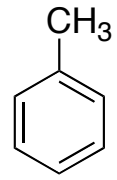
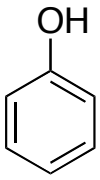
Nomenclature of substituted benzene rings

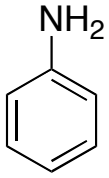
You should know the names of the following structures and be able to draw them from name:



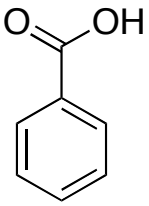
Toluene



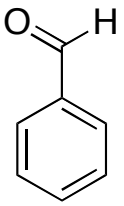
Phenol



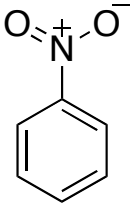
Aniline



Benzoic acid



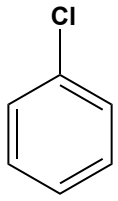
Benzaldehyde



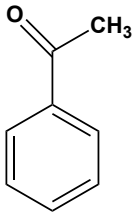
Nitrobenzene

Toluene = Methylbenzene
Phenol = Hydroxybenzene
Aniline = Aminobenzene

Other examples

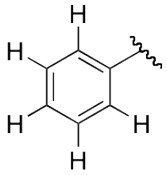


Chlorobenzene



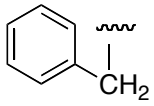
Acetophenone

Phenyl group = ϕ = Ph = C_6H_5

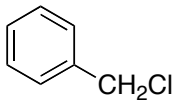


Aryl = Ar = aromatic group. It is a broad term, and includes any aromatic rings.

Benzyl = Bn =

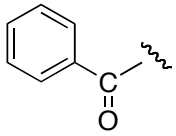


It has a -CH_2- (methylene) group attached to the benzene ring.
This group can be used to name particular compounds, such as the one shown below.

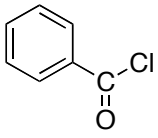


This compound has chlorine attached to a benzyl group, and is called benzyl chloride.

Benzoyl = Bz =

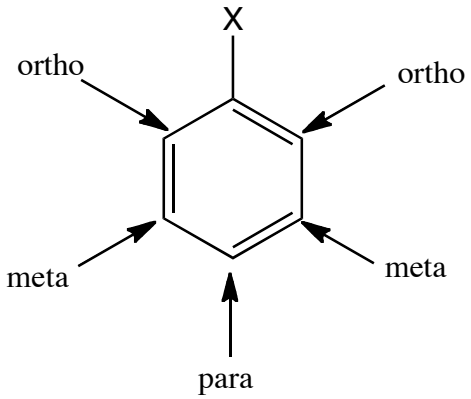


This is different from the benzyl group. It has a carbonyl attached to the benzene ring instead of a methylene group.

 is named benzoyl chloride.

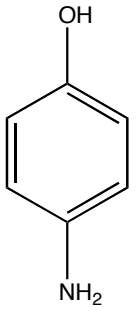
It is sometimes useful to name a compound with the aromatic part as a substituent rather than it forming a part of the parent name.

POLYSUBSTITUTED DERIVATIVES OF BENZENE
When you have two substituents on a benzene ring, *ortho*, *meta*, and *para* are used to tell where the second substitution is relative to the first one.



Ortho refers to 1,2-substitution and is abbreviated o-
Meta refers to 1,3-substitution and is abbreviated m-
Para refers to 1,4-substitution and is abbreviated p-

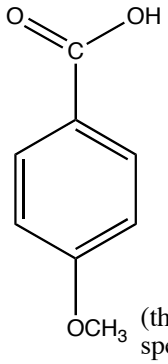
Examples:



p-aminophenol
(more correct, OH has priority)

or

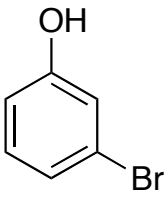
p-hydroxyaniline



p-methoxybenzoic acid

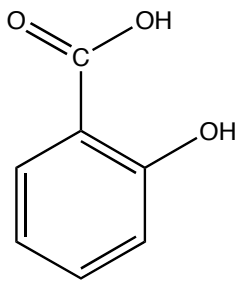
(this is an ether group, specifically methoxy)

Nomenclature: p-aminophenol or 4-aminophenol:
The amine and hydroxyl group are in the 1 and 4 positions, so they are *para* to each other. The parent structure in this molecule can be either aniline or phenol. For this course, it doesn't matter which parent structure you pick in the nomenclature with these substituents. Usually when naming the substituents, the atomic number takes priority, but there are many exceptions for historical reasons.

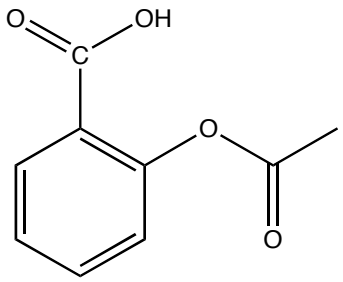


Nomenclature: *m*-bromophenol or 3-bromophenol
In this compound, the –OH (hydroxy) and –Br are in the 1 and 3 positions, so they are *meta* (or abbreviated *m*) to each other. The parent structure is phenol (phenol is a benzene

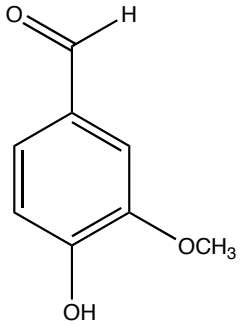
with a hydroxyl group directly attached, not to be confused with phenyl which means just a benzene ring as a substituent), so we call this meta-bromophenol.



2-hydroxybenzoic acid
aka salicylic acid

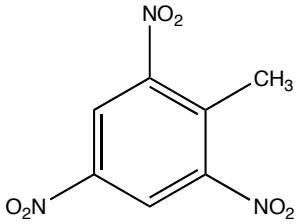


aspirin
acetylsalicylic acid

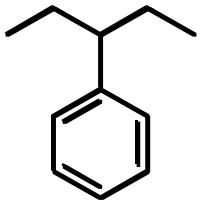


Nomenclature: 4-hydroxy-3-methoxybenzaldehyde (or vanillin from vanilla extract). The carbon substituent (an aldehyde group) gets priority.

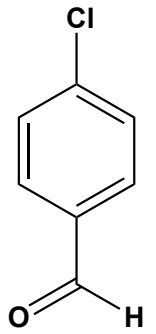
Note: we number the ring in a way such that the substituents have the lowest numbers (so it's not 4-hydroxy-5-methoxy-, but 4-hydroxy-3-methoxy-). The substituents are listed in alphabetical order before the parent compound, but this course will not be incredibly picky with the order.



Nomenclature: 2,4,6-trinitrotoluene (TNT)
An explosive

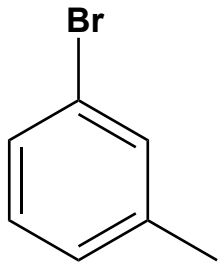


Nomenclature: 3-phenylpentane (pentan-3-ylbenzene is also an acceptable name, but it is more complicated and isn't the best name). (Note that this molecule is achiral: it has a plane of symmetry)



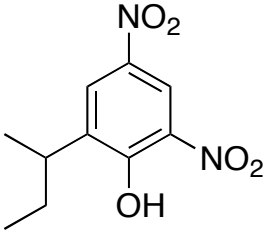
***para*-Chlorobenzaldehyde**

4-Chlorobenzaldehde



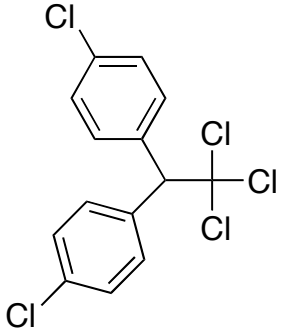
***meta*-Bromotoluene**

3-Bromotoluene



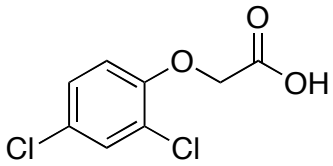
This is Amaize. It is used to enhance the yield of corn production.

The systematic name for this compound is 2-*sec*-butyl-4,6-dinitrophenol. It can also be called 6-(1-methylpropyl)-2,4-dinitrophenol.

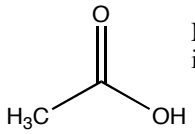


1,1,1-trichloro-2,2-bis-(4-chlorophenyl)ethane
Note: Although the two 4-chlorophenyl can also be named using di-, bis is used instead. bis is commonly used for large groups. The 4-chlorophenyl could also be called p-chlorophenyl

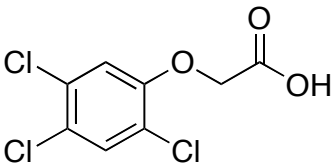
This compound is commonly known as DDT. DDT is an insecticide and helped to wipe out malaria in many parts of the world. The person who discovered its properties (Paul Müller) won the Nobel Prize in Medicine in 1948.



2,4-dichlorophenoxyacetic acid (2,4-D)

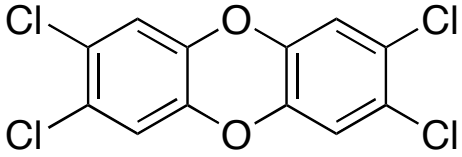


Note: Acetic acid is the parent structure

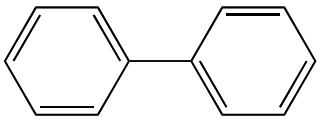


2,4,5-trichlorophenoxyacetic acid (2,4,5-T)

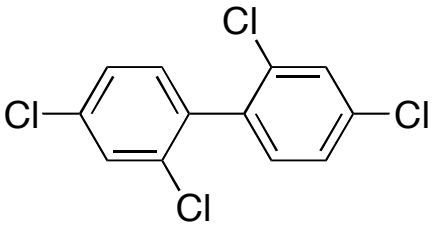
Agent Orange (2,4-D + 2,4,5-T), a broad leaf herbicide, was used in the Vietnam War to defoliate large areas. It was used in Edmonton on lawns as "Weed and Feed".



Dioxin is a potent toxin and carcinogen that can contaminate Agent Orange and can occur in pulp mill waste. While this is only an example of one dioxin, typically the term dioxin refers to this particular molecule.



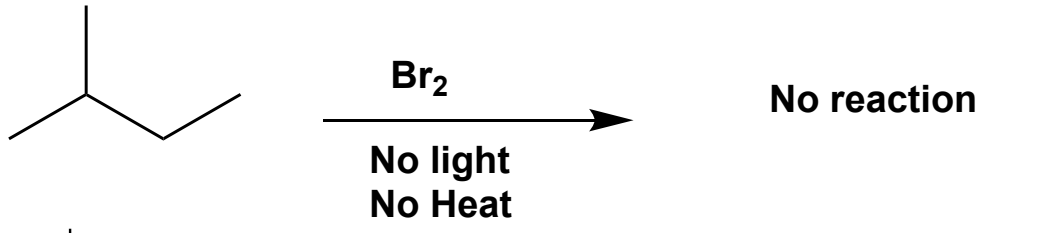
biphenyl

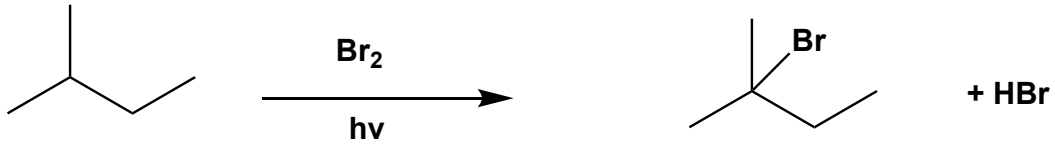


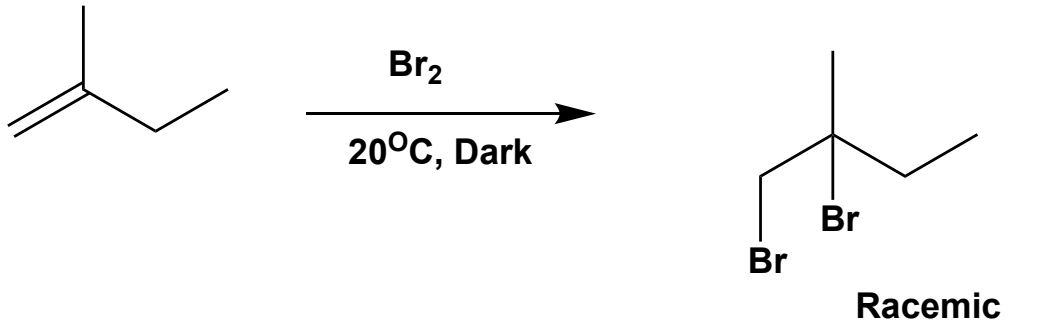
A polychlorinated biphenyl (PCB). PCBs were used in electrical transformers and are persistant organic pollutants.

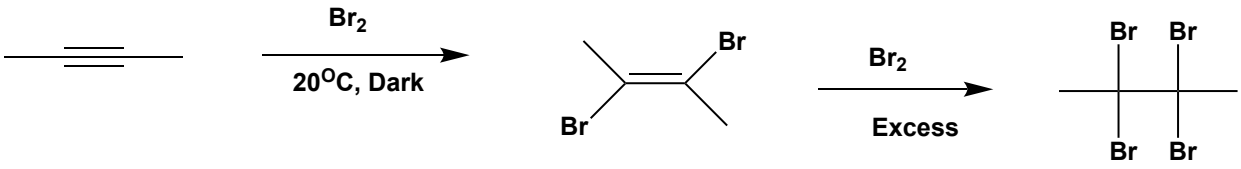
If the Cl's were Br's this would be a polybrominated biphenyl (PBB).

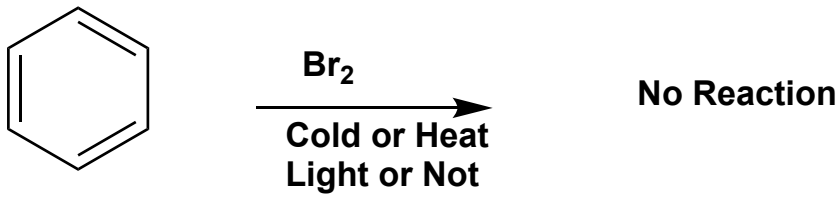
REVIEW


Br2
No light
No Heat
No reaction


Br2
hv
Br
+ HBr


Br2
20OC, Dark
Br
Br
Racemic


Br2
20OC, Dark
Br
Br
Br2
Excess
Br
Br
Br
Br


Br2
Cold or Heat
Light or Not
No Reaction

AROMATIC SUBSTITUTION REACTION

This reaction requires a catalyst, A Lewis Acid: Accepts a pair of electrons

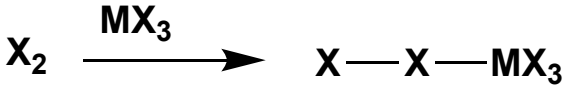
Examples of Catalyst

$H^{\oplus}$

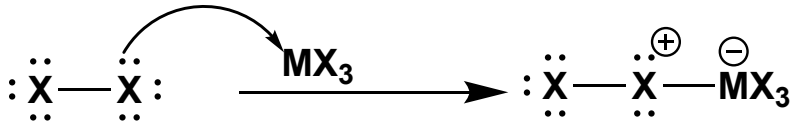
BX_3 X= Halogen

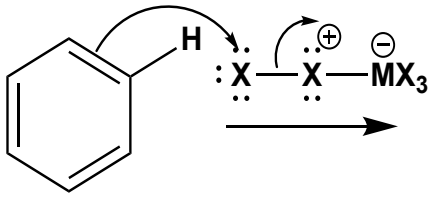
MX_3 M= Metal, Al, Fe

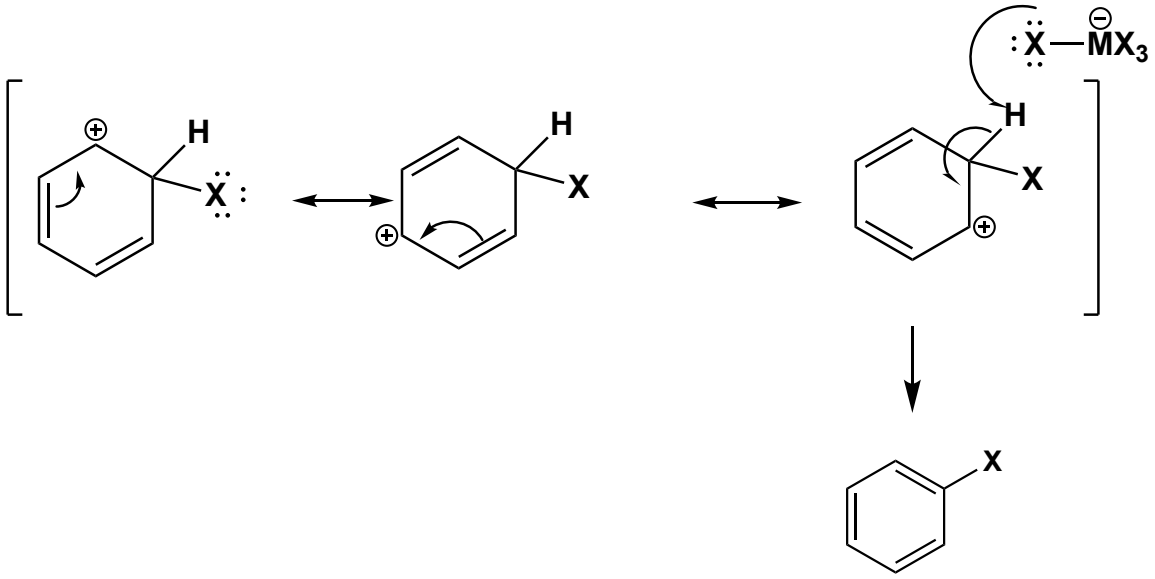
GENERAL REACTION MECHANISM



Where X= Halogen
M = metal, Al, Fe






H
X
H
X
H
X
X
MX3