

**I. BENZENE**

- A. Benzene is a six-carbon cyclic structure with alternating single and double bonds.
- B. STRUCTURE & STABILITY
- The structure of benzene can be represented in a number of ways.
    - All carbon atoms of benzene are  $sp^2$  hybridized.
    - Benzene is a flat molecule with bond angles of  $120^\circ$ .
  - Benzene is a very stable compound.
    - The stability of benzene is due to the resonance structures of benzene.
    - Benzene does not undergo the same types of reactions that alkenes or conjugated dienes undergo. (i.e., electrophilic additions)
- C. NOMENCLATURE OF BENZENE (15.1)
- Benzene is a parent name with substituents named according to standard IUPAC rules.
  - Disubstituted benzenes can be named using another convention.
    - An ortho-substituted benzene refers to a disubstituted benzene with the two substituents in a 1,2 relationship to each other.
    - A meta-substituted benzene refers to a disubstituted benzene with the two substituents in a 1,3 relationship to each other.
    - A para-substituted benzene refers to a disubstituted benzene with the two substituents in a 1,4 relationship to each other.
  - When benzene is a substituent on a parent system it is referred to as a phenyl group. Benzene is considered to be a substituent whenever the parent contains more than six carbon atoms. A  $\text{PhCH}_2$ - is referred to as a benzyl group.
  - When there are more than two substituents on a benzene ring the structure is numbered using the standard priority rules. The ortho-, meta-, para-, designation cannot be used to name substituted benzenes with three or more substituents.
  - There are a number of common names for monosubstituted benzenes.

**II. AROMATICITY & OTHER AROMATIC COMPOUNDS (15.3)**

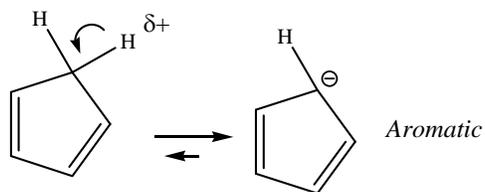
- A. There are three criteria used to define aromatic compounds.
- The molecule or the aromatic portion of a molecule must be cyclic.
  - The cyclic portion of the molecule must have a continuous, planar, conjugated system.
  - The cyclic, conjugated system must follow the Huckel Rule.
    - The Huckel Rule states that aromatic systems must have the appropriate number of pi electrons so that in the following equation,  $n =$  an integer (and remember, zero is an integer)

$$4n + 2 = \text{total \# of pi electrons in aromatic system}$$

- B. POLYCYCLIC AROMATIC COMPOUNDS (15.7)  
Some polycyclic compounds are aromatic. Generally these compounds are referred to by common names.
- C. AROMATIC IONS (15.4)  
Charged molecules may also be aromatic. These are referred to as aromatic ions. These ions can be positively charged or negatively charged.
- D. HETEROCYCLIC AROMATICS (15.5)  
Heterocyclic compounds may also be aromatic. These compounds contain at least one atom in the ring that is not a carbon atom.

**III. CHEMICAL CONSEQUENCES OF AROMATICITY & HOW BENZENE REACTS**

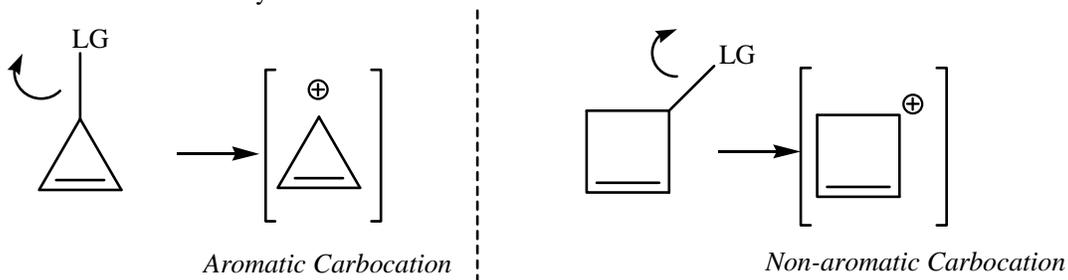
- A. ACIDITY OF PRECURSORS OF AROMATIC ANIONS
- Hydrogens of some compounds are unusually acidic (i.e., lower pKas than expected) due to aromatic stability of resulting conjugate base



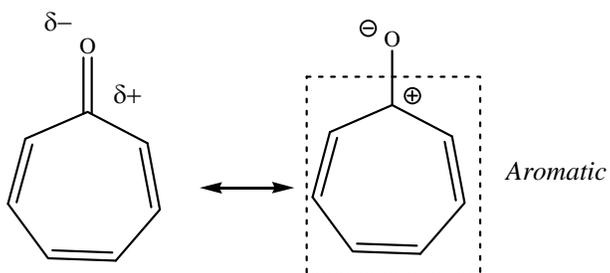
B. STABILITY OF REACTION INTERMEDIATES (Section 15.4)

1. Reactivity of some starting materials increased due to the generation of stable, aromatic carbocations

a. SN1 Reactivity



b. Nucleophilic Acyl Addition



2. Nucleophilicity of aromatic anions reduced due to aromatic stability