

15.1: NAMING AROMATIC COMPOUNDS

OBJECTIVES

After completing this section, you should be able to

1. draw the structure of each of the common aromatic compounds in Figure 16 (Common benzene derived compounds with various substituents), given their IUPAC-accepted trivial names.
2. write the IUPAC-accepted trivial name for each of the compounds in Figure 16, given the appropriate Kekulé, condensed or shorthand structure.
3. identify the ortho, meta and para positions in a monosubstituted benzene ring.
4. use the ortho/meta/para system to name simple disubstituted aromatic compounds.
5. draw the structure of a simple disubstituted aromatic compound, given its name according to the ortho/meta/para system.
6. provide the IUPAC name of a given aromatic compound containing any number of the following substituents: alkyl, alkenyl or alkynyl groups; halogens; nitro groups; carboxyl groups; amino groups; hydroxyl groups.
7. draw the structure of an aromatic compound containing any number of the substituents listed in Objective 6, above, given the IUPAC name.
8. provide the IUPAC name of a given aromatic compound in which the phenyl group is regarded as a substituent.
9. draw the Kekulé, condensed or shorthand structure of an aromatic compound in which the phenyl group is regarded as a substituent, given its IUPAC name.

KEY TERMS

Make certain that you can define, and use in context, the key terms below.

- arene
- benzyl group
- phenyl group

STUDY NOTES

You should already know the names and structures of several of the hydrocarbons shown in Figure 15.1. A compound containing a benzene ring which has one or more alkyl substituents is called an arene.

A phenyl group consists of a benzene ring with one of its hydrogens removed.

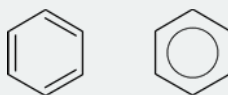


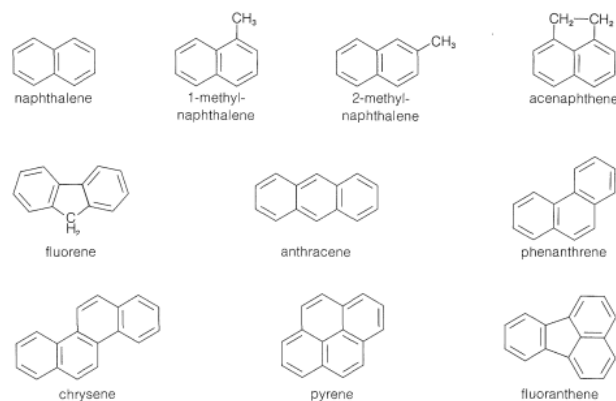
Figure 15.1.1: Two ways of representing a phenyl group

You should memorize the structures and formulas shown in Figure 16. You will meet these compounds frequently throughout the remainder of this course.

Note that the ortho/meta/para system cannot be used when more than two substituents are present in the benzene ring. The “numbering system” can be used instead of the ortho/meta/para system in most cases when only two substituents are present.

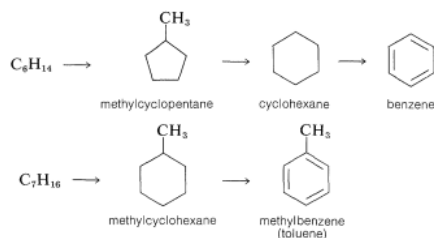
SOURCES OF AROMATIC COMPOUNDS

Initially aromatic compounds were isolated from coal tar. Coal tar, which is a distillate obtained when heating coal at 1000 °C in the absence of air, is a source of an amazing number of aromatic compounds. Many simple aromatic compounds, some of which includes nitrogen, oxygen, and sulfur, as well as hydrocarbons are obtained.



Some of the Aromatic Compounds Obtained from Coal Tar

Prior to World War II, coal tar was the only important source of aromatic hydrocarbons, but during the war the demand for benzene and toluene, a precursor to the explosive TNT, rose so sharply that other sources had to be found. Today, most of the benzene and almost all of the toluene produced in the United States are derived from petroleum. Although petroleum does contain some aromatic compound, it is primarily made up of alkanes of various chain lengths. Aromatic compounds are synthesized from petroleum by a process referred to in the petroleum industry as catalytic re-forming or hydroforming. This involves heating a C6-C10 alkane fraction of petroleum with hydrogen in the presence of a catalyst to modify the molecular structure of its components. Some amazing transformations take place, and the C6-C7 alkanes can be converted to cycloalkanes, which, in turn, are converted to arenes. Benzene, and methylbenzene (toluene) are produced primarily in this way.



NOMENCLATURE OF MONO-SUBSTITUTED BENZENES

Unlike aliphatic organics, nomenclature of benzene-derived compounds can be confusing because a single aromatic compound can have multiple possible names (such as common and systematic names) be associated with its structure. Common names are often used in the nomenclature of aromatic compounds. IUPAC still allows for some of the more widely used common name to be used. A partial list of these common names is shown in Figure 15.1.2 and there are numerous others. These common names take the place of the benzene base name. Methylbenzene is commonly known with the base name toluene, hydroxyphenol is known as phenol etc. It is very important to be able to identify these structures as they will be utilized in the nomenclature of more complex compounds.

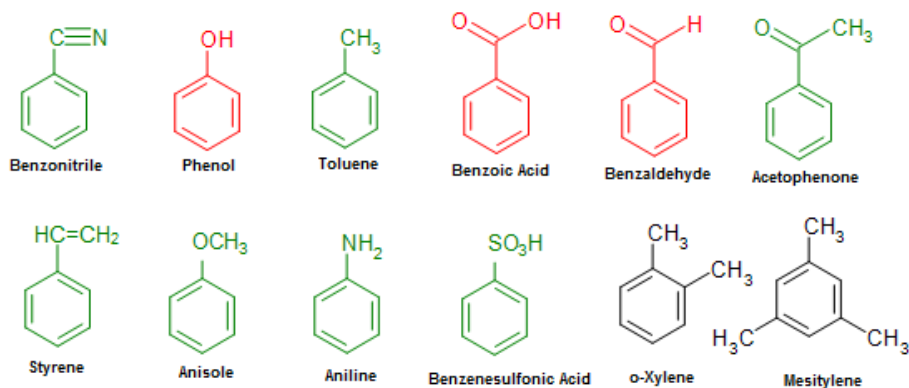
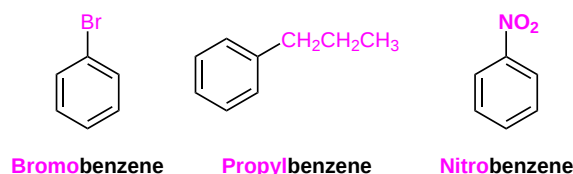


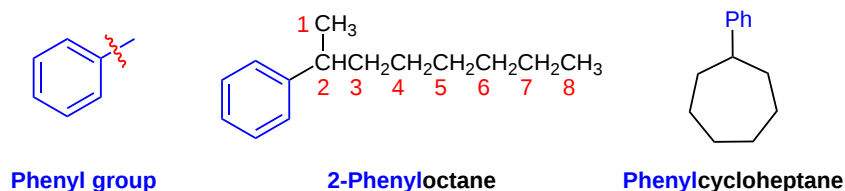
Figure 15.1.2: Common Names for Mono-Substituted Benzenes

Mono-substituted benzene rings, with a substituent not on the list above, are named with benzene being the parent name. These compounds are named as such: *Name of the substituent + Benzene*.

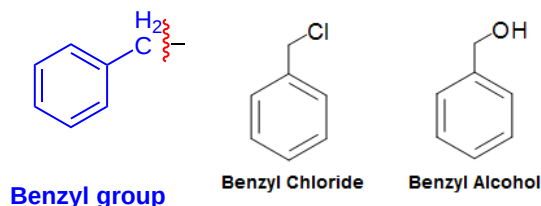


THE USE OF PHENYL AND BENZYL IN NOMENCLATURE

If the alkyl group attached to the benzene contains seven or more carbons the compound is named as a phenyl substituted alkane. The name phenyl (C_6H_5 -) is often abbreviated (Ph) and comes from the Greek word **pheno** which means "I bear light". This name commemorates the fact that benzene was first isolated by Michael Faraday in 1825 from the residue left in London street lamps which burned coal gas. If the alkyl substituent is smaller than the benzene ring (six or fewer carbons), the compound is named as an alkyl-substituted benzene following the rules listed above.



The benzyl group (abbrev. Bn), similar to the phenyl group and can be written as $\text{C}_6\text{H}_5\text{CH}_2\text{-R}$, $\text{PhCH}_2\text{-R}$, or Bn-R . Nomenclature of benzyl group based compounds are very similar to the phenyl group compounds. For example, a chlorine attached to a benzyl group would simply be called benzyl chloride, whereas an OH group attached to a benzyl group would simply be called benzyl alcohol.



NOMENCLATURE OF DISUBSTITUTED BENZENES

With disubstituted benzenes there are three distinct positional isomers which can occur and must be identified in the compounds name. Although numbering can be used to indicate the position of the two substituents it is much more common for the compounds to be named using prefixes. These prefixes are italicized and are often abbreviated with a single letter. They are defined as the following:

- **ortho- (o-):** 1,2- (next to each other in a benzene ring)
- **meta- (m):** 1,3- (separated by one carbon in a benzene ring)
- **para- (p):** 1,4- (across from each other in a benzene ring)

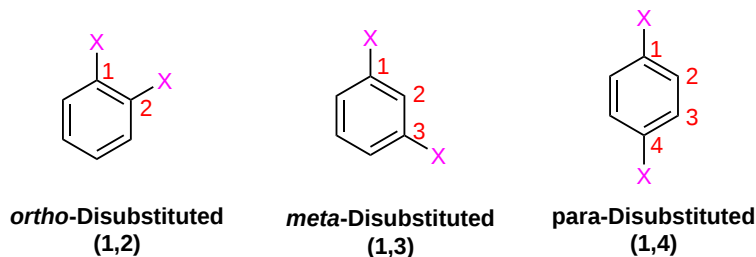
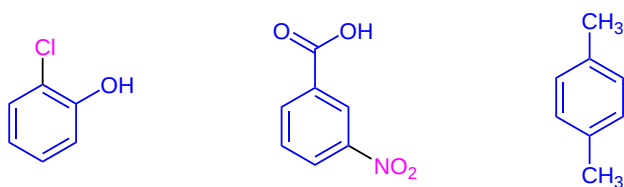
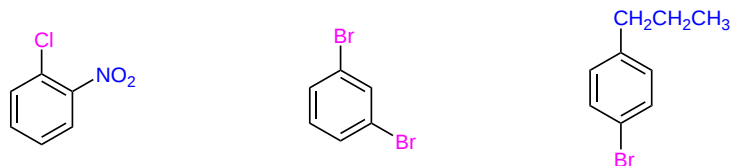


Figure 15.1.2. If any do appear then the compound is not named as a benzene but with a different parent name. These compounds are named as such: *Position prefix-Name of the substituent + Name of parent chain.*



ortho-Chlorophenol **meta-Nitrobenzoic acid** **para-Xylene**

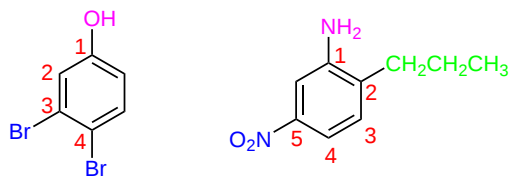
Figure 15.1.2 the compound is named as such: *Position prefix-Names of the substituents in alphabetical order + benzene*. Remember if two of the same substituent appears then the prefix *di-* is used before the substituent's name.



ortho-Chloronitrobenzene **meta-Dibromobenzene** **para-Bromopropylbenzene**

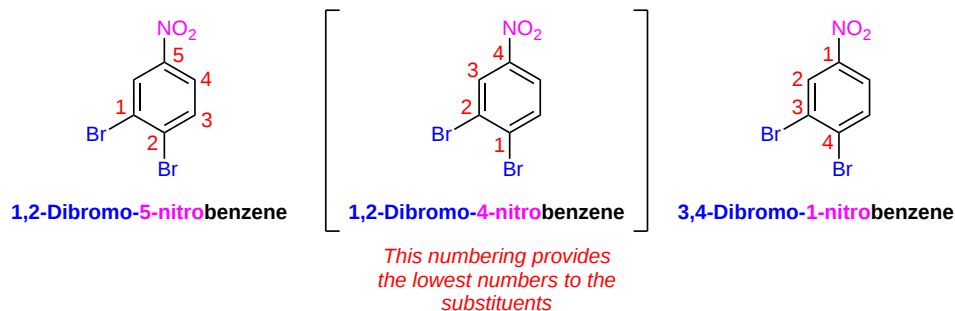
NOMENCLATURE OF BENZENES WITH THREE OR MORE SUBSTITUENTS

When three or more substituents are present the ortho, meta, para positional prefixes become inadequate and a numbering system for the ring must be applied. Here again it is important to check if any of the substituents are listed in **Figure 15.1.2**. If a substituent from **Figure 15.1.2** is present it is given the parent name in the nomenclature. Also, this substituent is given position one in the numbering system. The other substituents are numbered such that they get the lowest possible sum. In the compound's name the substituents are given their position number and listed alphabetically. Remember that di-, tri-, tetra- prefixes are still used to indicate multiple of the same substituent being present but are ignored for alphabetical listing.



3,4-Dibromophenol **5-Nitro-2-propylaniline**

Figure 15.1.2, the benzene ring is named in the same fashion as cycloalkanes. The lowest possible number is given to the substituents present. This is best done by arbitrarily giving a substituent position one and then numbering the rest of the substituents. Then this process is repeated with the other substituents. Which ever iteration provides the lowest overall sum of numbers will be used in the compound's name. The substituents are assigned a location number, listed alphabetically and the suffix *-benzene* is added.



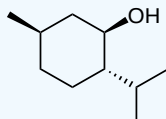
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EXERCISES

? EXERCISE 15.1.1



(True/False) The compound above contains a benzene ring and thus is aromatic.

Answer

False, this compound does not contain a benzene ring in its structure.

? EXERCISE 15.1.2

Benzene unusual stability is caused by how many conjugated pi bonds in its cyclic ring? ____

Answer

3

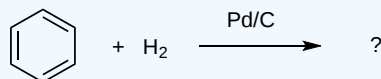
? EXERCISE 15.1.3

Menthol, a topical analgesic used in many ointments for the relief of pain, releases a peppermint aroma upon exposure to the air. Based on this conclusion, can you imply that a benzene ring is present in its chemical structure? Why or why not?

Answer

No, a substance that is fragrant does not imply a benzene ring is in its structure. See camphor example (figure 1)

? EXERCISE 15.1.4



Answer

No reaction, benzene requires a special catalyst to be hydrogenated due to its unusual stability given by its three conjugated pi bonds.

? EXERCISE 15.1.5

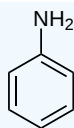
At normal conditions, benzene has ____ resonance structures.

Answer

2

? EXERCISE 15.1.6

Which of the following name(s) is/are correct for the following compound?



- a. nitrohydride benzene
- b. phenylamine
- c. phenylamide
- d. aniline
- e. nitrogenhydrogen benzene
- f. All of the above is correct

Answer

b, d

? EXERCISE 15.1.7

Convert 1,4-dimethylbenzene into its common name.

Answer

p-Xylene

? EXERCISE 15.1.8

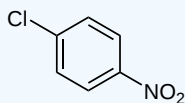
TNT's common name is: _____

Answer

2,4,6-trinitrotoluene

? EXERCISE 15.1.9

Name the following compound using OMP nomenclature:



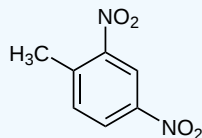
Answer

p-chloronitrobenzene

? EXERCISE 15.1.10

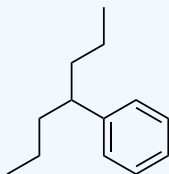
Draw the structure of 2,4-dinitrotoluene.

Answer



? EXERCISE 15.1.11

Name the following compound:

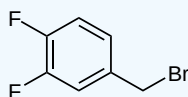


Answer

4-phenylheptane

✓ EXAMPLE 15.1.12

Which of the following is the correct name for the following compound?



- a. 3,4-difluorobenzyl bromide
- b. 1,2-difluorobenzyl bromide
- c. 4,5-difluorobenzyl bromide
- d. 1,2-difluoroethyl bromide
- e. 5,6-difluoroethyl bromide
- f. 4,5-difluoroethyl bromide

Solution

a

? EXERCISE 15.1.13

(True/False) Benzyl chloride can be abbreviated Bz-Cl.

Answer

False, the correct abbreviation for the benzyl group is Bn, not Bz. The correct abbreviation for Benzyl chloride is Bn-Cl.

? EXERCISE 15.1.14

Benzoic Acid has what R group attached to its phenyl functional group?

Answer

COOH

? EXERCISE 15.1.15

(True/False) A single aromatic compound can have multiple names indicating its structure.

Answer

True. TNT, for example, has the common name 2,4,6-trinitrotoluene and its systematic name is 2-methyl-1,3,5-trinitrobenzene.

? EXERCISE 15.1.16

List the corresponding positions for the OMP system (o-, m-, p-).

Answer

Ortho - 1,2 ; Meta - 1,3 ; Para - 1,4

? EXERCISE 15.1.17

A scientist has conducted an experiment on an unknown compound. He was able to determine that the unknown compound contains a cyclic ring in its structure as well as an alcohol (-OH) group attached to the ring. What is the unknown compound?

- Cyclohexanol
- Cycloheptanol
- Phenol
- Methanol
- Bleach
- Cannot determine from the above information

Answer

The correct answer is f). We cannot determine what structure this is since the question does not tell us what kind of cyclic ring the -OH group is attached on. Just as cyclohexane can be cyclic, benzene and cycloheptane can also be cyclic.

? EXERCISE 15.1.18

Which of the following statements is **false** for the compound, phenol?

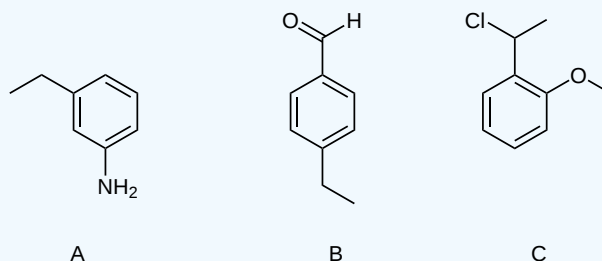
- Phenol is a benzene derived compound.
- Phenol can be made by attaching an -OH group to a phenyl group.
- Phenol is highly toxic to the body even in small doses.
- Phenol can be used as a catalyst in the hydrogenation of benzene into cyclohexane.
- Phenol is used as an antiseptic in minute doses.
- Phenol is amongst one of the three common names retained in the IUPAC nomenclature.

Answer

d

? EXERCISE 15.1.19

State whether the following is para, meta, or ortho substituted.

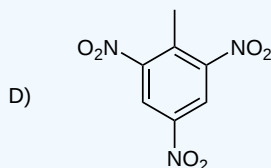
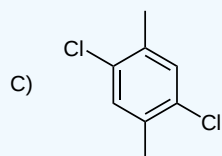
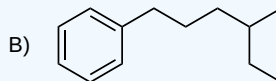
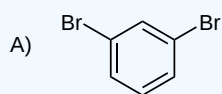


Answer

A – meta; B – para; C – ortho

? EXERCISE 15.1.20

Name the following compounds.



Answer

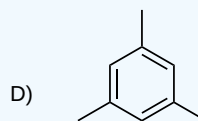
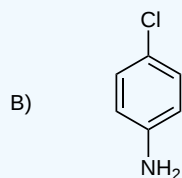
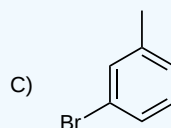
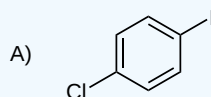
- 1,3-Dibromobenzene
- 1-phenyl-4-methylhexane
- 1,4-Dichloro-2,5-dimethylbenzene
- 2-methyl-1,3,5-trinitrobenzene. (Also known as trinitrotoluene, or TNT)

? EXERCISE 15.1.21

Draw the following structures

- p-chloriodobenzene
- m-bromotoluene
- p-chloroaniline
- 1,3,5-trimethylbenzene

Answer



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