Fulfilling the 2(N+1)2 Hirsch rule in smaller hollow fullerenes. Evaluation of long-range magnetic behavior and NMR patterns of C28, C284?, C24N4, and C28H4

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The formation of different 32 ?-electron systems derived from a prominent small fullerene given by C28, allows to evaluate several approaches ensuring an electronic shell closure in terms of the characteristic chemical shift anisotropy (CSA) and long-range magnetic response properties for spherical aromatic compounds. Our results show that the inclusion of extra electrons and the doping of the cage, are able to sustain a long-range shielding cone when an external field is oriented in a specific orientation. Such properties are inherent characteristics of spherical aromatic compounds, which are not obtained in the neutral C28 fullerene, and in the exo-bonded approach leading to C28H4. Thus, the doping of the cage is suggested as the most suitable approach to modify the overall count of electrons, leading to the expected response properties for further design of highly aromatic fullerenes. © 2018 Wiley Periodicals, Inc.

fullerenes

heterofullerenes

magnetic response

spherical aromaticity

Aromatic compounds

Aromatization

Chemical shift

Magnetism

Spheres

Aromaticities

Chemical shift anisotropy

Electronic shells

Heterofullerenes

Inherent characteristics

Magnetic response

Response properties

Specific orientation

Fullerenes