Chapter 4: Aromatic Compounds



benzaldehyde

Bitter almonds are the source of the aromatic compound benzaldehyde

Sources of Benzene

$$\begin{array}{c} C_6H_5CH = O \\ \text{benzaldehyde} \end{array}$$

$$\begin{array}{c} C_6H_5CH_2OH \\ \text{benzyl alcohol} \end{array} \xrightarrow{\text{oxidize}} \begin{array}{c} C_6H_5CO_2H \\ \text{benzoic acid} \end{array} \xrightarrow{\text{oxidize}} \begin{array}{c} C_6H_6 \\ \text{benzene} \end{array}$$

$$\begin{array}{c} C_6H_5CH_3 \\ \text{toluene} \end{array}$$

Some Facts About Benzene

Reacts mainly by substitution

$$C_6H_6 + Br_2 \xrightarrow{FeBr_3} C_6H_5Br + HBr$$

benzene bromobenzene

$$C_6H_6 + Cl_2 \xrightarrow{FeCl_3} C_6H_5Cl + HCl$$
benzene chlorobenzene

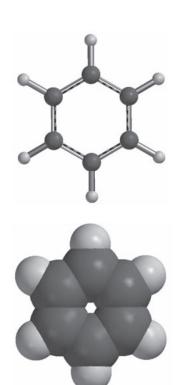


Friedrich August Kekule'

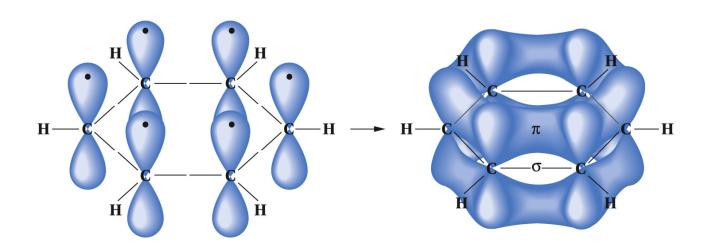
the Kekulé structures for benzene

$$\begin{bmatrix} H & H & H \\ H & H & H \\ H & H & H \end{bmatrix}$$

Benzene is a resonance hybrid of these two contributing structures.



The Orbital Model for Benzene

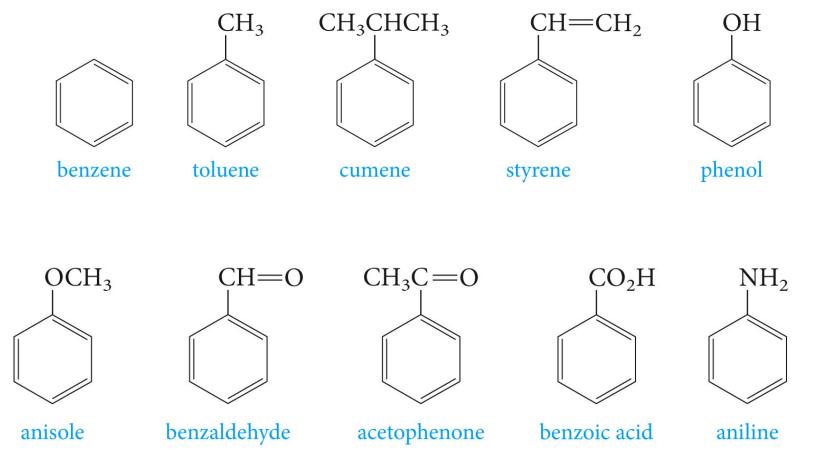


Symbols for Benzene

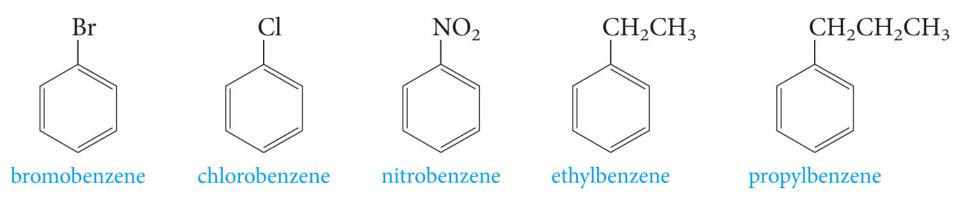


Nomenclature of Aromatic Compounds

Monosubstituted benzenes with common names



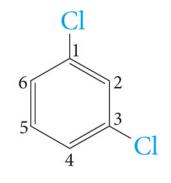
Monosubstituted benzenes that do not have common names



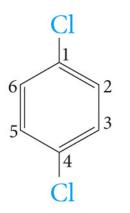
When two substituents are present, we use prefixes *ortho-*, *meta-*, and *para-*, usually abbreviated as o-, m-, and p-, respectively.

$$m$$
 p

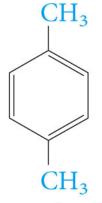
ortho-dichlorobenzene



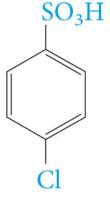
meta-dichlorobenzene



para-dichlorobenzene



para-xylene**

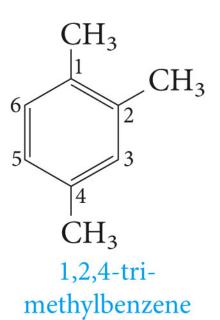


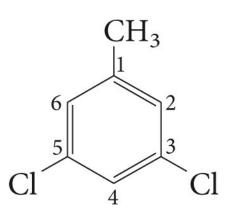
para-chlorobenzenesulfonic acid

Br
$$CH_3$$
 CH_3 CH_2 CH_3 CH_4 CH_3 CH_4 CH_5 CH_5

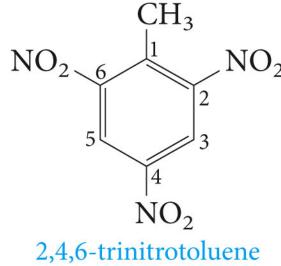
(note alphabetical order)

For more than two substituents, their positions are designated by numbering the ring.





3,5-dichlorotoluene



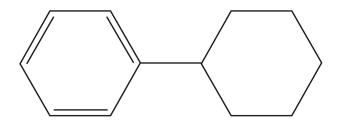
2,4,6-trinitrotoluene (TNT)

Aromatic hydrocarbons, as a class called Arenes (Ar) the aryl groups are therefore aromatic substituents.

$$C_6H_5-$$
 or $C_6H_5CH_2-$ or $C_6H_5CH_2-$ benzyl group

The symbol Ph is sometimes used as an abbreviation for phenyl group

Name the following structures

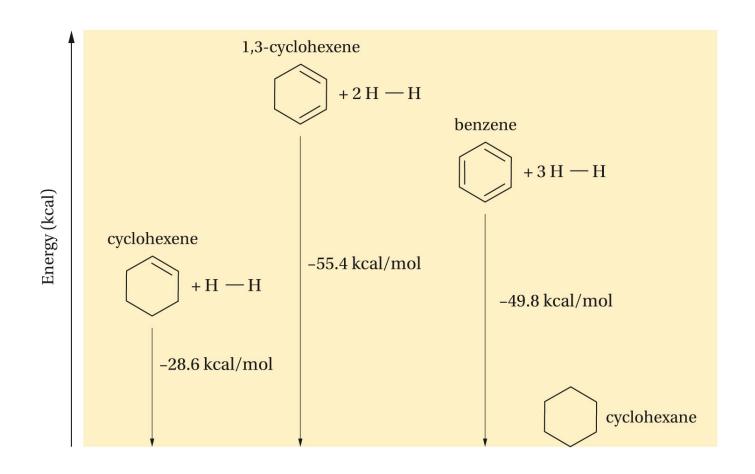


$$OH$$
 CH_2

The Resonance Energy of Benzene

$$C = C + H - H \longrightarrow -C - C - C - + \text{ heat (26-30 kcal/mol)}$$

$$H H$$



Electrophilic Aromatic Substitution

$$+ Cl_2$$
 $\xrightarrow{FeCl_3}$ $+ HCl$

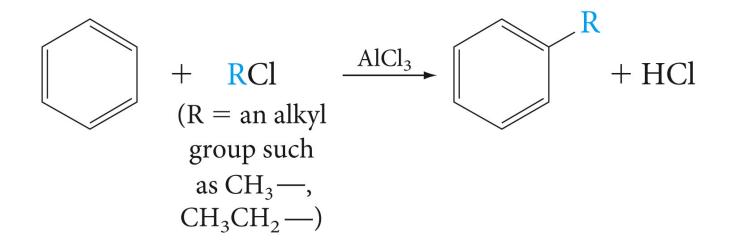
$$+ Br_2 \xrightarrow{FeBr_3} + HBr$$

$$+ HNO_3 + H_2SO_4 + H_2O$$

$$(HONO_2)$$

$$+ H2SO4 \xrightarrow{SO3} + H2O$$

$$(HOSO3H)$$



$$+ CH2 = CH2 H2SO4 CH2CH3$$

