AROMATICS

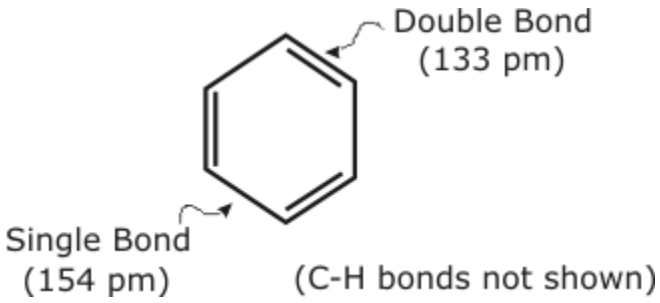
Benzene is a compound that chemists puzzled over for a very long time. Its chemical formula was determined to be C_6H_6 by Michael Faraday in 1825, but a suitable structural formula wasn't proposed until August Kekulé came up with one in 1865. Kekulé's ring structure was a very significant discovery because it helped explain the unique properties associated with benzene and benzene compounds.

Compounds that possess a benzene ring as part of their structure are classified as **aromatic** compounds. It is the presence of a benzene ring that distinguishes the aromatic hydrocarbons from the aliphatic hydrocarbons.

Carbon to Carbon Bonds in Benzene

The benzene ring consists of six carbon atoms, each of which is bonded to a hydrogen atom.

One way to satisfy the octet rule for carbon atoms in the benzene ring is to show the carbons with alternating single and double bonds. That way, each carbon atom has four bonds: a double bond (C=C), a single bond (C-C), and another single bond (C-H).



Now look carefully at the line diagram for the benzene ring above. What do you notice about the single and double bonds? Are they the same length?

Double carbon to carbon bonds are 14% shorter than single carbon to carbon bonds, yet *x*-ray crystallography studies show that all six carbon to carbon bonds in benzene ring are the same length (about 139 pm). The benzene ring is actually a flat hexagonal structure as illustrated by this image.

This structure suggests that all six of the carbon to carbon bonds are the same length. In other words, a distorted, unsymmetrical ring is not a suitable model for benzene.

The problem of producing a structural formula for benzene that is consistent with the flat ring observations has been addressed using the concept of resonance. It is a pretty simple idea.

Resonance means that there are two or more possible distributions of bonding electrons for a compound. The **resonance structure** (sometimes called resonance hybrid) is an average of the electron distributions.

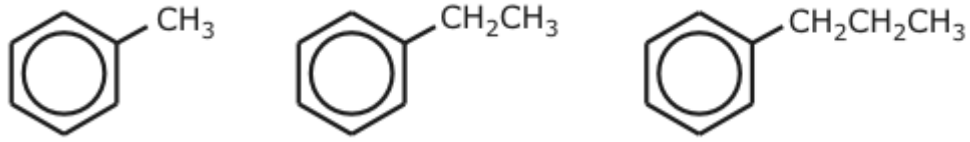
Naming Aromatic Hydrocarbons

One or more hydrogen atoms of a benzene molecule may be substituted with an alkyl group. The resulting compound is called an **alkyl benzene**.

Although all six of benzene's hydrogen atoms can be replaced by substituents, you will focus on those in which just one or two are replaced.

Monosubstituted Alkyl Benzenes

A benzene compound in which one hydrogen is replaced by an alkyl group is called a monosubstituted alkyl benzene. Consider these examples:



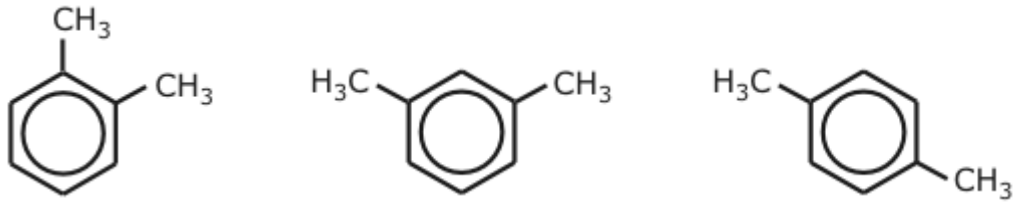
Naming monosubstituted alkyl benzene compounds requires a similar approach to the one you used for simple branched aliphatic compounds. The benzene ring is the parent and the alkyl group is the substituent. The ring carbon where the substituent is located is designated as carbon #1. This number is not included in the name.

Using these rules, what are the names of the monosubstituted alkyl benzene's above?

Methylbenzene is an ingredient in paint stripper. However, when you pick up a can of paint stripper and look at the ingredients list or the safety sheet, you are more likely to see the non-systematic name *toluene*. Toluene has been retained as an acceptable name for methylbenzene.

Disubstituted Alkyl Benzenes

When two hydrogen atoms on the benzene ring are replaced by alkyl groups, the result is a **disubstituted alkyl benzene**. The two alkyl groups may be the same or different. Consider these examples:



- What do you notice about the positions of the alkyl groups?
- What term is used to describe the possibility of three structures for C_8H_{10}?
- What implications might this have for naming?

Naming Aromatic Hydrocarbons

A reasonable question to ask now is: "are the rules different if the substituents are different?"

The answer is yes and no. No in the sense that you have to assign lowest possible numbers, but yes in the sense that you should number the alkyl groups based on alphabetical order.

When Benzene is the Substituent

There are instances when a benzene ring is bonded to a non-terminal carbon of an alkyl group and others where more than one benzene ring is connected to an alkyl group. In these cases, the alkyl groups become the parents and the benzene rings become the branches.

As a branch, the benzene ring is called a **phenyl** group.