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ACTIVE LEARNING IN CHEMISTRY EDUCATION

CHAPTER 27

INTRODUCTION TO ORGANIC COMPOUNDS

(Part 3)

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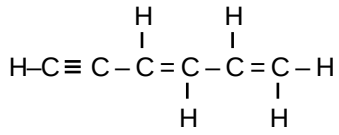
SECTION 27.1 Aromatic Compounds

An important class of carbon compounds exists which was not discussed in Chapters 25 or 26. This class of compounds was discovered during the early years of the study of organic chemistry. Because these compounds had sweet smelling odors they came to be known as the aromatics, although some of them have no such odor.

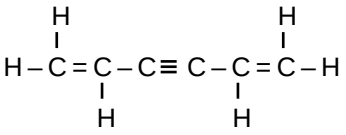
These compounds are still called *aromatics*, although the name no longer applies to any odor. Instead, compounds are now classified as aromatic if they contain a particular structure.

The alkanes, alkenes, and alkynes discussed in Chapter 25 are categorized according to whether they contained single, double, or triple bonds. Alcohols, ethers, aldehydes and the other classes of compounds discussed in Chapter 26 are categorized according to the presence of a specific functional group. The parent compound found in all aromatic molecules is *benzene*.

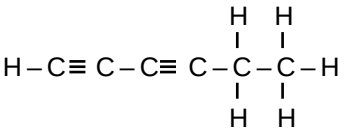
Benzene was discovered in 1825 by Michael Faraday who was at the time analyzing "illuminating gas." Benzene, itself, is the simplest member of the aromatic family. About ten years after its discovery, its formula was determined to be C_6H_6. However, the problem of determining the structure of benzene persisted for several decades. The molecule contains only one hydrogen atom for each carbon atom. Many different structures were proposed, some of which are shown below.



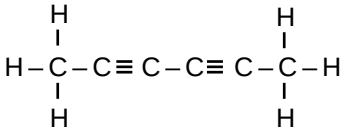
Structure 1



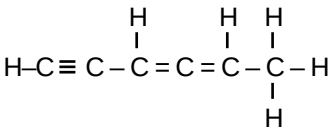
Structure 2



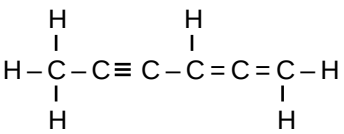
Structure 3



Structure 4



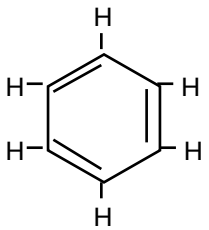
Structure 5



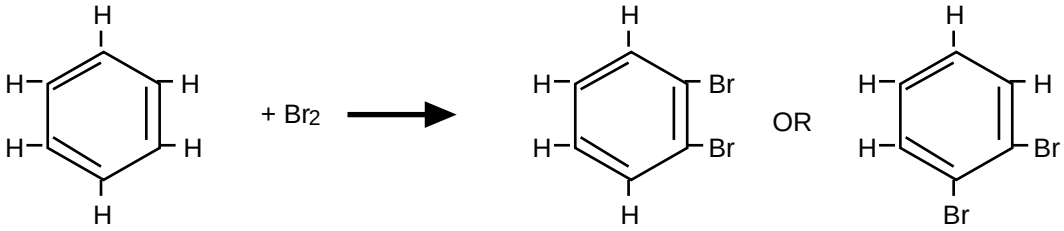
Structure 6

Benzene was found to be a rather stable molecule. Eventually, chemical testing revealed that none of these six "straight-chained" structures could explain the properties of benzene. Finally, in 1865, the chemical structure of benzene was predicted by the German chemist, Kekule. As the story goes, Kekule fell asleep one night sitting in front of a fire and had a dream about chains of carbon atoms behaving like twisting snakes. Suddenly, one of the snakes bit its own tail forming a ring, giving Kekule the inspiration to spend the rest of the night devising a ring structure for benzene. As a result, Kekule is remembered by his famous quote, "Let us learn to dream gentlemen, and then perhaps we shall learn the truth."

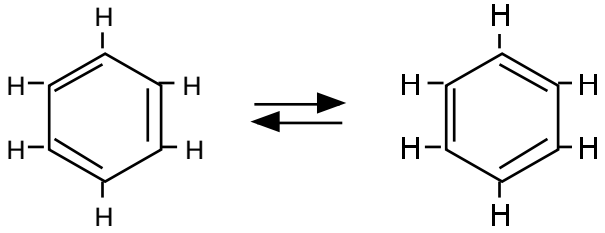
The structure which Kekule proposed was a ring consisting of six carbon atoms joined by alternating single and double bonds. Each carbon atom was also bonded to one hydrogen atom. The stability of the molecule needed to be explained, as did the fact that when it reacts in a one-to-one mole ratio with bromine, benzene forms only <u>one</u> di-substituted product (containing two bromine atoms), when two different products would be predicted as shown below.



Benzene



This evidence suggested that all of the bonds in benzene were equivalent. To solve this problem, Kekule suggested that the double bonds and single bonds in the ring shifted back and forth, and this shifting made all of the bonds sites equivalent:



However, benzene does not react like the alkenes which really do have double bonds. Today, we use the theory of *resonance* to describe the structure of benzene. This theory suggests that benzene does not contain single bonds or double bonds. Instead, the bonds between the carbon atoms are all identical. They are called *resonance hybrids* meaning that they have properties which are between single and double bonds, such as the length of the bonds. The length of carbon to carbon single bonds and carbon to carbon double bonds are 1.54 Angstroms and 1.34 Angstroms, respectively. The length of the carbon to carbon resonance hybrid bonds in the benzene ring is 1.39 Angstroms. According to this theory each carbon on the molecule would be identical. Therefore, only one product would be expected when benzene reacts with bromine. You may still see benzene represented with alternating single and double bonds, but it is understood that they are actually identical resonance hybrids. Some chemists use other symbols to represent benzene, including the structure shown below with the circle inside the ring. (The hydrogen atoms present on the ring are usually not written. They are assumed to be there, unless they are replaced by an atom of another element.)

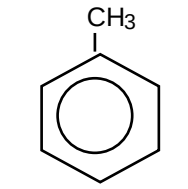
Benzene Benzene

Section 25.2 Naming Aromatic Compounds

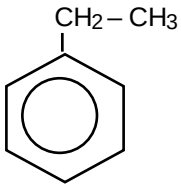
Aromatic compounds have both common names and IUPAC names. In Chapters 25 and 26 we did not include common names. However, because they are still widely used with aromatic compounds, we will include them in this chapter. When a hydrogen atom on the benzene ring is replaced by some other "substituent," the compound can be named as a derivative of benzene. In other words, benzene is considered to be the parent compound. Common substituents include:

bromo	–Br	nitro	$–NO_2$
chloro	–Cl	amino	$–NH_2$
fluoro	–F	hydroxy	–OH
iodo	–I	methyl	$–CH_3$
		ethyl	$–C_2H_5$

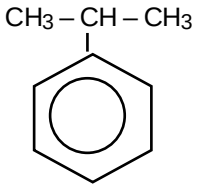
Naming the compounds in this way, gives the IUPAC names:



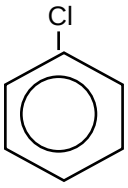
methylbenzene



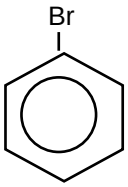
ethylbenzene



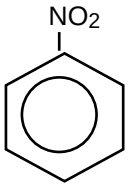
isopropylbenzene



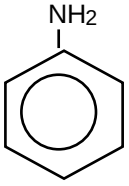
chlorobenzene



bromobenzene



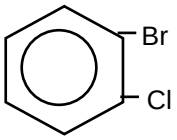
nitrobenzene



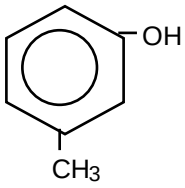
aminobenzene

Note how the IUPAC names always end with "benzene." When the ring contains only one substituent, it is not necessary to include numbers in the name, because all of the carbons are equivalent.

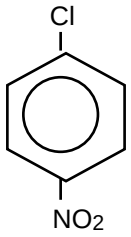
When the ring contains more than one substituent, the names become more complex. When the ring has two substituents, the prefixes *ortho*, *meta*, and *para* are used to describe the positions of the substituents. Ortho refers to adjacent positions, while meta describes two positions separated by one carbon atom. Para positions are located across from each other on the ring. The prefixes can be abbreviated as o-, m-, and p- as in the examples below. The substituents appear in the names in alphabetical order:



o-bromochlorobenzene

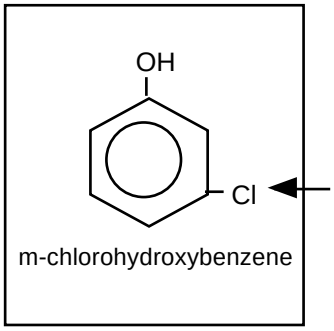


m-hydroxymethylbenzene



p-chloronitrobenzene

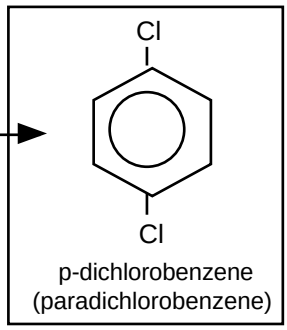
Prefixes are used when more than one <u>identical</u> substituent occurs on the ring. Note the use of the prefix "di" in the name of the structure below.



m-chlorohydroxybenzene

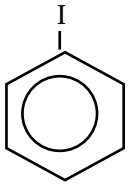
Prefixes are used when more than one <u>identical</u> substituent occurs on the ring. Note the use of the prefix "di" in the name of the structure shown at right.

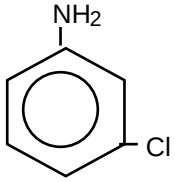
The structure at left has only two substituents. Note that in the IUPAC name the substituents are in alphabetical order (chloro before hydroxy).



p-dichlorobenzene
(paradichlorobenzene)

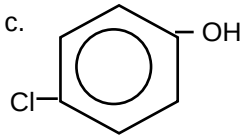
Problem 1. Give IUPAC names for the structures shown below. Write your answers in the space provided.

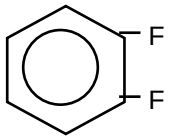
a. 

b. 

a._____

b._____

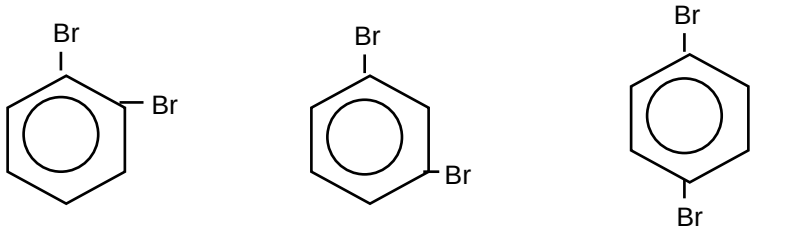
c. 

d. 

c._____

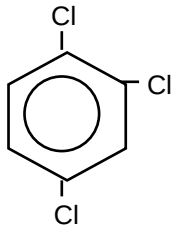
d._____

Structural isomers are compounds that have the same formula but different structures. Three structural isomers of dibromobenzene are possible. They are shown below with their IUPAC names.

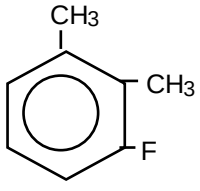


o-dibromobenzene (orthodibromobenzene)	m-dibromobenzene (metadibromobenzene)	p-dibromobenzene (paradibromobenzene)

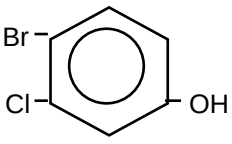
When the ring has three or more substituents, they are located by numbering the ring. The carbons in the ring are numbered so as to give the substituents the lowest possible numbers (as was the case with the cyclic compounds you studied in previously). The compound shown at right is called 1,2,4–trichlorobenzene.



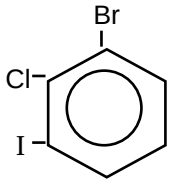
Prefixes like di, tri, etc., are not considered when putting names of substituents in alphabetical order. Consider the name of the structure at right. It is called 1-fluoro-2,3-dimethylbenzene. Note that "fluoro" comes before "methyl." The prefix "di" is ignored.



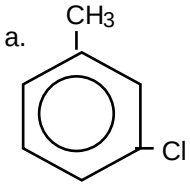
Note that the structure at right is 1-bromo-2-chloro-4-hydroxybenzene. It is <u>not</u> called 1-hydroxy-3-chloro-4-bromobenzene,because numbering the ring that way would give put higher numbers in the name.

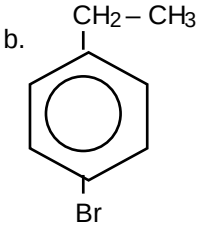


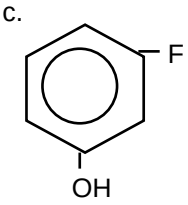
When numbering a ring in either of two ways gives the same set of numbers, then give the lowest number to the substituent which appears first in the name (see structure at right). It is called 1-bromo-2-chloro-3-iodobenzene. It is <u>not</u> called 1-iodo-2-chloro-3-bromobenzene.



Problem 2. Name the compounds shown below using the IUPAC system:

a. 

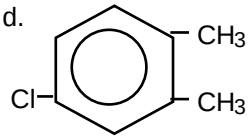
b. 

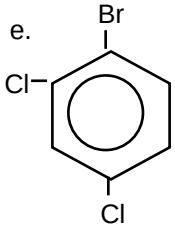
c. 

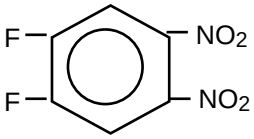
a. _____

b. _____

c. _____

d. 

e. 

f. 

d. _____

e. _____

f. _____

Problem 3. Draw structures which satisfy each of the following IUPAC names:

a. 1,2-dichloro-4-methylbenzene

b. 1,3,5-trimethylbenzene

c. o-diiodobenzene

d. m-hydroxyiodobenzene

e. p-diethylbenzene

f. 1,3-dibromo-5-chlorobenzene

Problem 4. The following IUPAC names are incorrect. Draw the structure that satisfies the name, and then write the correct name:

a. 2,3-dichlorobenzene

_____

b. 1-chloro-5,6-dibromobenzene

_____

c. 2-hydroxy-4,6-difluorobenzene

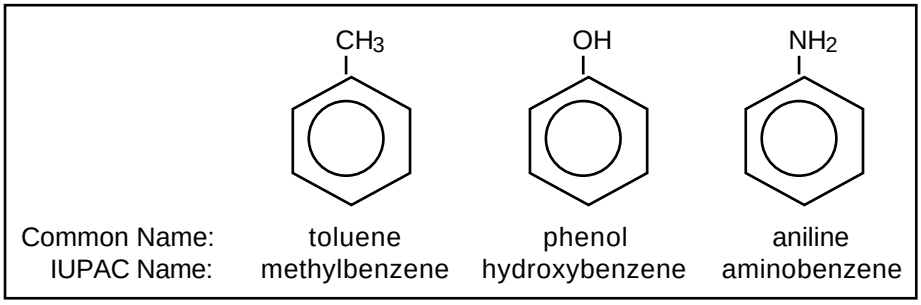
_____

d. 1-chloro-2-amino-5-chlorobenzene

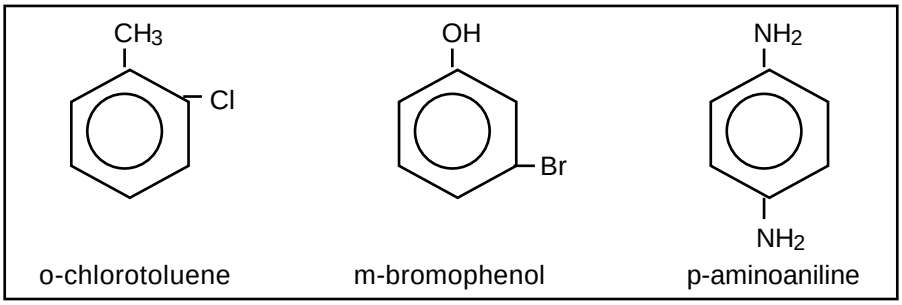
_____

Section 27.3 The Common Names of Aromatic (Benzene) Compounds

Remember, in the IUPAC system compounds are named as derivatives of benzene and, therefore, IUPAC names end with "benzene." Note the common names of the compounds shown below. The IUPAC names are also given.



We will now consider the common names of some benzene compounds that have two substituents on them. Note, however, that they are named as derivatives of toluene, phenol, or aniline, rather than benzene.



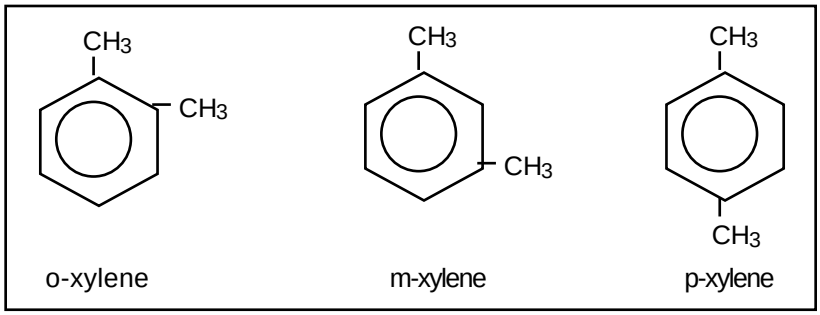
Problem 5. Give the IUPAC names of the three structures shown above.

a._____

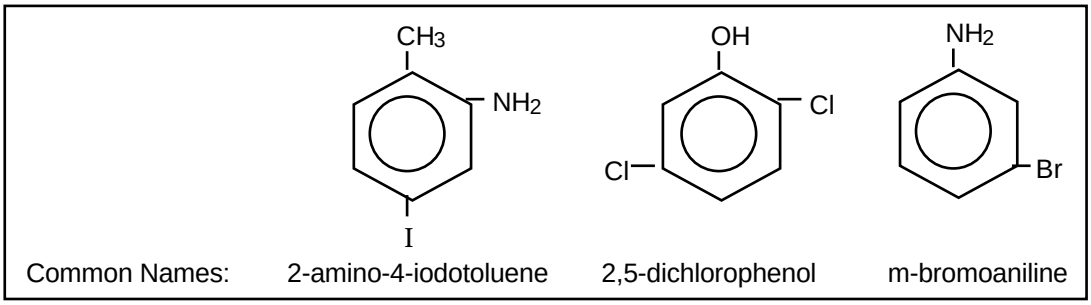
b._____

c._____

When the two substituents on the benzene ring are methyl groups, the compounds are known as xylenes in the common naming system. There are three forms of xylene:



Since xylenes are a special case, they should not be named as derivatives of toluene. For example, o-xylene should not be named o-methyltoluene. The common naming system, like the IUPAC system, makes use of the numbering of the ring for structures with three or more substituents. Note the common names of the structures below:



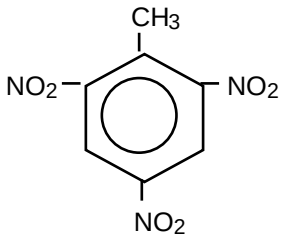
Problem 6. Give the IUPAC names of the three structures above.

a._____

b._____

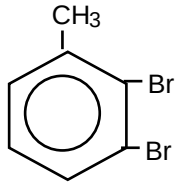
c._____

TNT is an abbreviation that comes from the common name for an explosive. Its structure is shown at right. Its common name is 2,4,6-trinitrotoluene. What is its IUPAC name?



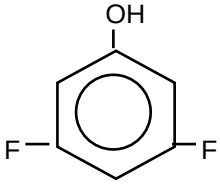
{1}_____

Examine the structure at right. Its common name is 2,3-dibromotoluene. Note that "methyl" is not part of its common name because the methyl group is part of the toluene structure. Since it is part of the parent compound in the common name (toluene), the methyl group is numbered as being on the number 1 carbon in the ring. That's why we do not call it 1,2-dibromotoluene.



Problem 7. Name the following compounds twice, using the common and IUPAC systems.

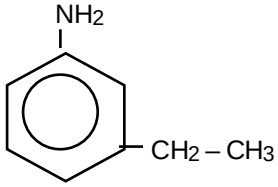
a.



Common: _____

IUPAC:_____

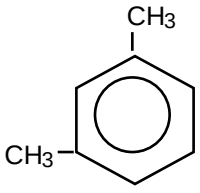
b.



Common: _____

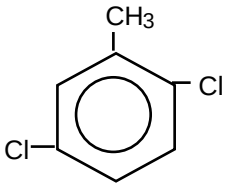
IUPAC:_____

c.



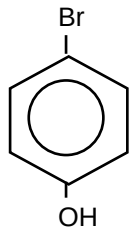
Common: _____

IUPAC:_____

d. 

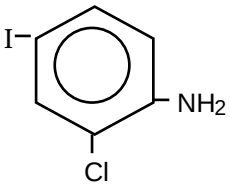
Common: _____

IUPAC:_____

e. 

Common: _____

IUPAC:_____

f. 

Common: _____

IUPAC:_____

Problem 8. The following common names are incorrect. Draw the structure that satisfies the name given, and then write the correct common name:

a. 4,5-dichlorophenol

_____

b. 2-bromotoluene

_____

c. 4,5-dibromoaniline

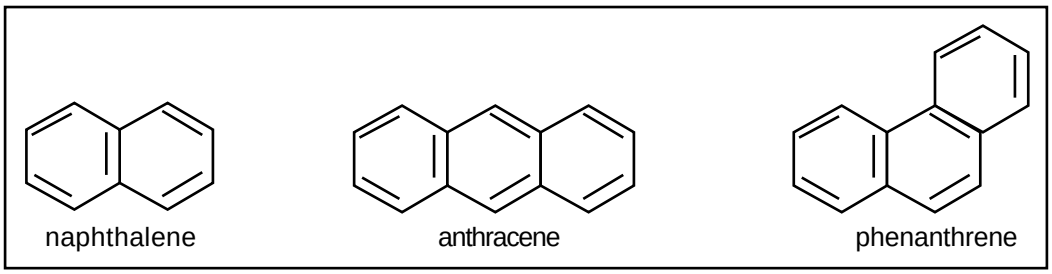
_____

d. 4-methyltoluene

_____

Section 27.4 Condensed Ring Structures

There are some common aromatic structures which are not composed of benzene rings with substituents on them. These compounds are known as *condensed ring structures*. They look somewhat like a number of benzene rings which have been bonded together. Three examples of condensed ring structures which are extracted from coal tar include:



Like p-dichlorobenzene, naphthalene is often used to make moth balls. Anthracene is used in the manufacture of dyes, and steroids are compounds which are based on the structure of phenanthrene. Since aromatic chemistry developed in a rather haphazard way for many years, many of these compounds were given common names (such as those above) which are still used today. These compounds do not actually exist in coal tar; instead, they are formed when coal tar is heated (distilled). It is believed that some condensed ring structures are formed whenever organic molecules are heated to a high temperature. This includes the burning of tobacco in cigarettes. The bad news is that many of these compounds have been shown to produce cancer. Workers at plants where coal tar is distilled have had higher than normal rates of skin cancer. Needless to say, condensed ring structures are also suspect in the development of lung cancer.

Section 27.5 Learning Outcomes

This is the end of your study of organic nomenclature in the ALICE program. You should know that organic chemistry is a very large field of study. New organic compounds and products are being made every year. Students of organic chemistry not only learn about the classification and nomenclature of compounds. This is actually only a very small part of what they study. Some of the most important research being done in science today, involves the study of reactions that organic compounds undergo. This field is very important in agriculture, medicine, manufacturing, and many other fields of human endeavor. Be sure that you have mastered each of the learning outcomes below.

_____1. Distinguish between organic structures which belong to the aromatic class of compounds and those which do not.

_____2. Draw the structure of simple aromatic molecules given their IUPAC names.

_____3. Write the IUPAC names of simple aromatic molecules given their structures.

_____4. Draw the structures of simple aromatic molecules given their IUPAC names.

_____5. Draw the structures of simple aromatic molecules given their common names.

_____6. Recognize the structure of condensed ring structures.

Section 27.6 Answers to Questions and Problems

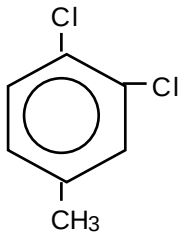
Questions:

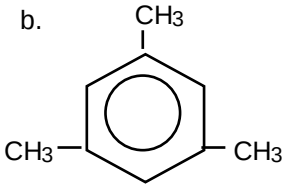
{1} 1-methyl-2,4,6-trinitrobenzene

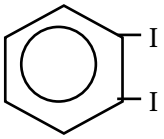
Problems:

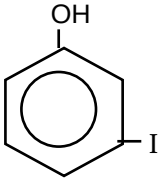
1. a. iodobenzene; b. m-aminochlorobenzene; c. p-chlorohydroxybenzene; d. o-difluorobenzene

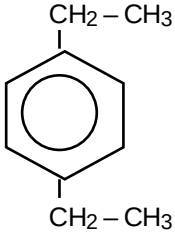
2. a. m-chloromethylbenzene; b. p-bromoethylbenzene; c. m-fluorohydroxybenzene;
   d. 4-chloro-1,2-dimethylbenzene; e. 1-bromo-2,4-dichlorobenzene;
   f. 1,2-difluoro-4,5-dinitrobenzene

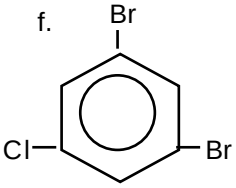
3. a. 

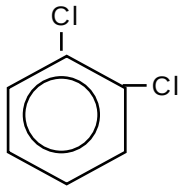
b. 

c. 

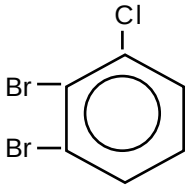
d. 

e. 

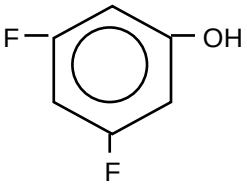
f. 

4. a. 

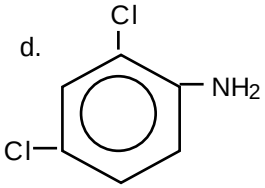
1,2-dichlorobenzene

b. 

1,2-dibromo-3-chlorobenzene

c. 

1,3-difluoro-5-hydroxybenzene

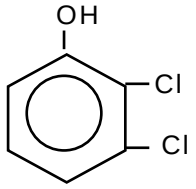
d. 

1-amino-2,4-dichlorobenzene

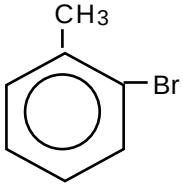
5. a. o-chloromethylbenzene
   b. m-bromohydroxybenzene
   c. p-diaminobenzene

6. a. 2-amino-4-iodo-1-methylbenzene
   b. 1,4-dichloro-2-hydroxybenzene
   c. m-aminobromobenzene

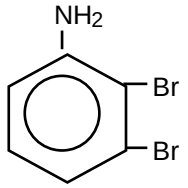
7. a. 3,5-difluorophenol
      1,3-difluoro-5-hydroxybenzene
   b. m-ethyltoluene
      1-amino-3-ethylbenzene
   c. m-xylene
      m-dimethylbenzene
   d. 2,5-dichlorotoluene
      1,4-dichloro-2-methylbenzene
   e. p-bromophenol
      p-bromohydroxybenzene
   f. 2-chloro-4-iodoaniline
      1-amino-2-chloro-4-iodobenzene

8. a. 

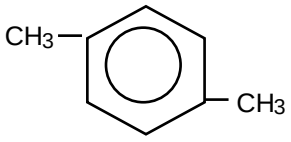
2,3-dichlorophenol

b. 

o-bromotoluene

c. 

2,3-dibromoaniline

d. 

p-xylene