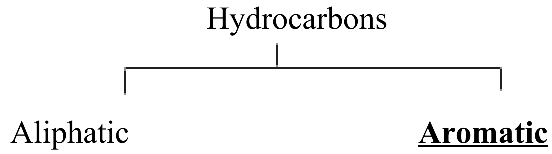
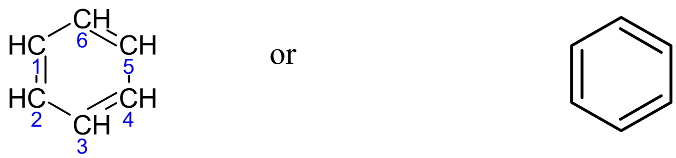
SCH4U1 Name:
OC03 Date:

AROMATIC HYDROCARBONS

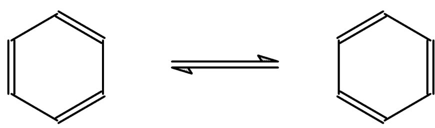


The aromatic hydrocarbons are benzene and compounds containing a benzene ring. Benzene has the chemical formula C_6H_6 and consists of a ring of six carbon atoms. Based on the chemical formula, one proposed structure for benzene was the following:

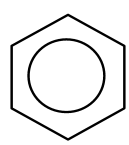


This structure would be called cyclohexatriene using the IUPAC system for naming aliphatic hydrocarbons that we have studied previously. However, the properties of benzene are very different than those of other double or triple bonded hydrocarbons. For example, benzene is a very stable molecule while alkenes and alkynes are both very reactive.

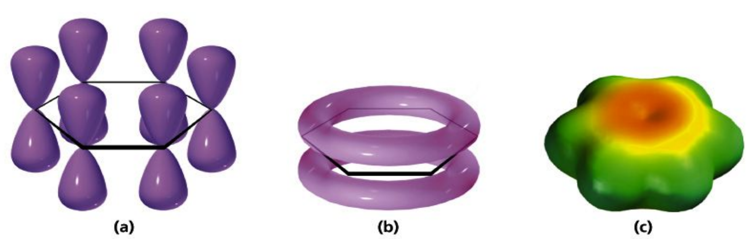
In fact, benzene has 6 *identical* carbon-carbon bonds in its structure. Benzene can be thought of as a hybrid of two "resonance forms" of cyclohexatriene:



Either of these structures is identified as benzene although neither is actually correct. Instead, a common way to represent benzene is a ring of 6 carbons with a circle in the middle:



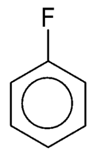
In other words, the electrons involved in the "double" bonds or pi bonds are shared equally among all 6 carbons. These pi electrons are said to be *delocalized* in this arrangement. Every carbon is sp^2 hybridization state with one electron involved in pi bonding. This means that benzene has a planar structure as shown in these models:



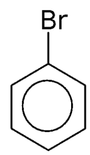
a) 6 half-filled *p* orbitals
b) π-bonding (delocalized electrons)
c) electron density diagram

Aromatic Nomenclature

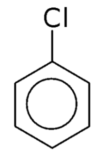
For many of the derivatives of benzene, we simply prefix the name of the substituent group to the word benzene. For example:



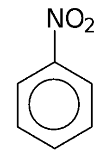
fluorobenzene



bromobenzene

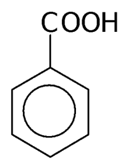


chlorobenzene

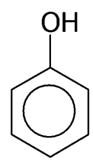


nitrobenzene

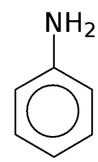
Some derivatives, however, have common names that do not follow the IUPAC system:



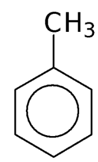
benzoic acid



phenol



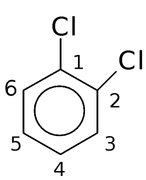
aniline



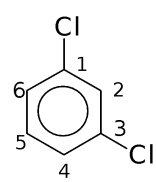
toluene

Benzoic acid and phenol are always known by these names and must be memorized. Aniline is also known as aminobenzene and toluene is also known as methylbenzene.

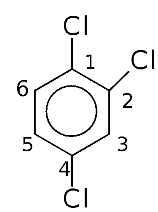
If several groups are substituted on the benzene ring, we also indicate their relative position. If all groups are the same, each substituted group is given a number to produce a sequence that gives the lowest combination of numbers.

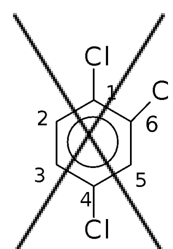


1,2-dichlorobenzene



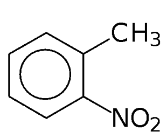
1,3-dichlorobenzene



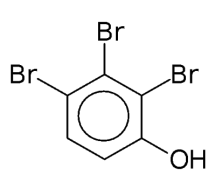


1,2,4-trichlorobenzene (*not 1,4,6 trichlorobenzene*)

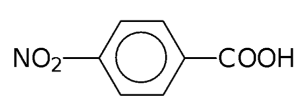
If the last named group has no number, it is understood to be at position 1. If a special name is used (e.g. phenol), the compound is named so the special group (e.g. the hydroxyl group on phenol) is at position 1.



2-nitrotoluene



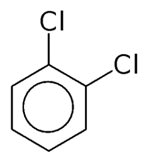
2,3,4-tribromophenol



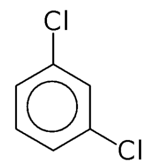
4-nitrobenzoic acid

Ortho, Meta and Para

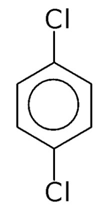
The various isomers of disubstituted benzene rings are often named using an alternative system. The names *ortho*, *meta* and *para* (prefixes *o*,*m* or *p*) identify the relative positions of two groups on the ring. Ortho means the two groups are on the 1,2 positions, meta means they are on the 1,3 positions and para means they are on the 1,4 positions.



o-dichlorobenzene

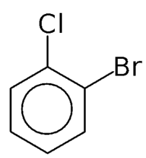


m-diclorobenzene

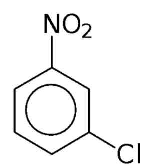


p-dichlorobenzene

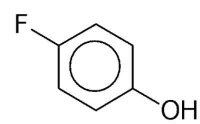
If the two groups are different, simply add the two prefixes with benzene. If one of the groups confers a special name, then the compound is named as a derivative of this compound.



o-bromochlorobenzene

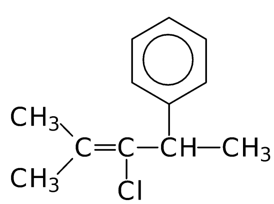


m-chloronitrobenzene



p-fluorophenol

Occasionally, benzene groups are found as substitutions or more complex hydrocarbon chains (e.g. alkenes or alkynes). In these compounds, the benzene is treated as a substitution and given the name *phenyl*. Be careful not to confuse a phenyl group with the compound phenol!



3-chloro-2-methyl-4-phenyl-2-pentene

ISOMERS

Structural Isomers are compounds with the same chemical formula but different arrangement of atoms. For example, the ortho, meta and para forms of dichlorobenzene shown above are all isomers with the chemical formula $C_6H_4Cl_2$. These compounds have the same molecular mass, but their physical and chemical properties are slightly different. **Geometric Isomers** are isomers where the atoms are arranged in the same way BUT they still have a different 3-dimensional arrangement. One form of this is *cis-trans* isomerism found in some alkenes.

To identify a pair of compounds as identical, isomers or different compounds, follow these clues.

1. Determine the chemical formula for the two compounds. Are they different? If YES, the compounds are <u>not</u> isomers but are different compounds.
2. If the chemical formula are the same, examine the spatial arrangement of atoms in the structure, Are the atoms joined in the same arrangement or are the atoms joined differently (structural isomerism)? Remember that there may be several ways to draw the same compound. If there are double bonds, examine if there are possible geometric (cis-trans) isomers.