

# Aromaticity in Phenyl Decorated closo-Monocarboranes. Planar-Spherical Aggregates Involving 7-12-Vertex Cages

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## Abstract

The characterized phenyl decorated closo-monocarboranes with variable sizes from 7- to 12-vertex cages, [Ph-closo-CB<sub>n</sub>H<sub>n</sub>]-,  $n = 6-11$ , allow us to address the role of the varying size and shape of the carborane cage in dual planar-spherical aromatic species. Our results show the formation of adjacent shielding cone characteristics enabled from both planar and spherical aromatic fragments, despite the different structures of the closo-monocarboranes. Under a field perpendicular to the phenyl ring, both shielding cones are enabled, which overlap at long-range regions, in contrast to other orientations leading to a short-range response from the planar aromatic fragment. Thus, a two- or one-aromatic circuit is enabled selectively within the same molecular unit, by controlling the orientation of the external field. Along with the series, a variable extension of the shielding cone from the carborane cage is observed, which is larger for the -CB<sub>11</sub>H<sub>11</sub> case, decreasing toward -CB<sub>6</sub>H<sub>6</sub>, denoting a similar extension from both the planar and spherical aromatic regions at the [4-Ph-closo-4-CB<sub>8</sub>H<sub>8</sub>]- (4) counterpart. The analysis of such multiple aromatic structures shows that, despite the different sizes and shapes of the closo cages, a similar aromatic behavior remains. In addition, the anisotropy of the induced magnetic field is given graphically, denoting a larger anisotropy for the planar aromatic moiety owing to its two-dimensional structure, which is suggested to discriminate between planar and spherical aromatic fragments within the same molecule.