

## Chemistry 110

Bettelheim, Brown, Campbell & Farrell

Eighth Edition

### Introduction to General, Organic and Biochemistry

#### Chapter 13

#### Benzene and its Derivatives

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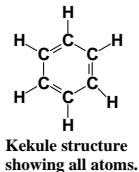
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### Aromatic Compounds

- **Aromatic compound:** a hydrocarbon that contains one or more benzene-like rings.
- **arene:** a term used to describe any given aromatic compound.
- **Ar-**, a symbol for an aromatic substituent group derived by removing an -H atom from an arene.
- **The Kekulé structure for benzene (1872):**



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### Benzene Resonance

- The theory of resonance, developed by Linus Pauling (1930), provided the first adequate description of the structure of benzene.
- According to the theory of resonance, certain molecules and ions are best described by writing two or more Lewis structures; the real molecule or ion is a resonance hybrid of these structures.
- Each individual Lewis structure is called a contributing structure.
- We show that the real molecule is a resonance hybrid of the two or more Lewis structures by using a double-headed arrow between them.

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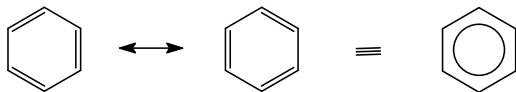
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### Benzene Resonance

➤ The resonance hybrid has some of the characteristics of each Lewis contributing structure



➤ The length of a carbon-carbon bond in benzene, for example, is midway between that of a carbon-carbon single bond and a double bond.

➤ The most important difference is that the benzene unsaturation does not add molecules, only ring substituents may be commonly changed by reaction.

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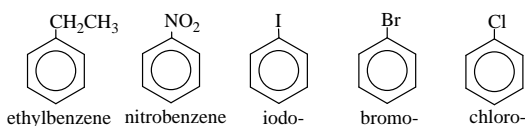
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### Naming of Benzene Derivatives

➤ The phenyl group ( $C_6H_5-$  or Ph-): the substituent group derived by removing one H from benzene.

➤ monosubstituted alkylbenzenes are named as derivatives of benzene; for example:



➤ the IUPAC system also retains certain common names for several of the simpler monosubstituted alkylbenzenes e.g.: toluene, styrene.

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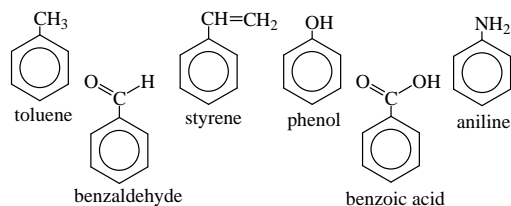
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### Naming of Benzene Derivatives

➤ the common names for these monosubstituted benzenes are also retained.



➤ When additional substituents are added to these compounds, they are named as derivatives of these compounds, locator numbers start with the substituent imparting the special name.

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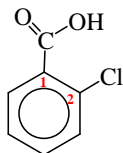
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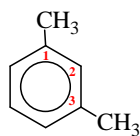
### Naming of Benzene Derivatives

When two substituents occur on a benzene ring, three isomers are possible; they may be located by

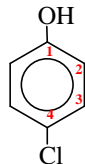
- numbering the atoms of the ring or
- using the locators ortho (o), meta (m), and para (p)



2-chlorobenzoic acid  
o-chlorobenzoic acid



1,3-dimethylbenzene  
m-xylene



4-chlorophenol  
p-chlorophenol

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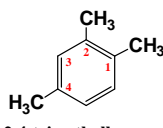
### Naming of Benzene Derivatives

For three or more substituents:

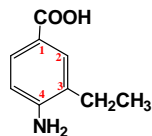
- If one of the substituents imparts a special name, name the molecule as a derivative of that parent, numbering from that substituent.
- If none of the substituents imparts a special name, number the substituents to give the smallest set of numbers, and list them in alphabetical order before the ending "benzene"



2,4-dinitrotoluene



1,2,4-trimethylbenzene



4-amino-3-ethylbenzoic acid

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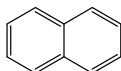
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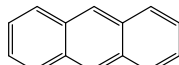
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### Polynuclear Aromatic Hydrocarbons

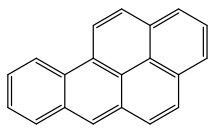
An aromatic hydrocarbon that contains two or more benzene rings, with each pair of rings sharing two adjacent carbon atoms, such as:



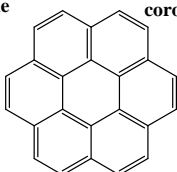
naphthalene



anthracene



benzo[a]pyrene



coronene

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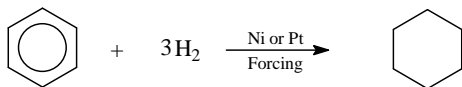
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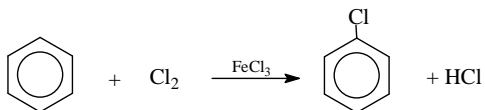
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## Reactions of Benzene

Benzene Undergoes Addition Only Under Forcing Conditions



It Mostly Undergoes Substitution



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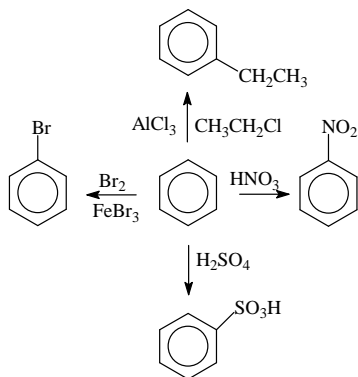
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## Other Substitution Reactions of Benzene



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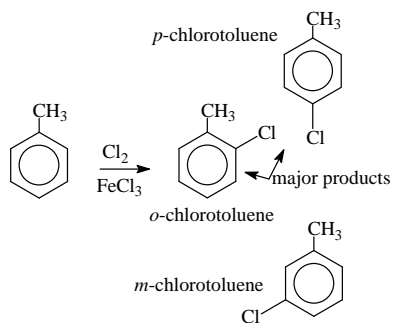
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## Substitution on Toluene



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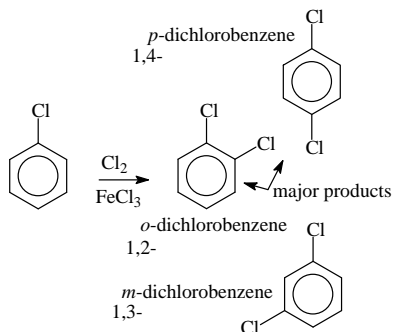
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### Substitution on Chlorobenzene




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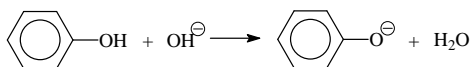
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### PHENOLS

- Phenols – The *hydroxy* group must be bonded directly to the benzene ring.
- Phenols are weakly acidic and ionize in basic solution forming water soluble phenoxide anions.



- Phenols are easily oxidized, the ring itself is attacked and phenols become dark on exposure to air.
- The antioxidant properties found in phenols are useful in food preservatives and in biological repair mechanisms.

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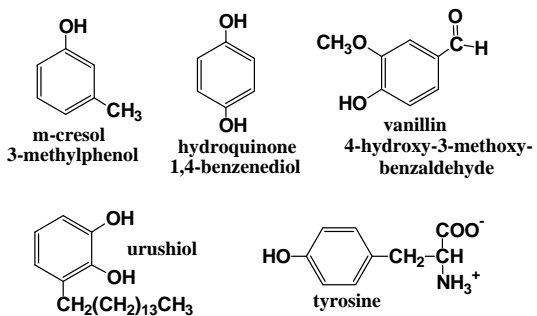
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### Some Common Phenols




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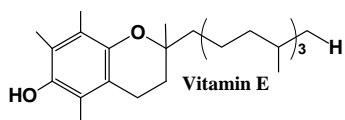
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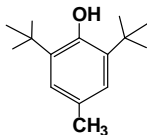
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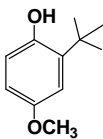
### Some Common Antioxidant Phenols



Vitamin E



2,6-di-*tert*-butyl-4-methylphenol  
Butylatedhydroxytoluene (BHT)



2-*tert*-butyl-4-methoxyphenol  
Butylatedhydroxyanisole (BHA)

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