

15.3: Nomenclature of Benzene Derivatives

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. In these sections, we will analyze some of the ways these compounds can be named.

Simple Benzene Naming

Some common substituents, like NO_2 , Br, and Cl, can be named this way when it is attached to a phenyl group. Long chain carbons attached can also be named this way. The general format for this kind of naming is:

(positions of substituents (if >1)- + # (di, tri, ...) + substituent)_n + benzene.

For example, chlorine (Cl) attached to a phenyl group would be named **chlorobenzene (chloro + benzene)**. Since there is only one substituent on the benzene ring, we do not have to indicate its position on the benzene ring (as it can freely rotate around and you would end up getting the same compound.)

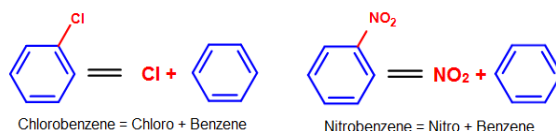


Figure 8. Example of simple benzene naming with chlorine and NO_2 as substituents.

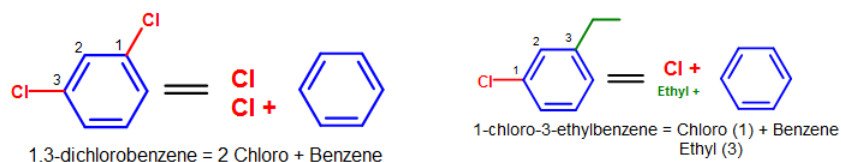


Figure 9. More complicated simple benzene naming examples - Note that standard nomenclature priority rules are applied here, causing the numbering of carbons to switch. See [Nomenclature of Organic Compounds](#) for a review on naming and priority rules.

Ortho-, Meta-, Para- (OMP) Nomenclature for Disubstituted Benzenes

Instead of using numbers to indicate substituents on a benzene ring, **ortho- (o-)**, **meta- (m-)**, or **para- (p-)** can be used in place of positional markers when there are **two** substituents on the benzene ring (disubstituted benzenes). 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)

Using the same example above in figure 9a (1,3-dichlorobenzene), we can use the ortho-, meta-, para- nomenclature to transform the chemical name into m-dichlorobenzene, as shown in the figure below.



Figure 10. Transformation of 1,3-dichlorobenzene into m-dichlorobenzene.

Here are some other examples of ortho-, meta-, para- nomenclature used in context:

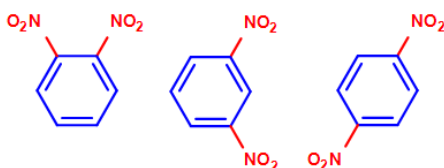


Figure 11. Example of o-, m-, p- nomenclature. Listed in order:
1) o-dinitrobenzene
2) m-dinitrobenzene
3) p-dinitrobenzene

However, the substituents used in ortho-, meta-, para- nomenclature do not have to be the same. For example, we can use chlorine and a nitro group as substituents in the benzene ring.

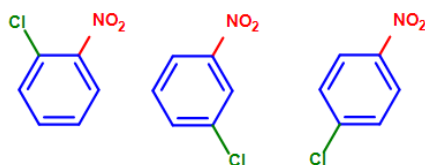
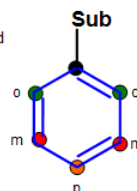


Figure 12. Example of o-, m-, p- nomenclature. Listed in order:
1) o-nitrochlorobenzene
2) m-nitrochlorobenzene
3) p-nitrochlorobenzene
Note that the two substituents do not have to be the same.

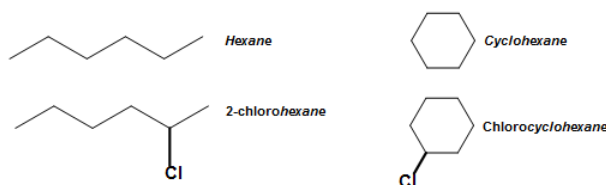
In conclusion, these can be pieced together into a summary diagram, as shown below:

Figure 13. A benzene ring with a primary substituent and the possible locations for the secondary substituent. As shown:
1,2- (green) = ortho, o-
1,3- (red) = meta, m-
1,4- (orange) = para, p-
For clarity, the benzene ring has been rotated 30° relative to the other benzenes in this article.



Base Name Nomenclature

In addition to simple benzene naming and OMP nomenclature, benzene derived compounds are also sometimes used as **bases**. The concept of a base is similar to the nomenclature of aliphatic and cyclic compounds, where the parent for the organic compound is used as a base (a name for its chemical name). For example, the following compounds have the base names **hexane** and **cyclohexane**, respectively. See Nomenclature of Organic Compounds for a review on naming organic compounds.



Benzene, similar to these compounds shown above, also has base names from its derived compounds. **Phenol** ($\text{C}_6\text{H}_5\text{OH}$), as introduced previously in this article, for example, serves as a base when other substituents are attached to it. This is best illustrated in the diagram below.

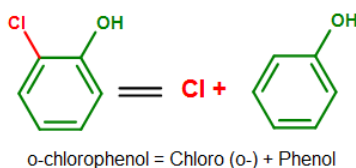


Figure 14. An example showing phenol as a base in its chemical name. Note how benzene no longer serves as a base when an OH group is added to the benzene ring.

Alternatively, we can use the numbering system to indicate this compound. When the numbering system is used, the carbon where the substituent is attached on the base will be given the first priority and named as carbon #1 (C_1). The normal priority rules then apply in the nomenclature process (give the rest of the substituents the lowest numbering as you could).

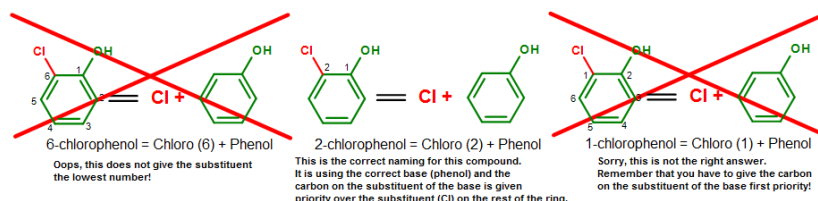


Figure 15. The naming process for 2-chlorophenol (o-chlorophenol). Note that 2-chlorophenol = o-chlorophenol.

Below is a list of commonly seen benzene-derived compounds. Some of these mono-substituted compounds (labeled in red and green), such as phenol or toluene, can be used in place of benzene for the chemical's base name.

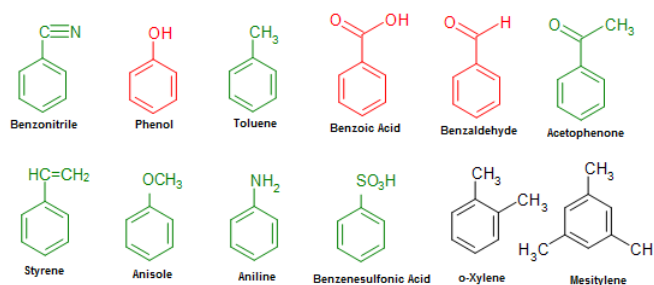


Figure 16. Common benzene derived compounds with various substituents.



Figure 17. 2,4,6-Trinitrotoluene, or **TNT**, a common explosive used for both industrial and military purposes, is consisted of a **toluene** base (labeled in blue), along with three **nitro** groups attached as substituents (labeled in red). The explosive is characteristic for its resistance to external shock and friction, making it useful in many applications where other highly sensitive explosives would simultaneously detonate.

Common vs. Systematic (IUPAC) Nomenclature

According to the indexing preferences of the *Chemical Abstracts*, **phenol**, **benzaldehyde**, and **benzoic acid** (labeled in red in **Figure 16**) are some of the common names that are retained in the IUPAC (systematic) nomenclature. Other names such as toluene, styrene, naphthalene, or phenanthrene can also be seen in the IUPAC system in the same way. While the use of other common names are usually acceptable in IUPAC, their use are discouraged in the nomenclature of compounds.

Nomenclature for compounds which has such discouraged names will be named by the simple benzene naming system. An example of this would include **toluene derivatives like TNT**. (Note that toluene by itself is retained by the IUPAC nomenclature, but its derivatives, which contains additional substituents on the benzene ring, might be excluded from the convention). For this reason, the **common chemical name** 2,4,6-trinitrotoluene, or TNT, as shown in figure 17, would not be advisable under the IUPAC (**systematic**) nomenclature.

To correctly name TNT under the IUPAC system, the simple benzene naming system should be used:

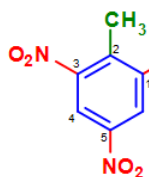


Figure 18. TNT, as named under the IUPAC nomenclature. Note that since the IUPAC nomenclature does not recognize toluene as the primary base of this compound, substituent priorities are reverted to normal defaults. As a result, TNT in IUPAC is named (systematic name): **2-methyl-1,3,5-trinitrobenzene**

Figure 18. Systematic (IUPAC) name of **2,4,6-trinitrotoluene** (common name), or TNT.

Note that the methyl group is individually named due to the exclusion of toluene from the IUPAC nomenclature.

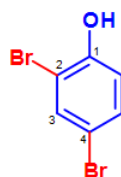


Figure 19. 2,4-dibromophenol, as shown in this diagram, is valid in both the common nomenclature as well as the IUPAC nomenclature. As mentioned previously, **phenol, benzoic acid, and benzaldehyde** substituents are allowed to be used in the IUPAC naming conventions and the base naming priority rules are applied in the nomenclature process.

Figure 19. The common name **2,4-dibromophenol**, is shared by the IUPAC systematic nomenclature. Only substituents **phenol, benzoic acid, and benzaldehyde** share this commonality.

Since the IUPAC nomenclature primarily rely on the simple benzene naming system for the nomenclature of different benzene derived compounds, the OMP (ortho-, meta-, para-) system is not accepted in the IUPAC nomenclature. For this reason, the OMP system will yield common names that can be converted to systematic names by using the same method as above. For example, o-Xylene from the OMP system can be named 1,2-dimethylbenzene by using simple benzene naming (IUPAC standard).

The Phenyl and Benzyl Groups

The Phenyl Group

As mentioned previously, the phenyl group (Ph-R, C_6H_5 -R) can be formed by removing a hydrogen from benzene and attaching a substituent to where the hydrogen was removed. To this phenomenon, we can name compounds formed this way by applying this rule: **(phenyl + substituent)**. For example, a chlorine attached in this manner would be named **phenyl chloride**, and a bromine attached in this manner would be named **phenyl bromide**. (See below diagram)

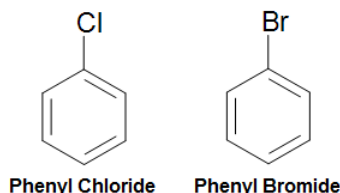


Figure 20. Naming of Phenyl Chloride and Phenyl Bromide

While compounds like these are usually named by simple benzene type naming (chlorobenzene and bromobenzene), the phenyl group naming is usually applied to benzene rings where a substituent with six or more carbons is attached, such as in the diagram below.

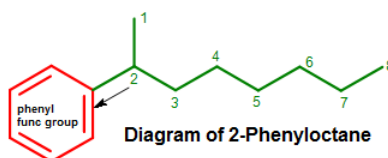


Figure 21. Diagram of **2-phenyloctane**.

Although the diagram above might be a little daunting to understand at first, it is not as difficult as it seems after careful analysis of the structure is made. By looking for the longest chain in the compound, it should be clear that the longest chain is eight (8) carbons long (octane, as shown in green) and that a benzene ring is attached to the second position of this longest chain (labeled in red). As this rule suggests that the benzene ring will act as a function group (a substituent) whenever a substituent of more than six (6) carbons is attached to it, the name "benzene" is changed to **phenyl** and is used the same way as any other substituents, such as **methyl, ethyl, or bromo**. Putting it all together, the name can be derived as: **2-phenyloctane** (phenyl is attached at the second position of the longest carbon chain, octane).

The Benzyl Group

The benzyl group (abbrev. Bn), similar to the phenyl group, is formed by manipulating the benzene ring. In the case of the benzyl group, it is formed by taking the phenyl group and adding a CH_2 group to where the hydrogen was removed. Its molecular fragment can be written as $C_6H_5CH_2$ -R, $PhCH_2$ -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.

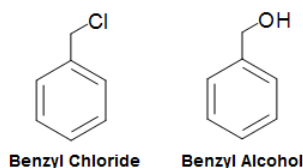


Figure 22. Benzyl Group Nomenclature

Additionally, other substituents can attach on the benzene ring in the presence of the benzyl group. An example of this can be seen in the figure below:

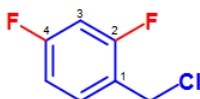
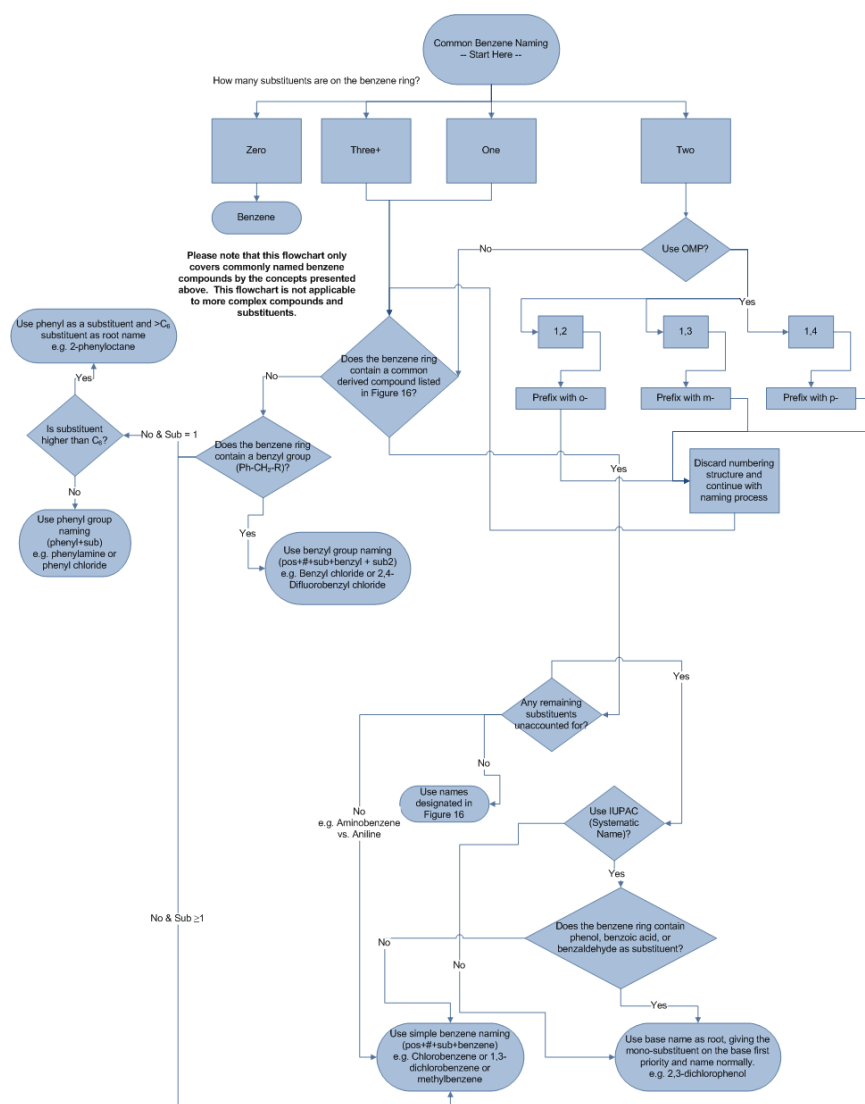


Figure 23. Nomenclature of 2,4-difluorobenzyl chloride. Similar to the base name nomenclatures system, the carbon in which the base substituent is attached on the benzene ring is given the first priority and the rest of the substituents are given the lowest number order possible.

Similar to the base name nomenclature system, the carbon in which the base substituent is attached on the benzene ring is given the first priority and the rest of the substituents are given the lowest number order possible. Under this consideration, the above compound can be named: **2,4-difluorobenzyl chloride**.

[Commonly Named Benzene Compounds Nomenclature Summary Flowchart](#)

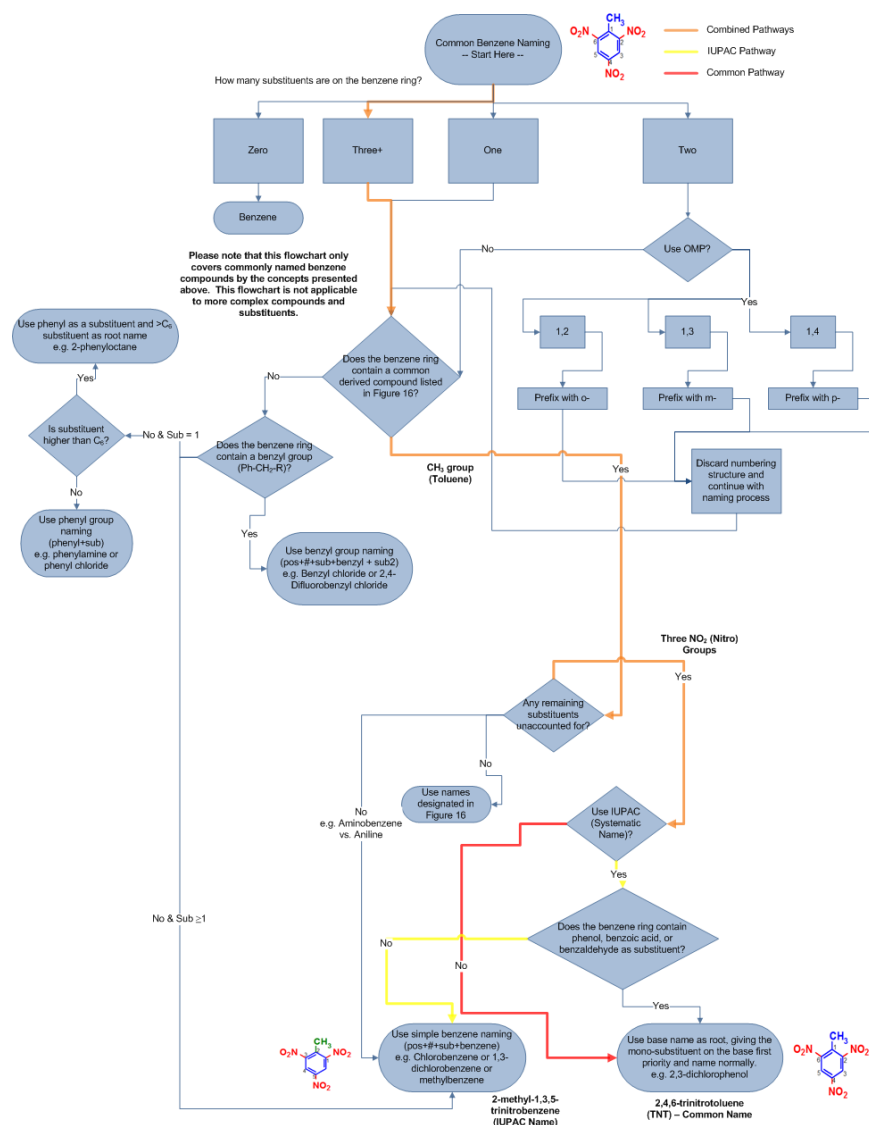


Summary Flowchart (Figure 24). Summary of nomenclature rules used in commonly benzene derived compounds.

As benzene derived compounds can be extremely complex, only compounds covered in this article and other commonly named compounds can be named using this flowchart.

Determination of Common and Systematic Names using Flowchart

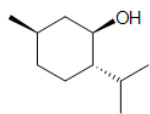
To demonstrate how this flowchart can be used to name TNT in its common and systematic (IUPAC) name, a replica of the flowchart with the appropriate flow paths are shown below:



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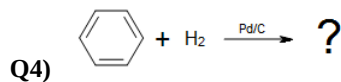
Practice Problems



Q1) (True/False) The compound above contains a benzene ring and thus is aromatic.

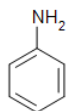
Q2) Benzene unusual stability is caused by how many conjugated pi bonds in its cyclic ring? ____

Q3) 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?



Q5) At normal conditions, benzene has ____ resonance structures.

Q6) Which of the following name(s) is/are correct for the following compound?

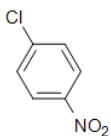


- a) nitrohydride benzene
- b) phenylamine
- c) phenylamide
- d) aniline
- e) nitrogenhydrogen benzene
- f) All of the above is correct

Q7) Convert 1,4-dimethylbenzene into its common name.

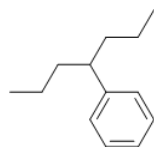
Q8) TNT's common name is: _____

Q9) Name the following compound using OMP nomenclature:

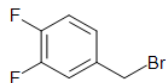


Q10) Draw the structure of 2,4-dinitrotoluene.

Q11) Name the following compound:



Q12) 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

Q13) (True/False) Benzyl chloride can be abbreviated Bz-Cl.

Q14) Benzoic Acid has what R group attached to its phenyl functional group?

Q15) (True/False) A single aromatic compound can have multiple names indicating its structure.

Q16) List the corresponding positions for the OMP system (o-, m-, p-).

Q17) 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?

- a) Cyclohexanol
- b) Cycloheptanol
- c) Phenol
- d) Methanol
- e) Bleach
- f) Cannot determine from the above information

Q18) Which of the following statements is **false** for the compound, phenol?

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

Answer Key to Practice Questions

Q1) False, this compound does not contain a benzene ring in its structure.

Q2) 3

Q3) No, a substance that is fragrant does not imply a benzene ring is in its structure. See camphor example (figure 1)

Q4) No reaction, benzene requires a special catalyst to be hydrogenated due to its unusual stability given by its three conjugated pi bonds.

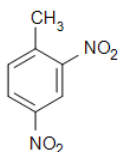
Q5) 2

Q6) b, d

Q7) p-Xylene

Q8) 2,4,6-trinitrotoluene

Q9) p-chloronitrobenzene



Q10)

Q11) 4-phenylheptane

Q12) a

Q13) False, the correct abbreviation for the benzyl group is Bn, not Bz. The correct abbreviation for Benzyl chloride is Bn-Cl.

Q14) COOH

Q15) True. TNT, for example, has the common name 2,4,6-trinitrotoluene and its systematic name is 2-methyl-1,3,5-trinitrobenzene.

Q16) Ortho - 1,2 ; Meta - 1,3 ; Para - 1,4

Q17) 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.

Q18) d

Contributors

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