

C50Cl10, a planar aromatic fullerene. Computational study of ¹³C-NMR chemical shift anisotropy patterns and aromatic properties

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The isolated-pentagon-rule (IPR) is a prime determinant of fullerene stabilization accounting for the difficult isolation of hollow C_n (n < 60) species. In this connection, the isolation and structural characterization of D_{5h}-C₅₀Cl₁₀ as an IPR-violating fullerene are of interest owing to the study of factors providing further stability. Herein, we use DFT calculations to explore its aromatic behavior. In this connection the C₅₀Cl₁₀ structure is considered as a fullerene displaying a planar-aromatic character provided by the face-to-face disposition of two IPR structural motifs, mediated by ten exobonded sp³-carbons. In addition, the D_{5h}-C₅₀Br₁₀ counterpart appears to be another promising structure as the target for explorative synthesis. Owing to the curvature of its IPR motif, an interesting variation in the ¹³C-NMR patterns relative to corannulene is described, where the relation between C_I and C_{II} signals is useful to evaluate the degree of the curvature of the π -surface. The charge distribution of C₅₀Cl₁₀ reveals a more electron-deficient IPR dome in comparison to C₆₀, envisaging an enhanced chemistry related to bare fullerenes. In addition, the -Cl and -Br exobonded atoms provide effective π -holes, suggesting such oblate fullerenes as interesting two-dimensional five-fold symmetric synthons useful for the formation of supramolecular species. Hence, an interesting chemistry and supramolecular array derivatives are potential applications to be further explored towards the development of novel nano-devices. © the Owner Societies.