

Alkynes and Aromatic Compounds

By

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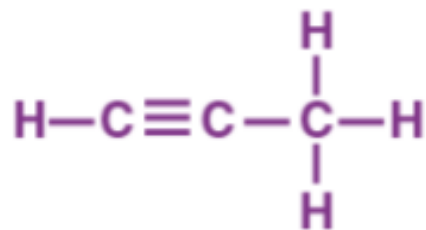
Lecture 3

Alkynes contain carbon-carbon triple bonds.

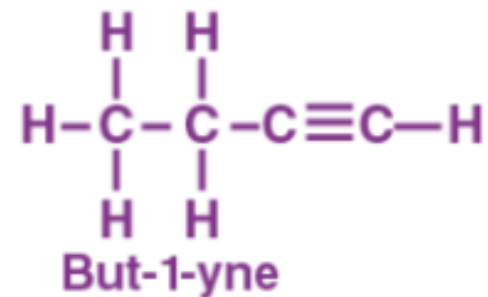
- ❑ General formula: C_nH_{2n-2} (for one triple bond)
- ❑ The nomenclature system for alkynes is identical to that of alkenes, except the suffix -yne is used to indicate a the triple bond.
- ❑ Alkynes do not have cis and trans- isomer
- ❑ triple bonds are shorter and stronger than double bonds
- ❑ he extra π linkage (alkynes have two π bonds) makes the triple bond even more reactive. Thus, alkynes are very reactive



Ethyne



Propyne



But-1-yne

Isomerism in Alkynes

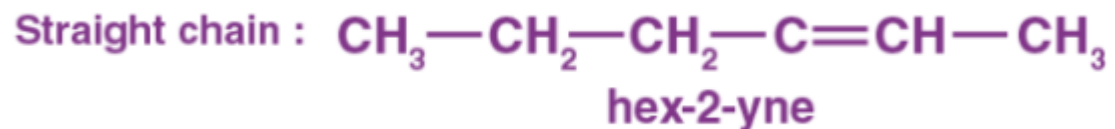
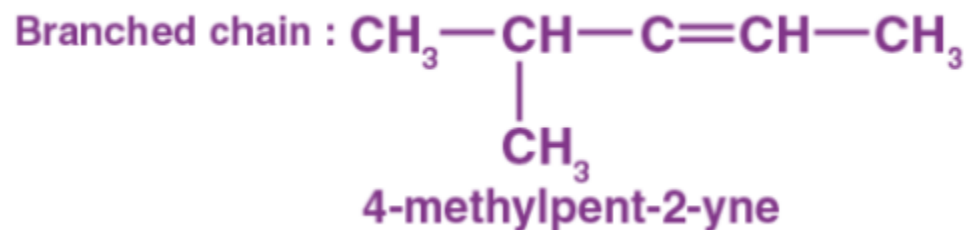
Alkynes show three types of isomerism

- 1) Chain isomerism
- 2) Position isomerism
- 3) Functional isomerism

1. Chain isomerism

It is due to the different arrangement of carbon atoms in the chain that is straight chain or branched.

Example: 4-methylpent-2-yne and hex-2-yne



2. Position isomerism

It is due to the difference in the location of the triple bond

Example: Pent-1-yne and pent-2-yne



pent-1-yne



pent-2-yne

3. Functional isomerism

Alkynes are isomeric with alkenes both being represented by the general formula $\text{C}_n\text{H}_{2n-2}$.

Example: But-1-yne and buta-1,3-diene



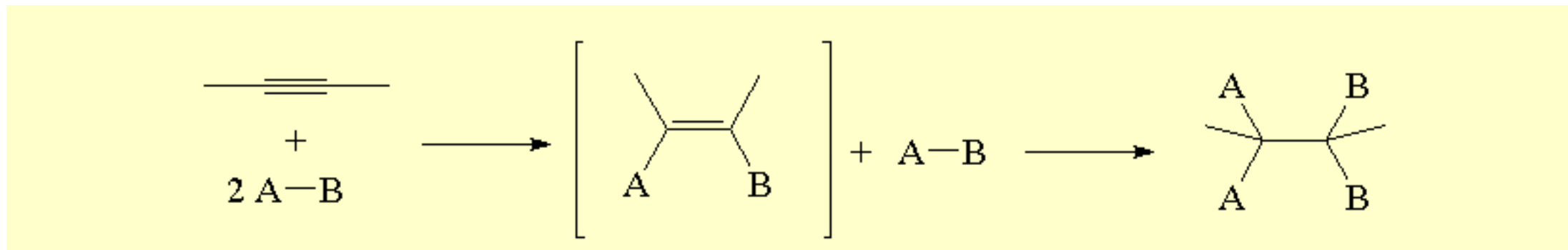
but-1-yne



buta-1,3-diene

Reactions of Alkynes

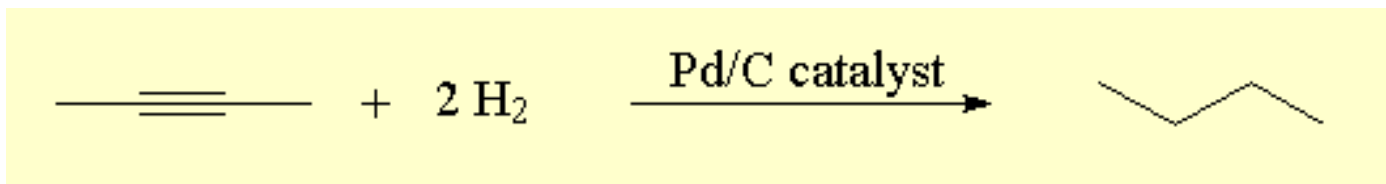
General type of reaction is an electrophilic addition reaction. Like alkenes, the electrons of the p bonds are available for reaction. As there are two p bonds the addition can occur twice.



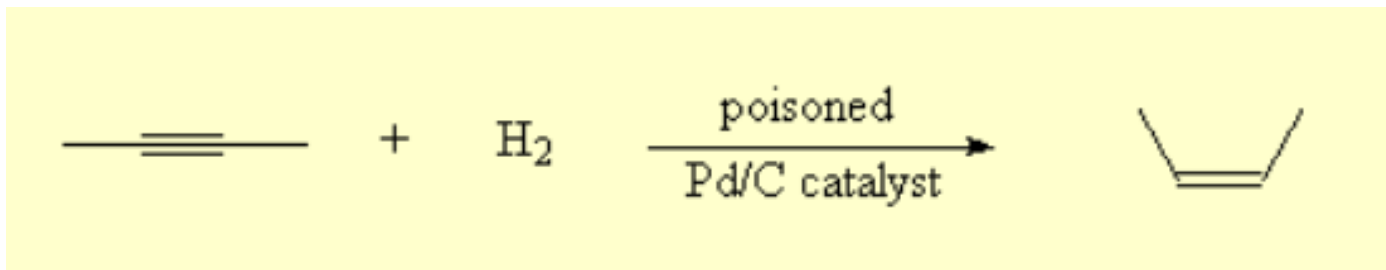
- 1) Hydrogenation \blacklozenge addition of hydrogen.
- 2) Halogenation
- 3) Hydrohalogenation
- 4) Acid-base reaction

1. Hydrogenation ⇨ addition of hydrogen.

- Require a catalyst (Pt/C or Pd/C) to help break strong H-H bond
- Form a saturated hydrocarbon from an unsaturated one

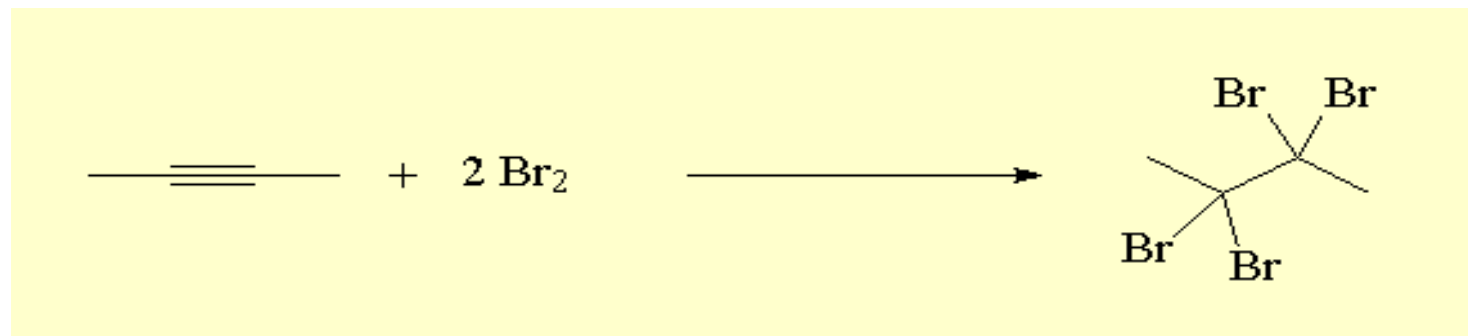


- Partial hydrogenation is possible if a poisoned or deactivated catalyst is used
- In the case of partial hydrogenation, (Z) alkenes are obtained from non terminal alkynes



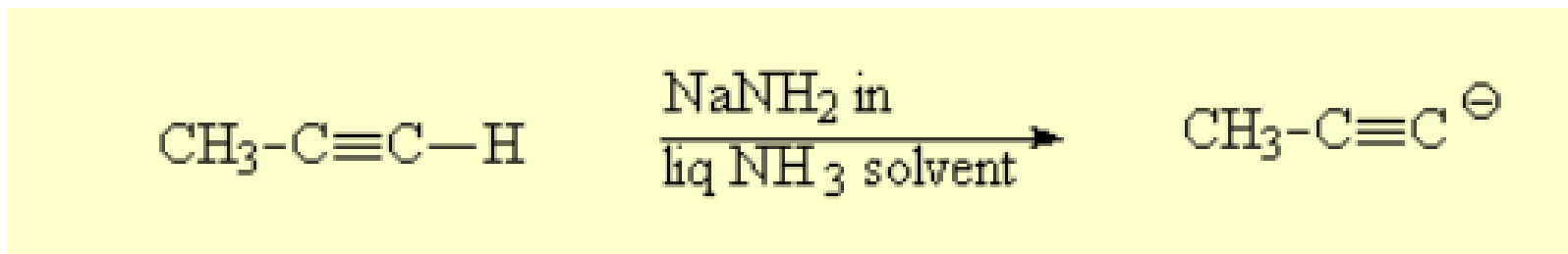
2. Halogenation

- No catalyst required for addition of Cl₂ or Br₂
- Normally an excess of halogen is used to ensure complete reaction



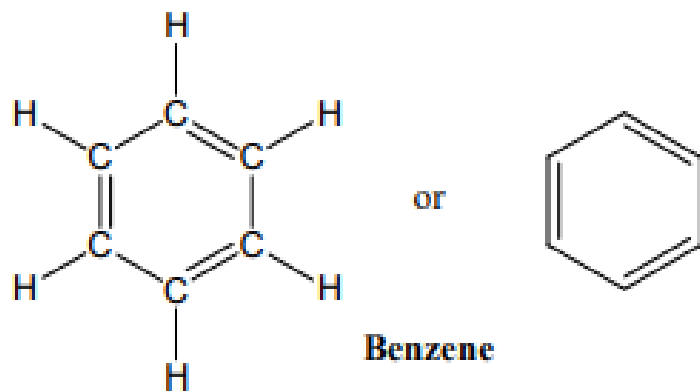
4. Acid-base reaction

- Terminal alkynes only
- Require a very strong base, usually Na⁺NH₂⁻ in liquid NH₃ as solvent



Aromatic Compounds

- Aromatic compounds are those that contain the benzene ring (C₆H₆) or its structural relatives.
- Aliphatic compounds do not contain benzene rings

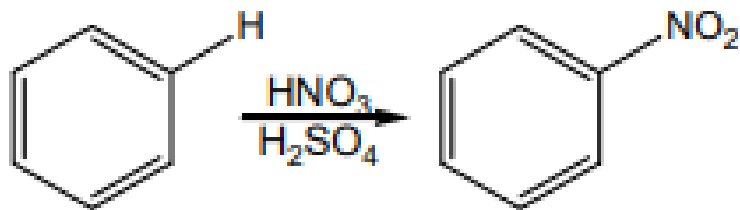


Physical Properties of Aromatic Compounds

- Just like alkanes and alkenes, aromatic compounds are nonpolar, and therefore insoluble in water (unless other substituents, such as OH groups, are present). They are also usually less dense than water.
- Many aromatic compounds are obtained from petroleum and coal tar.
- Benzene and toluene are commonly used as solvents, and are the starting materials for the synthesis of other useful organic compounds.
- Some foods contain aromatic compounds, which can be synthesized by some plants. Some aromatic amino acids and vitamins are listed as essential, because we lack the ability to synthesize them, and must obtain them from our diet.

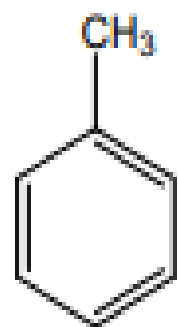
Chemical Properties of Aromatic Compounds

- Aromatic compounds are chemically stable (unlike alkenes). They do NOT undergo any of the reactions of alkenes which we have discussed.
- The major reaction of interest is a substitution reaction in which a hydrogen is replaced by some other group:

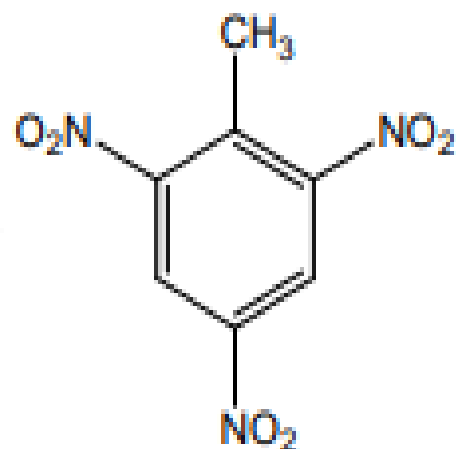
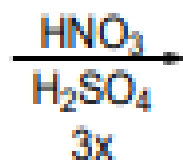


a nitration reaction

- This is an industrially important reaction, because there are mechanisms for converting the nitro group to many other possible functional groups.

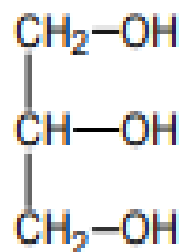


toluene

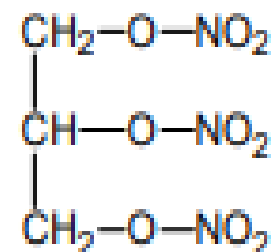
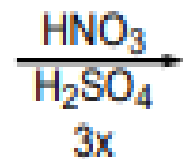


2,4,6-trinitrotoluene (TNT)

A powerful explosive; a sharp pressure wave from a detonator causes the molecule to rearrange into carbon dioxide, water vapor, nitrogen (N₂), and other gases, which expand rapidly and destructively



glycerol /
glycerin

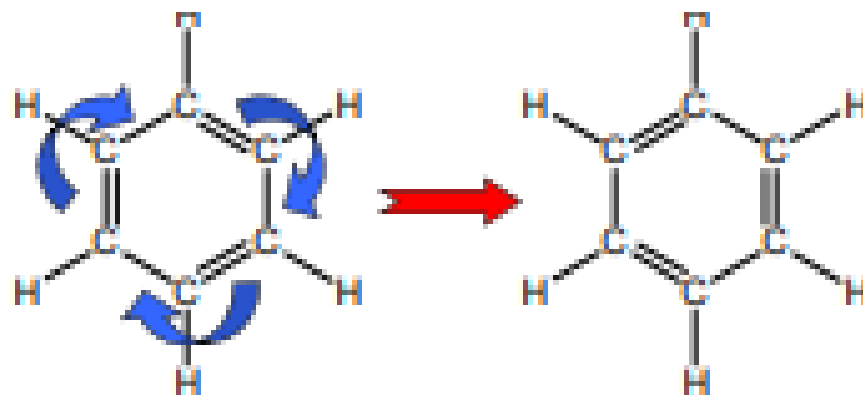


Nitroglycerin

An oily, colorless, extremely unstable liquid; it is usually mixed with an absorbent material, such as clay, to make **dynamite** (Alfred Nobel, 1866)

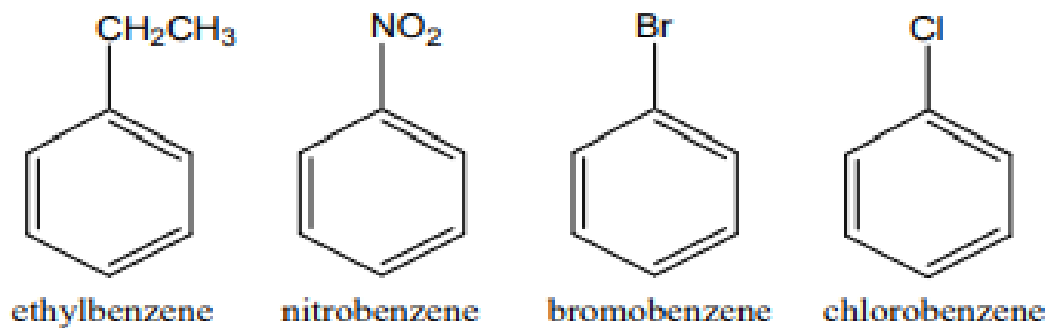
The Structure of Benzene

- The name “aromatic” originally referred to fragrant oils having similar chemical properties (such as oil of wintergreen, vanilla extract, etc.), including a very low carbon-to-hydrogen ratio.
- The molecular structure of benzene was a puzzle for a long time after its discovery; although the formula indicates the presence of double bonds, benzene does not undergo the typical alkene reactions.
- The ring structure of benzene was proposed by August Kekulé in 1865; he suggested that the double bonds switch positions to give two equivalent structures:

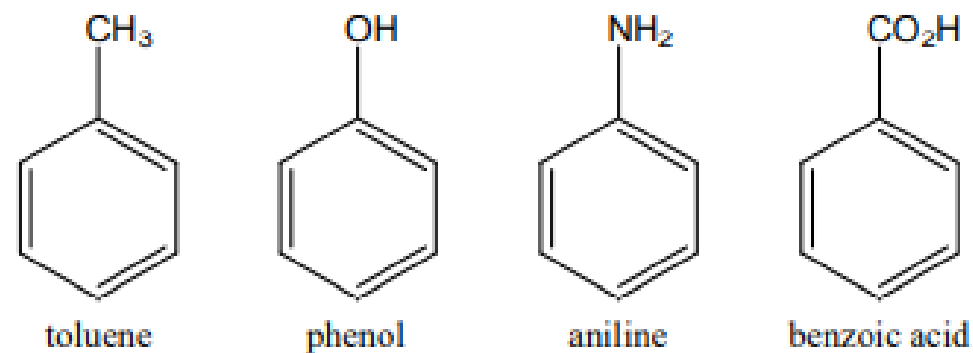


Nomenclature of Benzene Derivatives

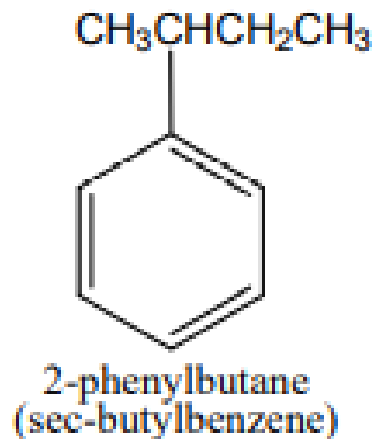
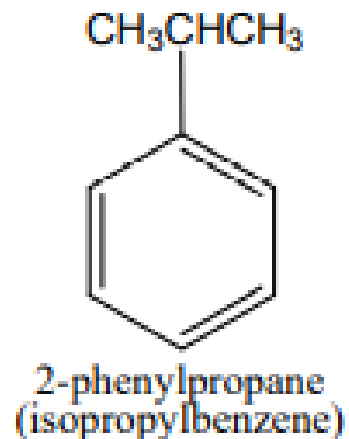
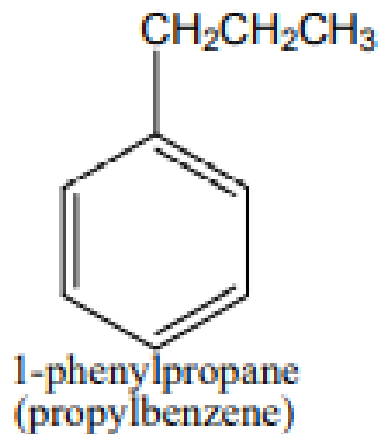
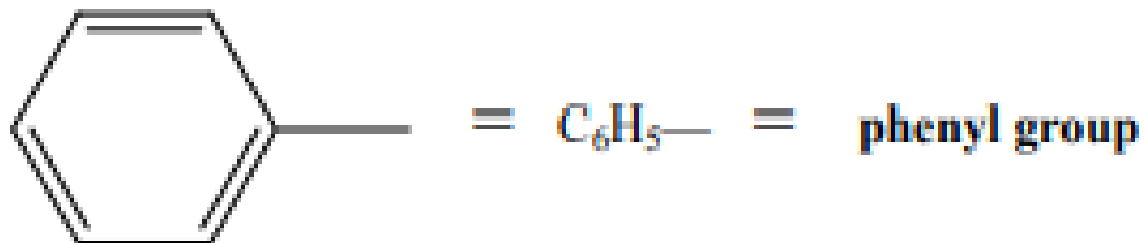
Rule 1. When a single hydrogen of the benzene ring is replaced, the compound can be named as a derivative of benzene.



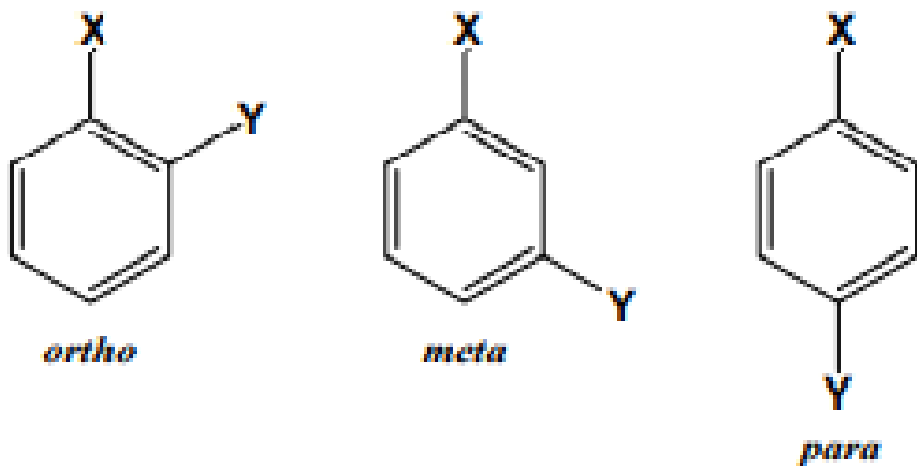
• **Rule 2.** A number of benzene derivatives are known by their common (trivial) names rather than by their formal IUPAC names.



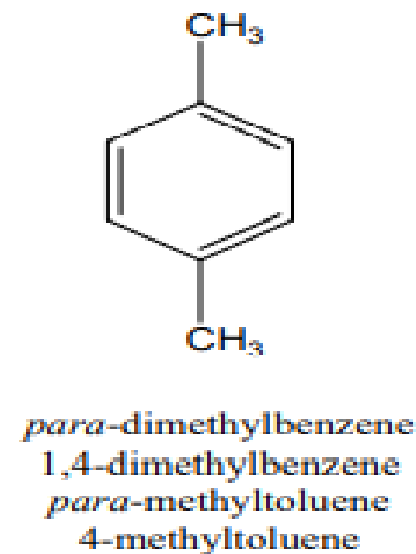
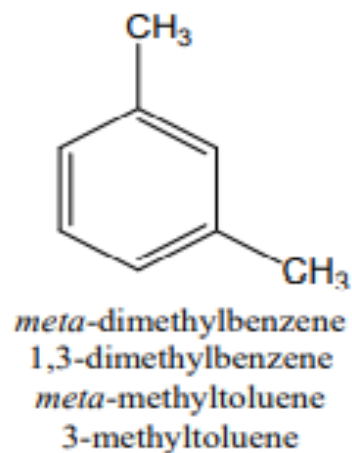
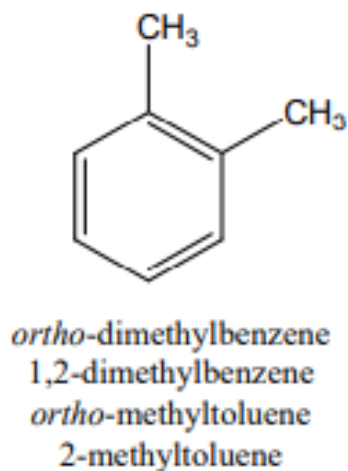
• **Rule 3.** Compounds formed by replacing a hydrogen of benzene with a more complex hydrocarbon group can be named by naming the benzene ring as the substituent, called the phenyl group.



- **Rule 4.** When two groups are attached to a benzene ring, three isomeric structures are possible:



- In naming these compounds, either the ortho / meta / para prefixes may be used, or position numbers (begin numbering at the group which comes first in alphabetical order)



- **Rule 5.** When two or more groups are attached to the benzene ring, their positions can be indicated by numbering the carbon atoms of the ring to obtain the lowest possible numbers for the attachment positions. Groups are arranged in alphabetical order

