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Research Abstract

Hückel Calculations and Aromaticity
in Two and Three Dimensions

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Aromaticity, one of the old concepts has been revisited many times giving the theories of chemical bonding, structure and stability. Although it is a concept, it has a deciding role on the properties of molecules. Earlier concept of aromaticity was restricted to two dimensional conjugated π systems and later extended to various types of three dimensional systems.

Extensive ab initio calculations have been carried out for planar and non planar systems with and without π electrons. Calculations were performed with Hartree-Fock (HF) and Density functional theory (B3LYP functional) methods using 6-31G* basis sets. Aromaticity indices like Degree of aromaticity, Nucleus independent chemical shift (NICS) and Reactivity index were used in the present study. Hückel calculation, a simple but powerful approach toward explaining the stabilities, physical properties, and chemical reactivities have been performed for some three dimensional systems.

Benzene and other conjugated systems were found to be aromatic based on the three indices mentioned. On protonation the aromaticity of benzene ring increases although there is an energy barrier. In Corranulene the criteria of planarity is lost but the system still behaves as aromatic. Water clusters were found to be slightly aromatic due to the delocalization of electrons through hydrogen bonding. Among fullerene derivatives it has been observed that aromaticity can change with the number of electrons, structural parameters as well as encapsulation. A remarkable change in aromaticity is observed for two dimensional graphene sheets on folding to three dimensional tubes.

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