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NOTE

The Structural Aspects of Benzene

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A new explanation for the structure of benzene is proposed which is in coincidence with the geometry and chemical reactions of benzene.

Benzene, C_6H_6 was first isolated by Michael Faraday in 1825 from the liquid condensed by compressing oil gas. Kekule in 1866, suggested that the six carbons were connected in a hexagonal ring with alternating single and double carbon-to-carbon bonds, and with each carbon connected to a single hydrogen.

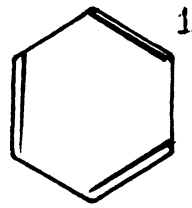

Fig. 1

This concept was controversial on three accounts: First, benzene did not behave as expected, as judged by the behaviour of the other compounds with carbon-to-carbon double bonds. Second, there should be two different dibromo substitution products of benzene with the bromine of adjacent carbons but only one such compound could be isolated[1].

Fig. 2

Third, if benzene actually possessed three single and three double bonds, as a Kekule structure, we would expect to find three short bonds (1.34 Å) and three long bonds (1.48 Å) probably as in 1,3-butadiene. Actually, X-ray diffraction studies show that the six carbon-carbon bonds in benzene are equal and have a length of 1.39 Å.[2]

Thus the fact is that, of the many bond structures that have been proposed for benzene, either before or after Kekule's time, no single one may be accepted as satisfactory[3].

New model

To explain the chemical reactions and geometry of benzene a new structure is proposed. In the proposed model there is no double bond between two consecutive carbon atoms.

This model suggests that the six carbons were connected in a hexagonal ring with carbon-to-carbon single bond, called primary single bond, and with each carbon connected to a single hydrogen.

And this model also suggests the existence of three single bonds between carbon atoms of hexagonal ring in *para* positions. So these bonds are called secondary single bonds.

Thus the three secondary bonds are connecting the carbon skeleton of benzene

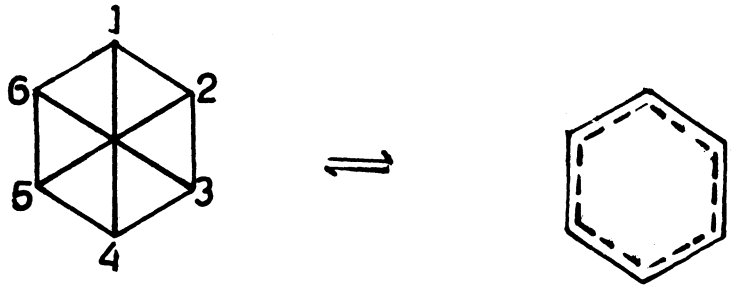

Fig. 3

in the following way.

1. First secondary bond between C_1 and C_4.
2. Second secondary bond between C_2 and C_5.
3. Third secondary bond between C_3 and C_6.

In all these bonds, nuclei is separated by 2.8 Å, which is too far apart for effective bonding[4]. Therefore these secondary bonds are weak bonds. Since these secondary bonds cross over each other in the centre of benzene, a magnetic flux is created. And due to repulsion these bonds are broken into six half bonds. Hence each half bond have a length of 1.4 Å. Consequently all the six half bonds have been rearranged and equally distributed between the six carbons of hexagonal ring. In this way all of C—C bonds of benzene have the same length with 1.5 bonds between the carbons[5].

Evidence

If we add the energies of all bonds in benzene, we can see that calculated and actually found values of benzene are same for the heat of atomization.

The actual value is 1323 Kcal/mol. If we use E value for a C—C secondary bond obtained from C_2H_6 79.1 kcal/mol[6]. C—C primary bond obtained from cyclohexane, 81 kcal/mol[6] and C—H bonds from methane, 99.5 kcal/mol. We get a total of 1325.1 kcal/mol for the proposed model of benzene.

Thus calculated value (1325.1 kcal/mol) and actual value (1323 kcal/mol) are resonably close.

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