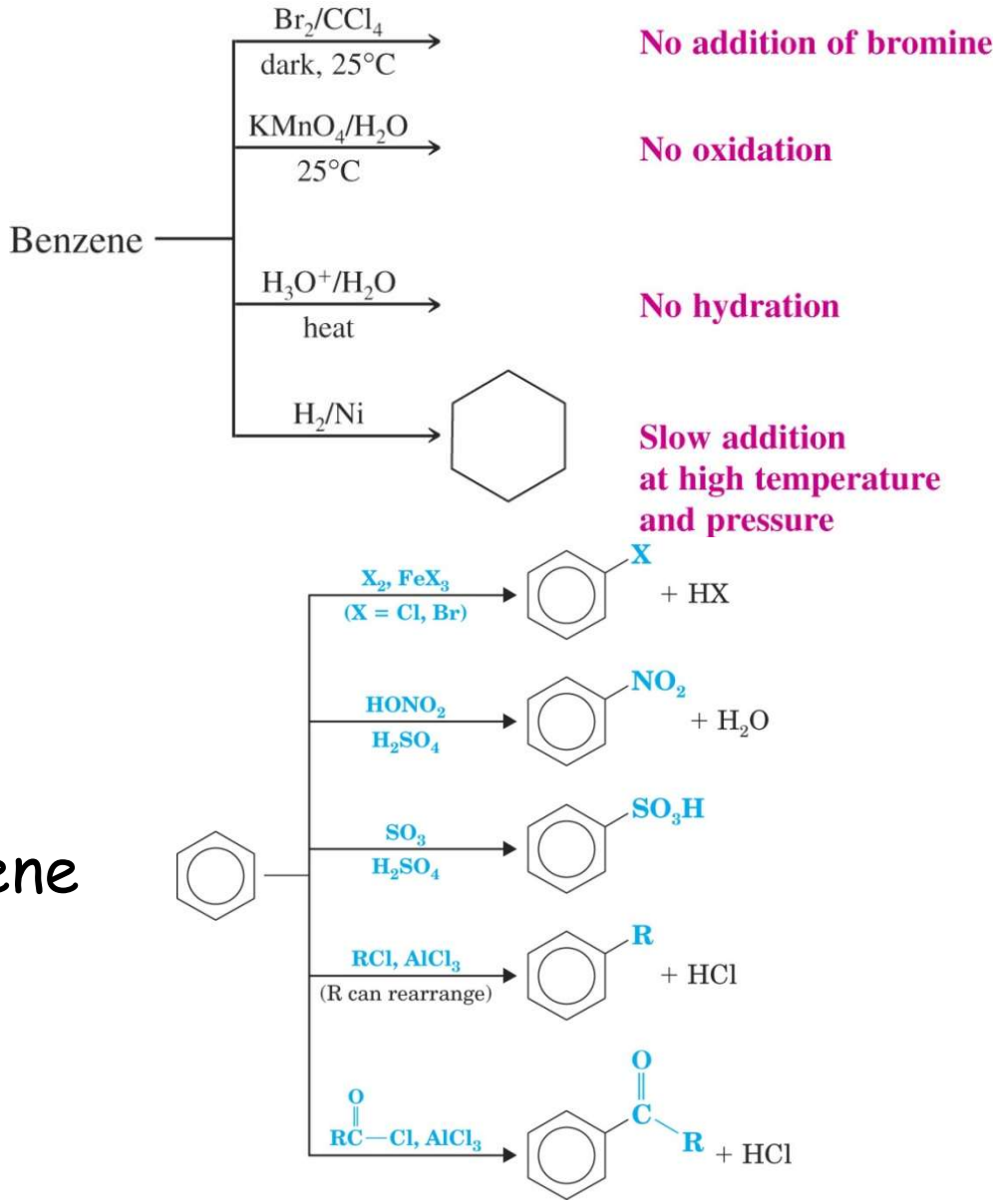
- Benzene is **planar**
  - All C-C-C bond angles are **120°**
  - All **six** carbon atoms are sp^2-hybridized with *p* orbital perpendicular to the plane of the ring



- A molecule is aromatic only if it :
  - is **cyclic**
  - is **conjugated**
  - is **planar** and
  - contains a total of **4*n* + 2 π electrons**, where *n* is an integer (*n* = 0, 1, 2, 3,…)

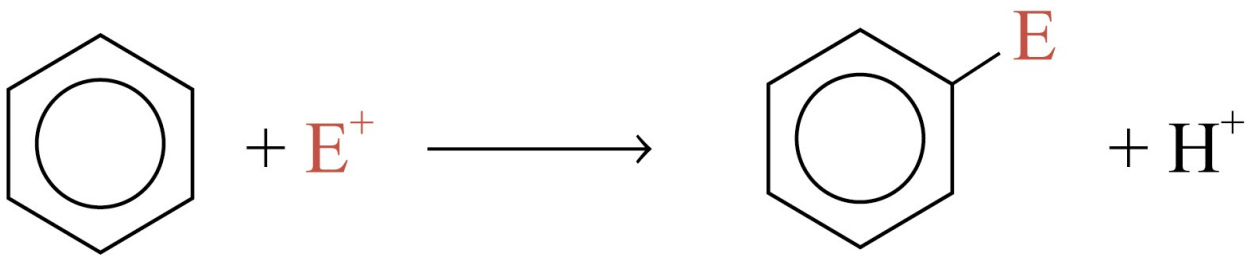
Chemical Properties

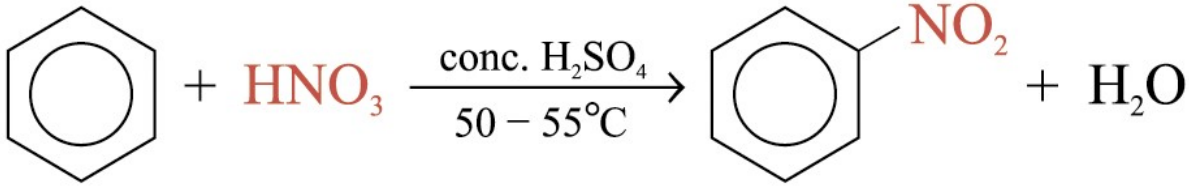
- Even though benzene is highly unsaturated it does **not undergo** any of the regular reactions of alkenes such as addition or oxidation



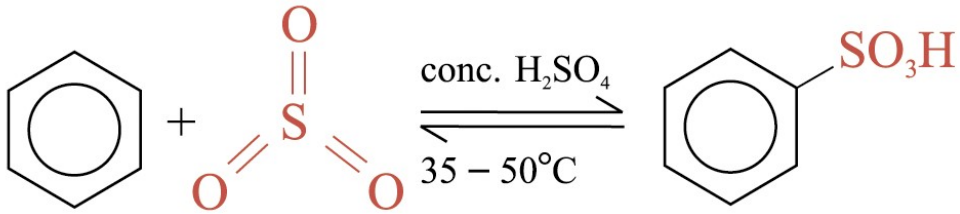
- The aryl group (Ar) is derived by removal of a hydrogen atom from an arene

Electrophile Aromatic Substitution Reactions

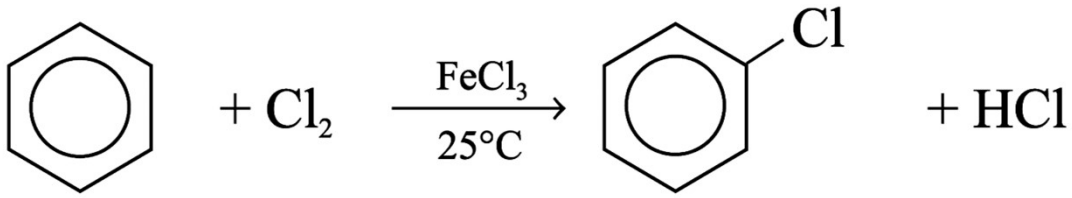




Nitrobenzene

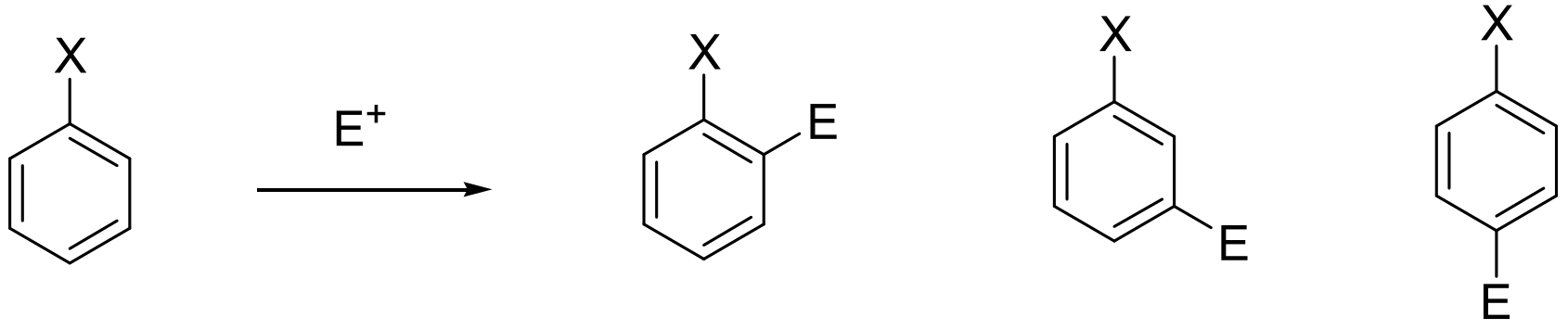


Benzenesulphonic acid



Chlorobenzene

Electrophile Aromatic Substitution Reactions



Octo- **Meta-** **Para-**

- If X is **Electron Donating (alkyl, amine, OH, O-R)**, reaction is **fast** and product of **Octo, para-** substituent **>** **meta-**
- If X is **Electron withdrawing (NO_2, COOH,)**, reaction is **Slow** and product of **meta-** substituent **>** **octo-** and **para-**
- If X is **halogen (F, Cl, Br, I)**, reaction is **slow** and product of **octo-** and **para-** substituents **>** **meta-**