BOOKS

1) Organic Chemistry Structure and Function, K. Peter C. Vollhardt, Neil Schore, 6th Edition

2) Organic Chemistry, T. W. Graham Solomons, Craig B. Fryhle

3) Organic Chemistry, Jonathan Clayden Nick Greeves Stuart Warren, 2th Edition

4) Organic Chemistry, John E. McMurry,8th. Edition

5) Reaksiyon Mekanizmaları: Metin Balcı, 2.Baskı.

1. AROMATIC COMPOUNDS

1. AROMATIC COMPOUNDS

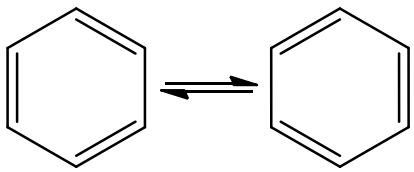
Benzene has only as many hydrogen atoms as it has carbon atoms. Benzene, having the formula of C_6H_6, should be a highly unsaturated compound because it has an index of hydrogen deficiency equal to 4. Benzene is colorless liquid bp ~80°C. In 1825, Faraday isolated benzene from a compressed illuminating gas that had been made by pyrolyzing whale oil.

Eventually, chemists began to recognize that benzene was a member of a new class of organic compounds with unusual and

interesting properties. Benzene does not show the behavior expected of a highly unsaturated compound.

1.1 The Structure for Benzene

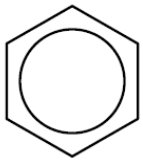
In 1865, August Kekulé, proposed the first definite structure for benzene, a structure that is still used today. Kekulé suggested that the carbon atoms of benzene are in a ring, that they are bonded to each other by alternating single and double bonds, and that one hydrogen atom is attached to each carbon atom. This structure satisfied the requirements of the structural theory that carbon atoms form four bonds and that all the hydrogen atoms of benzene are equivalent:



Experimental evidence bears this out. Spectroscopic measurements show that the molecule of benzene is planar and that all of its carbon–carbon bonds are of equal length. Moreover, the carbon–carbon bond lengths in benzene are 1.39 Å, a value in between that for a carbon–carbon single bond

between sp^2-hybridized atoms (1.47 Å) and that for a carbon–carbon double bond (1.34 Å).

The hybrid structure of benzene is represented by inscribing a circle inside the hexagon as shown in formula below.

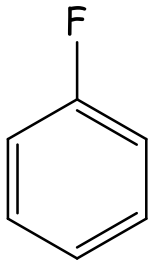


- All C⎓C bond lengths the same (1.39 Å) (compare with C—C single bond 1.54 Å, C=C double bond 1.34 Å)
- Electron density in all six C-C bonds is identical
- Structure is planar, hexagonal
- C–C–C bond angles: 120°
- Each C has sp^2 and has a *p* orbital perpendicular to the plane of the six-membered ring

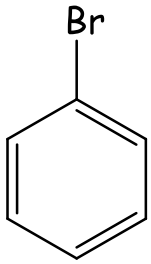
1.2 Nomenclature of Benzene Derivatives

Two systems are used in naming monosubstituted benzenes.

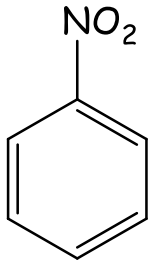
- In many simple compounds, benzene is the parent name and the substituent is simply indicated by a prefix.



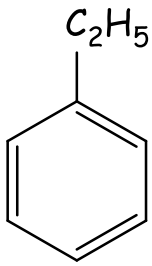
Fuorobenzene



Bromobenzene

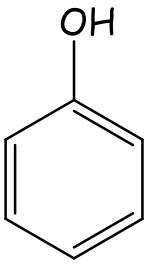


Nitrobenzene



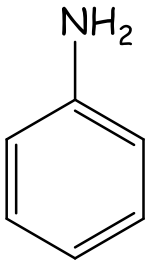
Ethylbenzene

- For other simple and common compounds, the substituent and the benzene ring taken together may form a commonly accepted parent name.



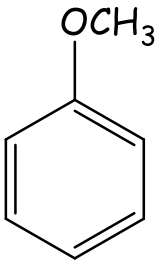
Hydroxybenzene

Phenol



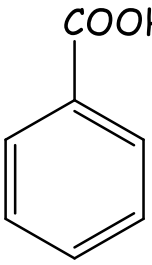
Benzeneamine

Aniline



Methoxybenzene

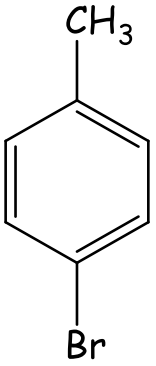
Anisole



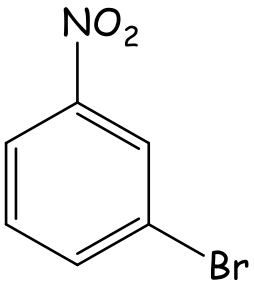
Benzenecarboxylic acid

Benzoic acid

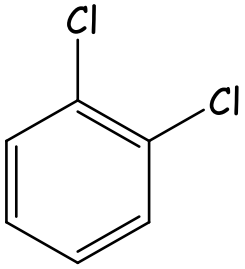
- When two substituents are present, their relative positions are indicated by the prefixes ortho-, meta-, and para- (abbreviated o-, m-, and p-) or by the use of numbers



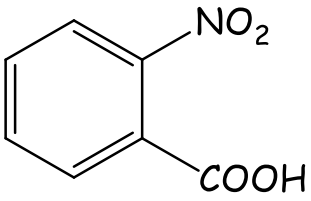
1-Bromo-4-methylbenzene
p-Bromotoluene



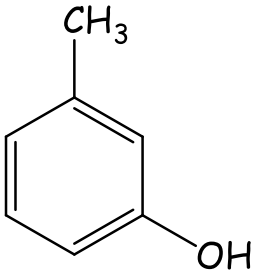
1-Bromo-3-nitrobenzene
m-Bromonitrobenzene



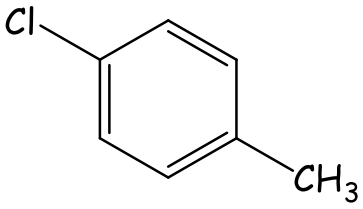
1,2-Dibromobenzene
o-dichlorobenzene



2-Nitrobenzoic acid
(*o*-Nitrobenzoic acid)

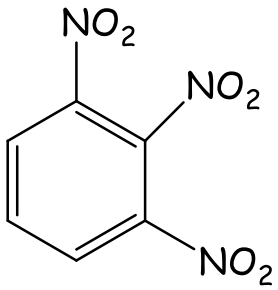


3-Methylphenol
(*m*-Methylphenol)

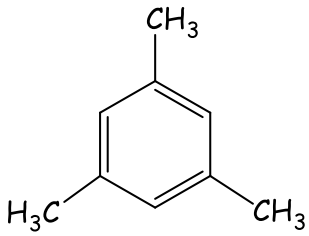


4-Chlorotoluene
(*p*-Chlorotoluene)
(1-Chloro-4-methyl-benzene)

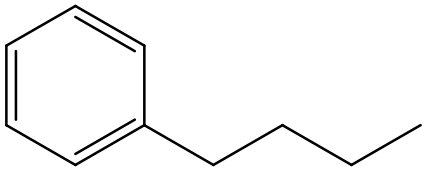
- If more than two groups are present on the benzene ring, their positions must be indicated by the use of *numbers*.



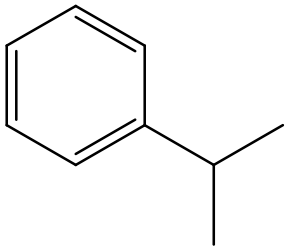
1,2,3-Trinitrobenzene



1,3,5-Methylbenzene



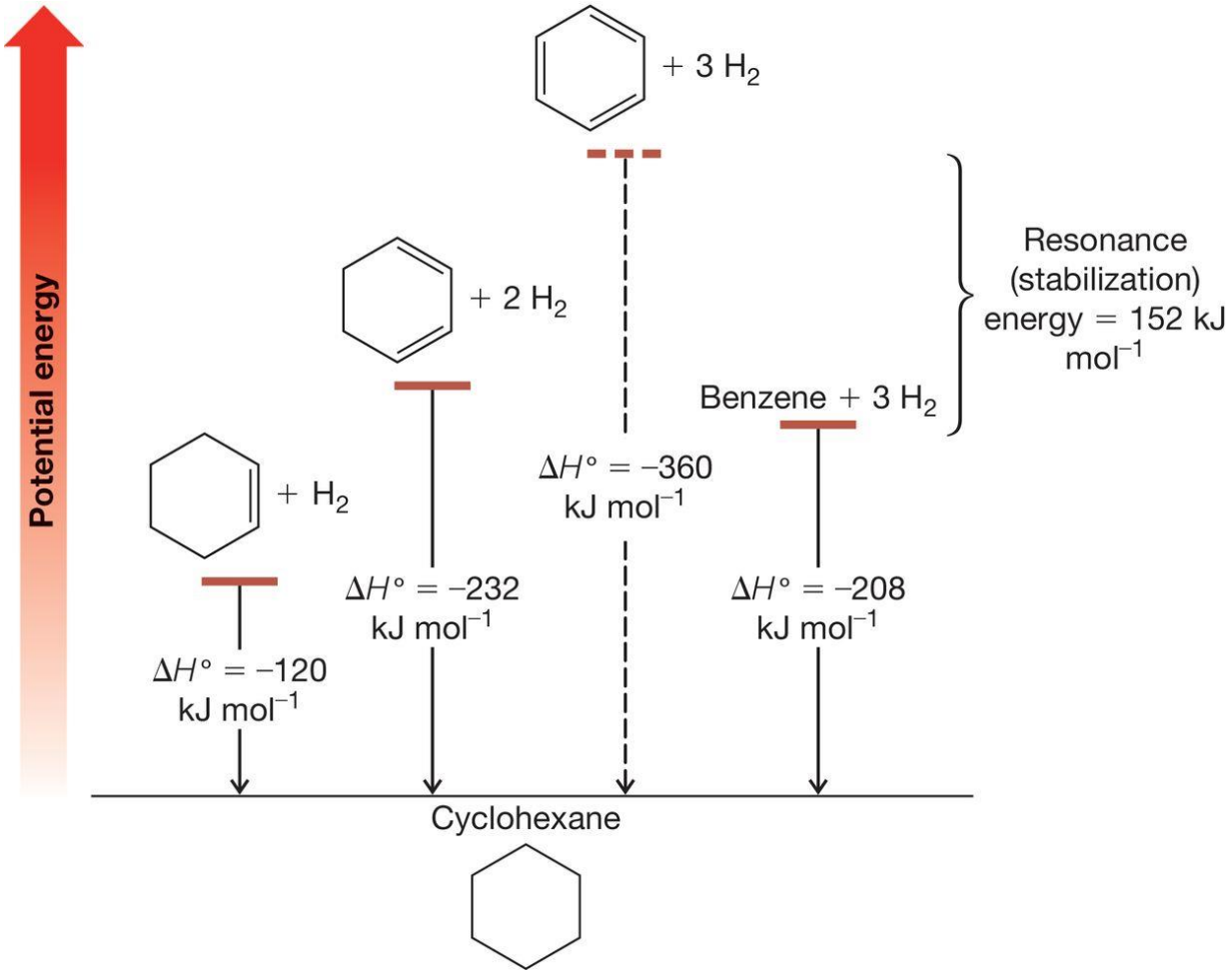
Butylbenzene



Isopropylbenzene

1.3 The Resonance Explanation of the Structure of Benzene

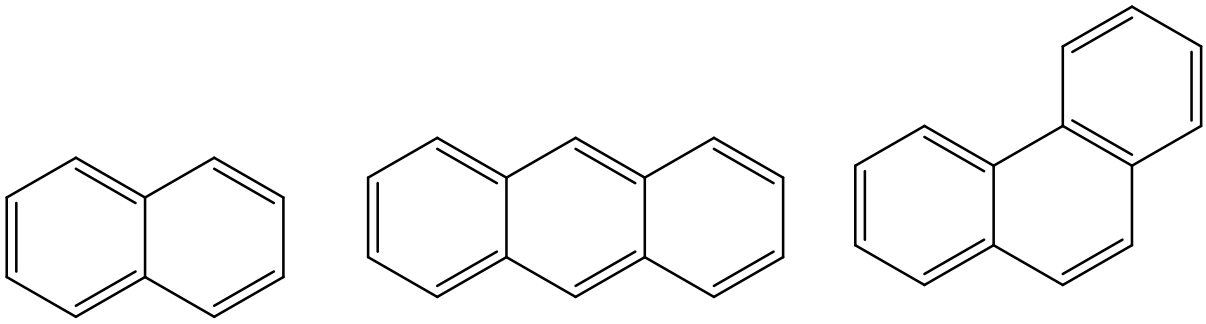
Benzene is unusually unreactive. Does this mean that it is also especially stable thermodynamically? Look at $\Delta H°$ hydrogenation:



The difference in energy between hypothetical 1,3,5-cyclohexatriene (which if it existed would have higher energy) and benzene is called *resonance energy*, and it is an indication of the extra stability of benzene due to electron delocalization. Special stability is now called aromaticity. All cyclic 6 pi electron arrangements are aromatic, including transition states.

1.4 Benzenoid Aromatic Compounds

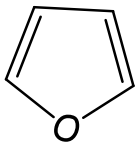
Representatives of one broad class of benzenoid aromatic compounds are called polycyclic aromatic hydrocarbons (PAH). Benzenoid polycyclic aromatic hydrocarbons consist of molecules having two or more benzene rings fused together.



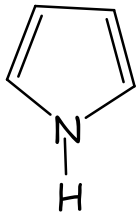
Naphtalene Antracene Phenantrene

1.5 Heterocyclic Aromatic Compounds

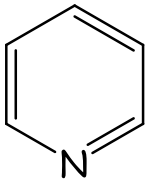
Cyclic compounds that include an element other than carbon are called heterocyclic compounds. Heterocyclic compounds containing nitrogen, oxygen, or sulfur are by far the most common.



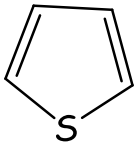
Furan



Pyrrole



Pyridine



Thiophene