

QFL-0341 Estrutura e reatividade de compostos orgânicos

2019

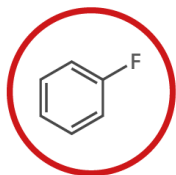
Nomenclatura de compostos aromáticos



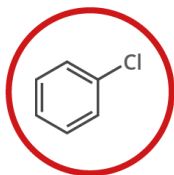
BENZENE DERIVATIVES IN ORGANIC CHEMISTRY

A WIDE VARIETY OF IMPORTANT ORGANIC COMPOUNDS ARE DERIVED FROM BENZENE, BY REPLACING ONE OF THE HYDROGENS WITH A DIFFERENT FUNCTIONAL GROUP. THEY CAN HAVE BOTH COMMON & SYSTEMATIC NAMES, WHICH CAN BE CONFUSING; HERE, COMMON NAMES ARE SHOWN PRIMARILY, WITH SYSTEMATIC NAMES SHOWN IN ITALICS.

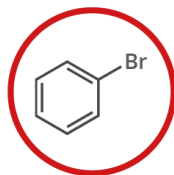
● HALOGEN-CONTAINING ● HYDROCARBON DERIVATIVES ● OXYGEN-CONTAINING ● NITROGEN-CONTAINING ● SULFUR-CONTAINING ● POLYAROMATICS



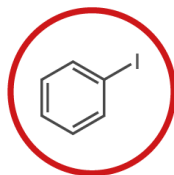
FLUOROBENZENE
Fluorobenzene
 C_6H_5F



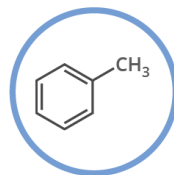
CHLOROBENZENE
Chlorobenzene
 C_6H_5Cl



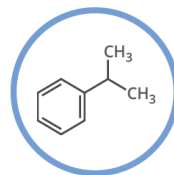
BROMOBENZENE
Bromobenzene
 C_6H_5Br



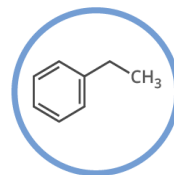
IODOBENZENE
Iodobenzene
 C_6H_5I



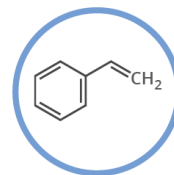
TOLUENE
Methylbenzene
 C_7H_8



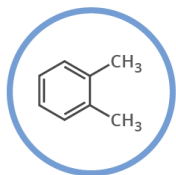
CUMENE
Isopropylbenzene
 C_9H_{12}



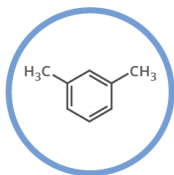
ETHYLBENZENE
Ethylbenzene
 C_8H_{10}



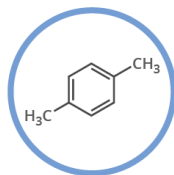
STYRENE
Vinylbenzene
 C_8H_8



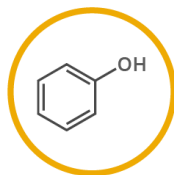
ORTHO-XYLENE
1,2-dimethylbenzene
 C_8H_{10}



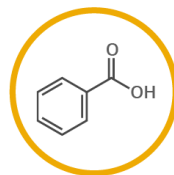
META-XYLENE
1,3-dimethylbenzene
 C_8H_{10}



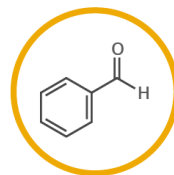
PARA-XYLENE
1,4-dimethylbenzene
 C_8H_{10}



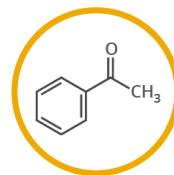
PHENOL
Hydroxybenzene
 C_6H_5OH



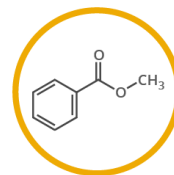
BENZOIC ACID
Benzenecarboxylic Acid
 C_6H_5COOH



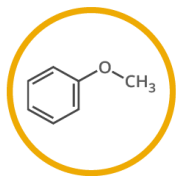
BENZALDEHYDE
Benzenecarbaldehyde
 C_6H_5CHO



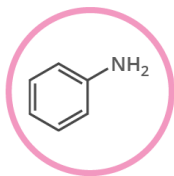
ACETOPHENONE
1-phenylethanone
 $C_6H_5COCH_3$



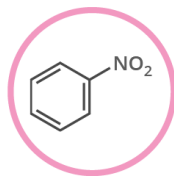
METHYL BENZOATE
Methyl Benzoate
 $C_8H_8O_2$



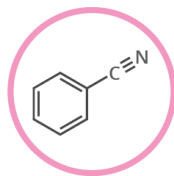
ANISOLE
Methoxybenzene
 $C_6H_5OCH_3$



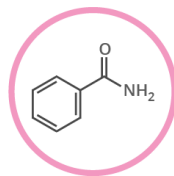
ANILINE
Aminobenzene
 $C_6H_5NH_2$



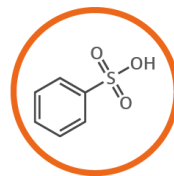
NITROBENZENE
Nitrobenzene
 $C_6H_5NO_2$



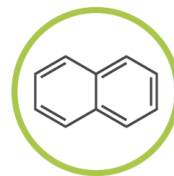
BENZONITRILE
Benzonitrile
 C_6H_5CN



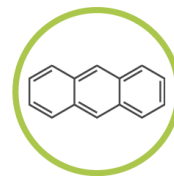
BENZAMIDE
Benzamide
 $C_6H_5CONH_2$



BENZENESULFONIC ACID
Benzenesulfonic Acid
 $C_6H_5SO_3H$



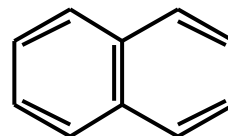
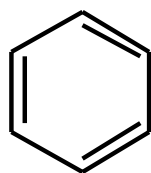
NAPHTHALENE
Naphthalene
 $C_{10}H_8$



ANTHRACENE
Anthracene
 $C_{14}H_{10}$

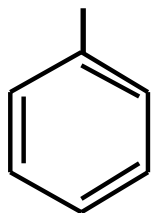
Aromatic Compounds

Arene: A compound containing one or more benzene rings.



Naphthalene

Aryl group: When we remove a H atom from an arene (Ar-).

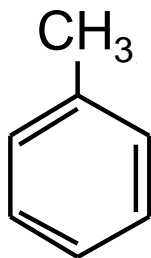


Phenyl $C_6H_5^-$

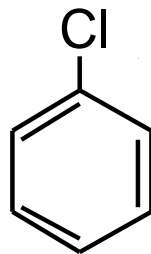
Naming of Aromatic Compounds

Aromatic compounds are named:

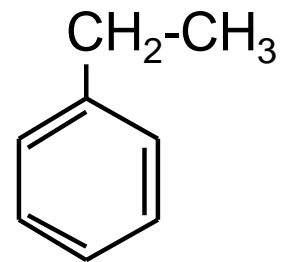
- With benzene as the parent chain.
- Name of substituent comes in front of the “benzene”.



methylbenzene



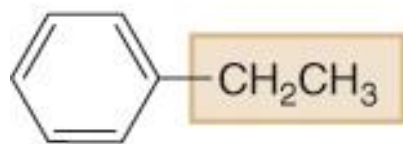
chlorobenzene



ethylbenzene

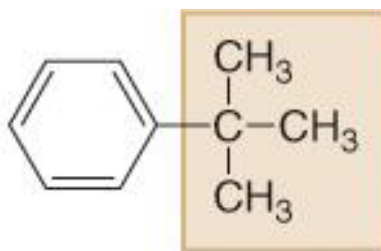
Nomenclature of Benzene Derivatives

- To name a benzene ring with one substituent, name the substituent and add the word benzene.



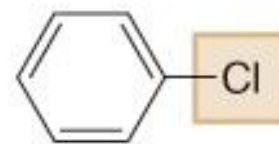
ethyl group

ethylbenzene



tert-butyl group

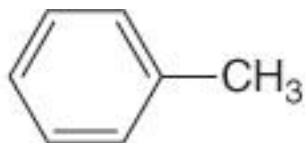
tert-butylbenzene



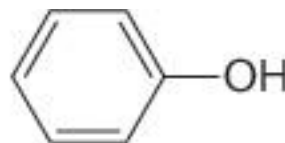
chloro group

chlorobenzene

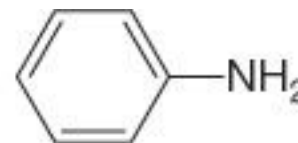
- Many monosubstituted benzenes have common names which you must also learn.



toluene
(methylbenzene)



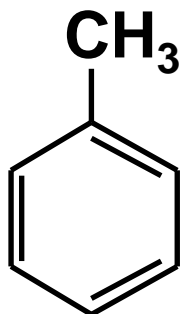
phenol
(hydroxybenzene)



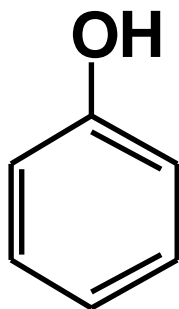
aniline
(aminobenzene)

Naming of Aromatic Compounds

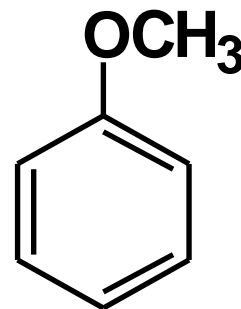
Some substituted benzenes have common names.



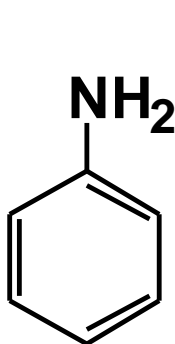
Toluene



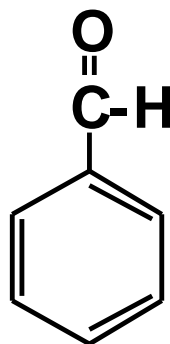
Phenol



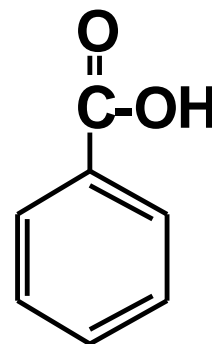
Anisole



Aniline



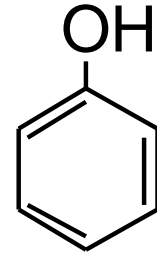
Benzaldehyde



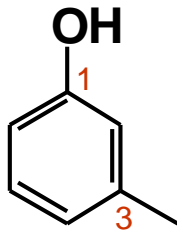
Benzoic acid

Phenol

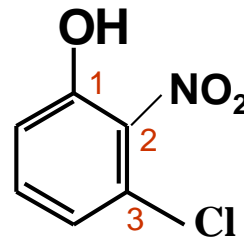
- **Phenol** is the IUPAC name for benzene with a hydroxyl group.



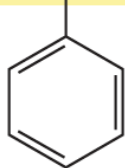
Phenol



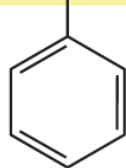
3-Methylphenol
(m-Cresol)



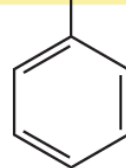
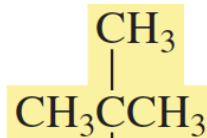
3-Chloro-2-nitrophenol



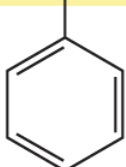
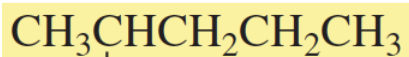
isopropilbenzeno



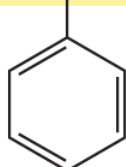
sec-butilbenzeno



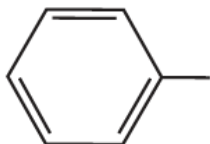
tec-butilbenzeno



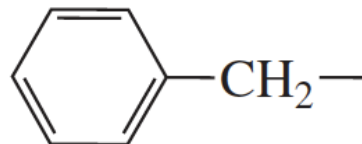
2-fenilpentano



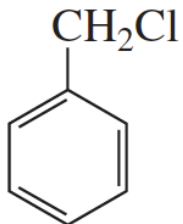
3-fenilpentano



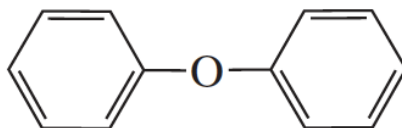
Grupo fenila



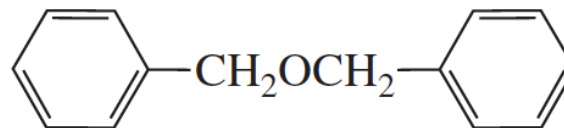
Grupo benzila



cloro-metilbenzeno



Éter difenílico

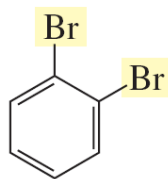


Éter dibenzílico

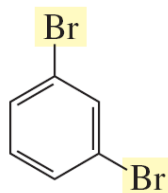
Nomenclatura de benzenos dissustituídos e polissustituídos

Benzenos dissustituídos

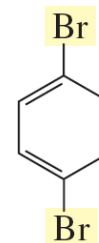
- **substituintes iguais:** posição indicada por número ou prefixos (*o*, *m*, *p*)



1,2-dibromobenzeno
o-dibromobenzeno

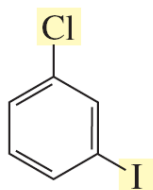


1,3-dibromobenzeno
m-dibromobenzeno

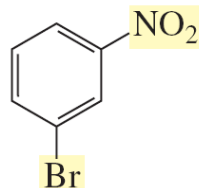


1,4-dibromobenzeno
p-dibromobenzeno

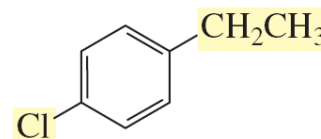
- **substituintes diferentes:** indicação por ordem alfabética



1-cloro-3-iodobenzeno
m-cloro-iodobenzeno



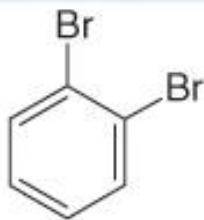
1-bromo-3-nitrobenzeno
m-bromo-nitrobenzeno



1-cloro-4-etilbenzeno
p-cloro-etilbenzeno

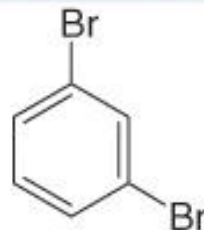
- There are three different ways that two groups can be attached to a benzene ring, so a prefix—**ortho**, **meta**, or **para**—can be used to designate the relative position of the two substituents.

1,2-disubstituted benzene
ortho isomer



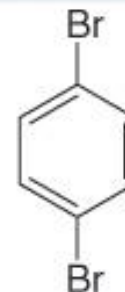
ortho-dibromobenzene
or
o-dibromobenzene
or 1,2-dibromobenzene

1,3-disubstituted benzene
meta isomer



meta-dibromobenzene
or
m-dibromobenzene
or 1,3-dibromobenzene

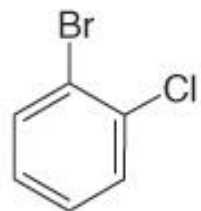
1,4-disubstituted benzene
para isomer



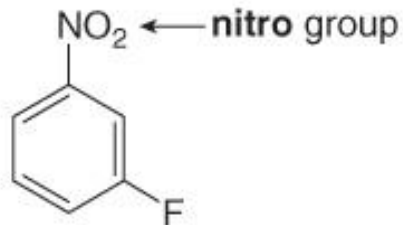
para-dibromobenzene
or
p-dibromobenzene
or 1,4-dibromobenzene

- If the two groups on the benzene ring are different, alphabetize the names of the substituents preceding the word benzene.
- If one substituent is part of a common root, name the molecule as a derivative of that monosubstituted benzene.

Alphabetize two different substituent names:

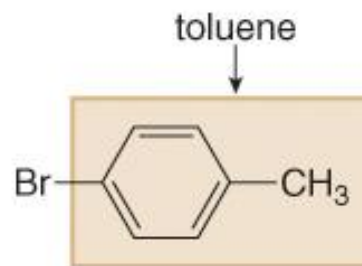


***o*-bromochloro-
benzene**

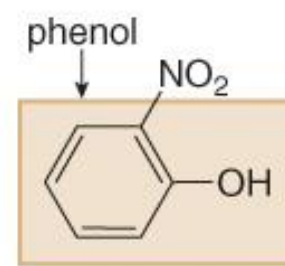


***m*-fluoronitro-
benzene**

Use a common root name:



***p*-bromotoluene**

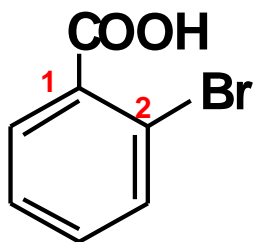


***o*-nitrophenol**

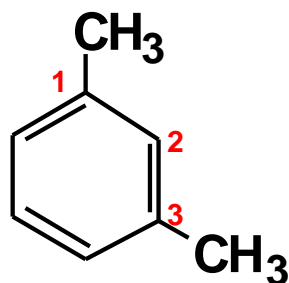
Naming of Aromatic Compounds

When **two groups** are attached to benzene, the ring is numbered to give the lower numbers to the substituents.

- Start numbering from a special name (if we have).
- If we do not have, number them to get the smallest set of numbers.
- List them by alphabetical order.

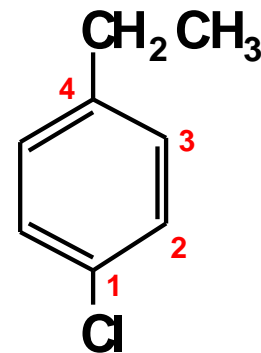


2-Bromobenzoic acid



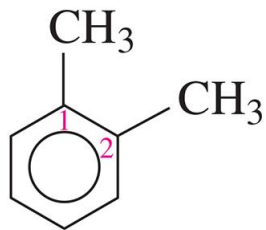
3-methyltoluene

1,3-Dimethylbenzene

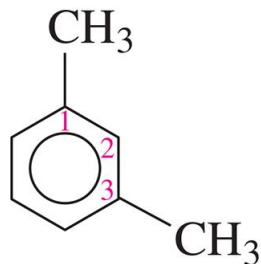


1-Chloro-4-ethylbenzene

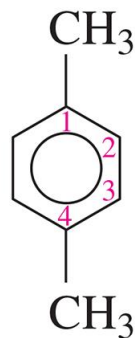
- The common name **xylene** is used for the isomers of dimethylbenzene.



1,2-Dimethylbenzene
(*o*-xylene)



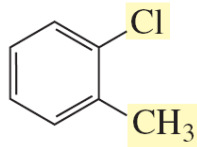
1,3-Dimethylbenzene
(*m*-xylene)



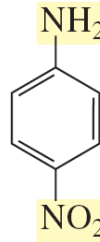
1,4-Dimethylbenzene
(*p*-xylene)

- If three or more substituents are attached to the benzene ring, they are numbered in the direction to give the lowest set of numbers and then named alphabetically.

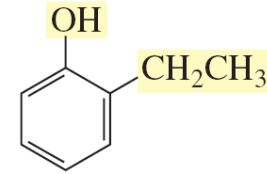
Um dos substituintes incorporado ao nome (posição 1)



2-clorotolueno
o-clorotolueno

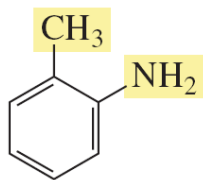


4-nitroanilina
p-nitroanilina

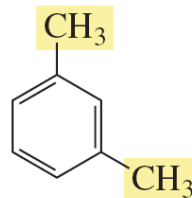


2-etilfenol
o-etilfenol

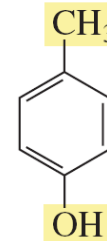
Ambos os substituintes incorporados ao nome



o-toluidina



m-xileno



p-cresol

**usado como conservante
até ser proibido por
razões ambientais**

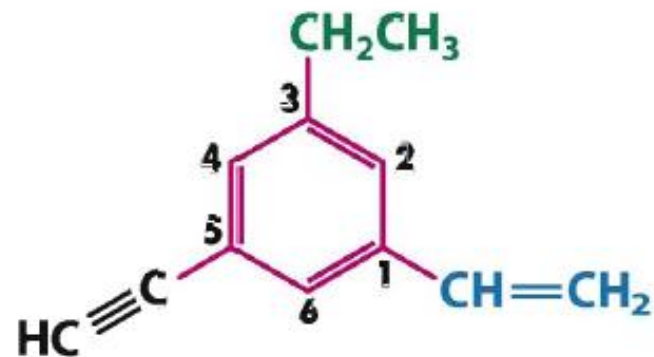
Benzeno trissubstituido



**1-Bromo-
2,3-dimethylbenzene**



1,2,4-Trinitrobenzene

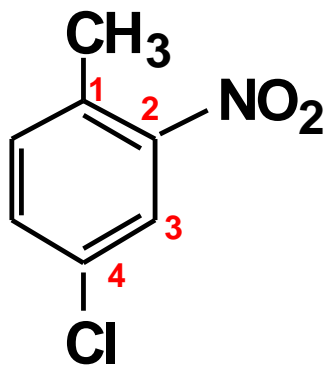


**1-Ethenyl-3-ethyl-
5-ethynylbenzene**

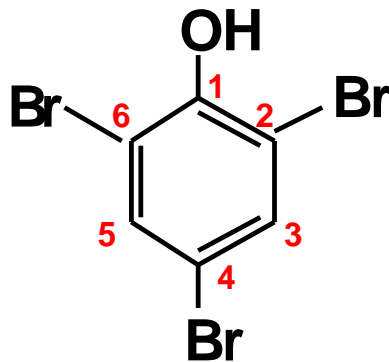
Naming of Aromatic Compounds

If we have **three or more substituents**:

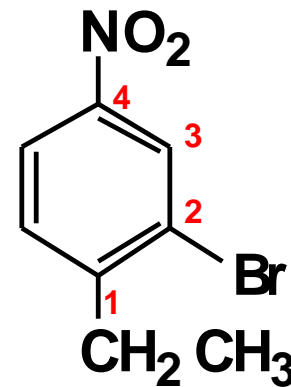
- Start numbering from a special name (if we have).
- If we do not have, number them to get the smallest set of numbers.
- List them by alphabetical order.



4-Chloro-2-nitrotoluene



2,4,6-Tribromophenol

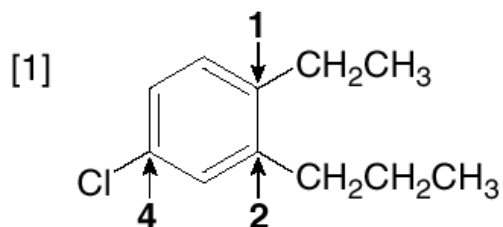


2-Bromo-1-ethyl-4-nitrobenzene

For three or more substituents on a benzene ring:

1. Number to give the lowest possible numbers around the ring.
2. Alphabetize the substituent names.
3. When substituents are part of common roots, name the molecule as a derivative of that monosubstituted benzene. The substituent that comprises the common root is located at C1.

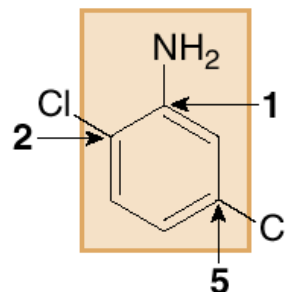
Examples of naming polysubstituted benzenes



- Assign the lowest set of numbers.
- Alphabetize the names of all the substituents.

4-chloro-1-ethyl-2-propylbenzene

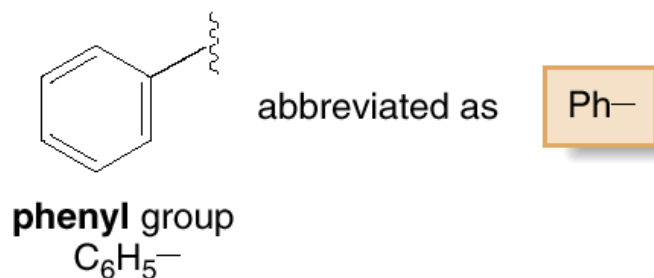
[2]



- Name the molecule as a derivative of the common root **aniline**.
- Designate the position of the NH₂ group as "1," and then assign the lowest possible set of numbers to the other substituents.

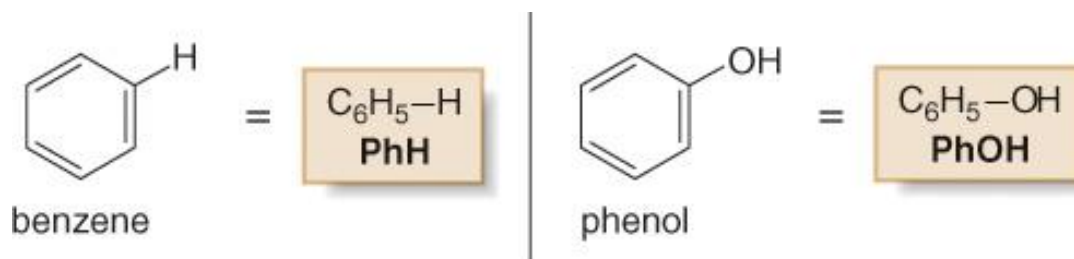
2,5-dichloroaniline

- A benzene substituent is called a **phenyl group**, and it can be abbreviated in a structure as “**Ph-**”.

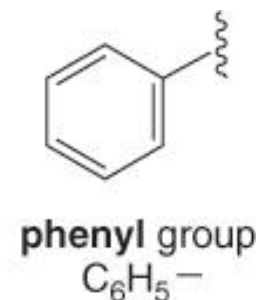
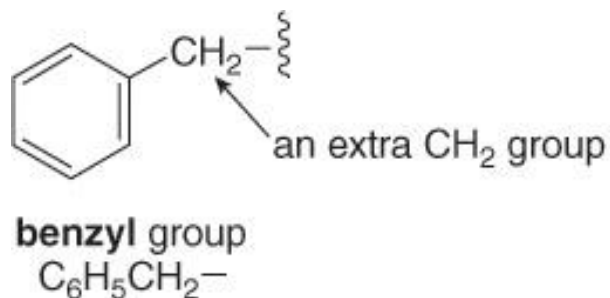


- A phenyl group (C_6H_5-) is formed by removing one hydrogen from benzene (C_6H_6).

- Therefore, benzene can be represented as **PhH**, and **phenol** would be **PhOH**.

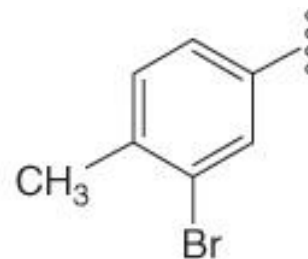
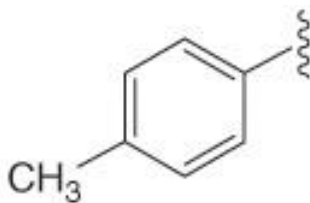


- The **benzyl group**, another common substituent that contains a benzene ring, differs from a phenyl group.



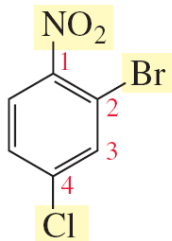
- Substituents derived from other substituted aromatic rings are collectively known as **aryl groups**.

Examples of
aryl groups

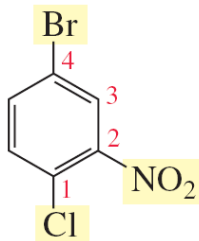


Benzenos polissubstituídos

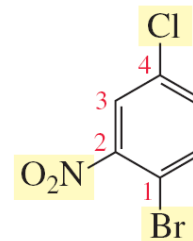
números mais baixos possíveis e em ordem alfabética



2-bromo-4-cloro-1-nitrobenzeno

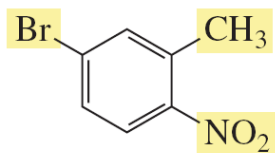


4-bromo-1-cloro-2-nitrobenzeno

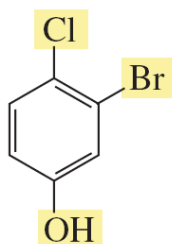


1-bromo-4-cloro-2-nitrobenzeno

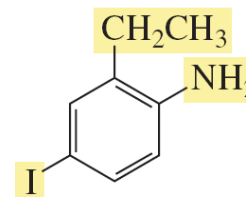
um dos substituintes incorporado ao nome (posição 1)



5-bromo-2-nitrotolueno

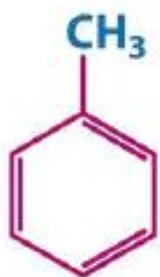


5-bromo-4-clorofenol

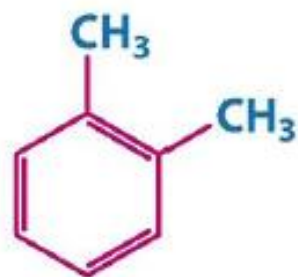


2-etil-4-iodoanilina

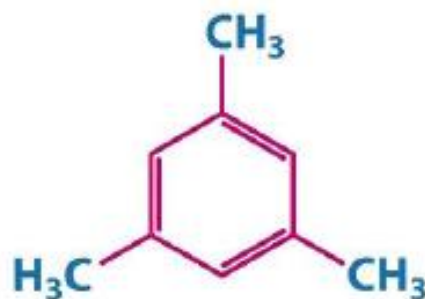
Conhecidos por nomes vulgares



Methylbenzene
(Toluene)

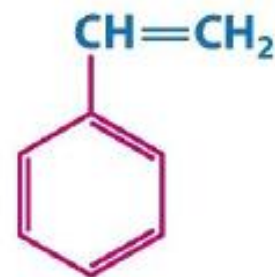


1,2-Dimethylbenzene
(*o*-Xylene)



1,3,5-Trimethylbenzene
(Mesitylene)

(Common industrial and laboratory solvents)



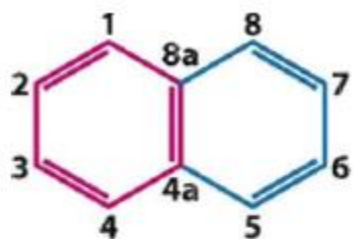
Ethenylbenzene
(Styrene)

(Used in polymer
manufacture)



Methoxybenzene
(Anisole)

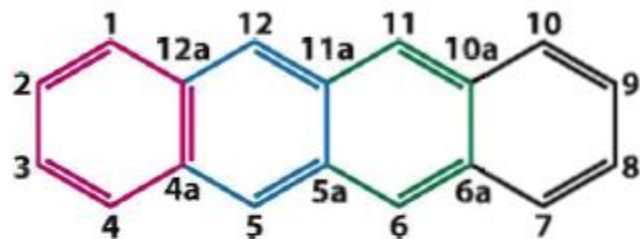
(Used in perfume)



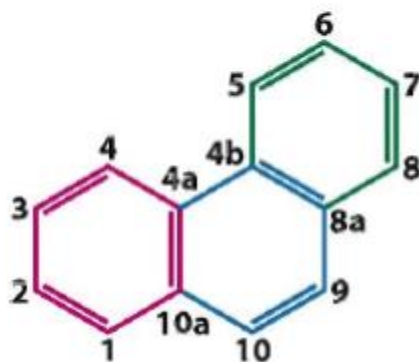
Naphthalene



Anthracene

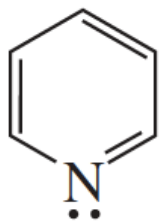


**Tetracene
(Naphthacene)**

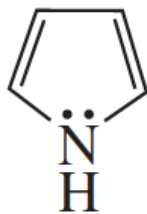


Phenanthrene

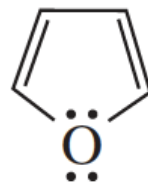
Substâncias heterocíclicas aromáticas



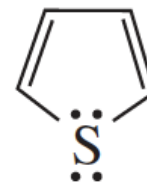
pyridine



pyrrole



furan



thiophene

Substância heterocíclica: composto cíclico onde pelo menos um dos átomos do anel é um átomo diferente do carbono.

Piridina é aromático

