Class - B.Sc. Part II (Subsidiary)
Subject - chemistry
Paper - Gr. C, Subsidiary
Topic - Structure of Benzene
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Structure of Benzene

The structure of benzene has been derived given as below:—

(1) molecular formula :— on the basis of elemental analysis and molecular weight determination, the molecular formula of benzene comes to be C_6H_6. This indicated that benzene was a highly unsaturated compound (compare it with n-hexane)

(2) open chain structure :— Benzene could be constructed as a straight chain or ring compound having double (C=C) or triple (C≡C) bonds. But benzene did not behave like alkenes or alkynes, it did not decolorize bromine in carbon tetrachloride or cold aqueous $KMnO_4$. It did not add water in presence of acids.

Benzene + Br_2/CCl_4 ⟶ No reaction

Benzene + dil./cold $KMnO_4$ ⟶ No reaction
Benzene + H_2O/H^+ ⟶ No reaction

(3) Evidence of cyclic structure :-

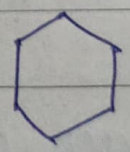
a. Substitution of benzene :- Benzene reacts with bromine in presence of $FeBr_3$ to form monobromobenzene.

$$C_6H_6 + Br_2 \xrightarrow{FeBr_3} C_6H_5Br + HBr$$

It shows that only one monobromo and no isomeric products were obtained, which indicates that all six hydrogen atoms in benzene were identical. This could be possible only if benzene had a cyclic stru. of six carbons and to each carbon was attached one hydrogen.

b. Addition of Hydrogen :- Benzene reacts with three moles of hydrogen in presence of Ni to give cyclohexane.

$$C_6H_6 + 3H_2 \xrightarrow[150^\circ C \text{ pressure}]{Ni}$$



cyclohexane

This confirmed that the cyclic structure of benzene and also show the presence of three carbon - carbon double bonds.