THEORETICAL DETERMINATION OF NUCLEAR MAGNETIC SHIELDING IN PLANAR BENZENE ISOMERS

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Magnetic susceptibilities and magnetic shielding at the nuclei of proton and carbon in a series of molecules with chemical formula C_6H_6 and a planar structure, i.e., benzene, fulvene, 3,4-dimethylenecyclobutene, trimethylenecyclopropane, and the hypothetical cyclohexatriene, have been evaluated at the coupled Hartree-Fock level of accuracy, using conventional common origin schemes, basis sets of London orbitals, and procedures adopting continuous transformation of the origin of current density. The results are rationalized via models of the charge flow induced in the electron cloud by a magnetic field perpendicular to the molecular plane. The connection between magnetic properties and the concept of aromaticity is discussed.