

# Aromatic character of $O_h$ - $C_{24}N_{24}$ . A cavernous nitride fullerene bearing $N_4$ -macrocycle motifs

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Spherical fullerenes offer noteworthy structures usually involving six- and five-membered faces, with application in technological issues. In this sense, cavernous spherical-like structures bearing larger holes provide interesting examples for further understanding of structure-properties relationship.

Here, we explored the magnetic response of a proposed cavernous nitride fullerene,  $C_{24}N_{24}$ , which has a  $O_h$ -symmetry with six  $N_4$ -macrocyclic and eight 1,3,5-triazine faces displaying 48-? electrons.  $C_{24}N_{24}$  exhibits a local aromatic behavior owing to the contrasting antiaromatic response of the  $N_4$ -macrocyclic faces and the aromatic character of the 1,3,5-triazine faces. Thus, the overall structure is ascribed as a local aromatic species, where the triazine faces exhibit the characteristic shielding cone for aromatic rings. Furthermore, the constructive combination of local shielding cones in  $C_{24}N_{24}$  delivers a related shielding-cone response, as expected for a perfect aromatic cage. Hence, the local aromatic/nonaromatic/antiaromatic sections exhibit an additive or subtractive interaction, leading to a characteristic response inherent to the nature of the spherical cage. We expect that further study of the interplay between different aromatic and antiaromatic faces in fullerene-like cages can deliver interesting pseudo-aromatic or pseudo-antiaromatic spherical species. © 2019 Wiley Periodicals, Inc.

aromaticity

cavernous

fullerene

magnetic fields

Aromatic compounds

Fullerenes

Magnetic fields

Nitrides

Shielding

Spheres

1,3,5-triazines

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Aromaticities

cavernous

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Structure-properties relationships

Aromatization