

Interplay Between Planar and Spherical Aromaticity: Shielding Cone Behavior in Dual Planar-Planar, Planar-Spherical and Spherical-Spherical Aromatics

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The shielding cone concept is one of the most characteristic aspects of planar aromatic species. Herein, we explored how two neighbor aromatic moieties behave as dual planar-planar, planar-spherical, and spherical-spherical species given by biphenyl, [PhCB₁₁H₁₁]⁺, and [CB₁₁H₁₁]²⁺, respectively. Our results show two separate aromatic regimes given by Clar's sextet and spherical aromatic states, with independent shielding cones sharing shielding regions of moderate strength, which can be extended for networks involving multiple independent aromatic states. © 2020 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim

benzene

carborane

NICS

shielding cone

spherical aromaticity

Aromatic compounds

Aromatization

Shielding

Aromatic moieties

Aromatic species

Aromaticities

Dual-planar

Spheres