PROPERTIES AND USES

Physical properties:

Structure:- The representation of the benzene molecule has evolved from the kekule ring formula (1), often abbreviated to a more realistic structure described by (2), in which all six carbon-to-carbon bonds are identical.

Resonance:- Benzene has great thermal stability, lower energy than the compound corresponding to (1), with three double bonds. When benzene is decomposed to carbon & hydrogen, it absorbs more energy than that predicted by Kekule's formula. This is because it assumes the resonant structure which is intermediate between the two structures shown below, in which the charges are spread equally.

Physical Constants for benzene :

Property	Numerical Value
Formula weight	78.11
Melting point, ^{o}C	5.533
Boiling point, ^{o}C	80.10
Density, at –3.77 ^{o}C, kg/m^{3}	873.7
Vapor pressure, at 26.075 ^{o}C, kPa	13.33

Refractive index	1.49792
Viscosity, at 20 ^{o}C, cP	0.6468
Surface tension, at 25 ^{o}C,mN/m	28.18
Critical temperature, ^{o}C	289.45
Crtical pressure, kPa	4924.4
Critical density, kg/m^3	300
Flash point (closed cup), ^{o}C	-11.1
Ignition temperature in air, ^{o}C	538
Flammability in air, vol%	1.5-8.0
Heat of fusion, kJ/(kg.mol)	9847
Heat of vaporization at 80.1 ^{o}C, kJ/(kg.mol)	33871
Heat of combustion at constant pressure & 25 ^{o}C,kJ/g	41.836
Solubility in water at 25 ^{o}C, g/100g water	0.180
Solubility of water in benzene at 25 ^{o}C, g/100g benzene	0.05

Chemical properties:

The reactions of benzene are of 3 distinct types: substitution, addition, and rupture of the ring.

Substitution: Under suitable conditions, one or more of hydrogen atoms of benzene can be replaced by atoms such as halogens, or by groups such as nitro & sulfonic acid groups.

Electrophilic substitution: When a monosubstitution product of benzene is subjected to the action of an electrophile, the rate of further substitution is increased by some groups and decreased by some other groups. It also influence thedirection of the second substitution.

Nucleophilic substitution of benzene derivatives: When the benzene ring is substituted with a sufficient number of highly electronegative groups, it becomes electrophilic itself and will react with nucleophilic substituting reagents.

Oxidation: Benzene can be oxidized to a number of different products. An important reaction is the catalytic oxidation of benzene to maleic anhydride and byproducts. The oxidation proceeds with air or oxygen at elevated temperatures with a vanadium pentoxide and molybdenum oxide catalyst.

Reduction: Benzene can be reduced to cyclohexane. At room temperature & ordinary pressure, benzene, either alone or in hexane or cyclohexane solution, is quantitatively reduced with hydrogen using nickel catalyst.

Pyrolysis: When benzene is passed through a red-hot iron tube, bubbled through molten lead or pumice, or passed at elevated temperatures over vanadium compounds, condensation takes place with the formation of biphenyl. At temperatures above 750^{o}C, benzene decomposes largely into carbon & hydrogen.

Halogenation: Depending on the conditions, either substitution or addition products can be obtained by the halogenation of benzene. Chlorine or bromine reacts with hot benzene in the presence of carriers such as ferric halides to give substitution products such as chlorobenzene or bromobenzene.

Nitration: The nitration of benzene to a monoderivative occurs readily in yields as high as 98% when a mixture of concentrated nitric and sulfuric acids is used at 50-55^{o}C.

Sulfonation: Benzene can be sulfonated with concentrated or fuming sulfuric acid to benzenesulfonic acid.

Alkylation: Alkylbenzenes, such as ethylbenzene & cumene, are produced commercially by the reaction of benzene with ethylene & propylene in the liquid or vapor phase in presence of anhydrous aluminium chloride or solid phosphoric acid as the catalyst

Uses:

Benzene has many uses and demand continues to grow despite increasing restrictions and environmental regulations. Styrene monomer is the largest use of benzene, followed by cumene/phenol, cyclohexane, and nitrobenzene. Those derivatives are used to produce a wide range of plastics, fibers, resins and films. Benzene is also an excellent solvent for waxes, resins, rubber and various other organic materials, but toxicological properties greatly limit use. Benzene, like other aromatics, has a high octane number and was a valued gasoline-blending component until its use was restricted by the pollution control laws.