Consequences of Curvature on Induced Magnetic Field: The Case of Helicenes

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Helicenes consist of several fused rings twisted around an axis, forming a cylindrical helix, with ?-delocalized electrons in the non-planar rings. Induced magnetic fields dissecting the orbital contributions of [6]-, [7]-, and [14]helicene are discussed. Computations show a deshielding cone produced by the ?-electrons along the helical axis. Unexpectedly, the response of the core electrons produces a shielding cone, which is cumulative and sensitive to the curvature of the systems owing to the overlap of the other ring responses. A warning is provided regarding the evaluation of the delocalization in curved systems in which the x- and y-components of the induced magnetic field become relevant.

aromaticity

electron delocalization

helicenes

magnetic responses

Magnetic fields

Aromaticities

Delocalizations

Delocalized electron

Electron delocalization

Helicenes

Induced magnetic fields

Magnetic response

Orbital contribution

Electrons