Expansion of Magnetic Aromaticity Criteria to Multilayer Structures: Magnetic Response and Spherical Aromaticity of Matryoshka-Like Cluster [Sn@Cu12@Sn20]12?

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Structural characterization of the discrete [Sn@Cu12@Sn20]12? cluster exposed a fascinating architecture composed of three concentric structural layers in which an endohedral Sn atom is enclosed in a Cu12 icosahedron, which in turn is embedded in an Sn20 dodecahedron. Herein, the possibility of sustaining aromatic behavior for this prototypical multilayered species was evaluated, in order to extend this concept to more complex clusters on the basis of magnetic response and bonding analysis by the AdNDP approach. This revealed characteristic features of spherical aromatics, given by the ability to sustain the shielding cone property, similar to archetypal aromatics. The favorable bonding pattern in the [Sn@Cu12@Sn20]12? cluster fulfills the 2(N+1)2 Hirsch rule for aromaticity; thus, the cluster could be regarded as a first member of aromatic multilayered structures. The set of four 13c?2e aromatic bonds that was identified in the internal SnCu12 structure results in spherical aromatic character of this multilayered cluster. This insight builds a bridge between the traditional concept of Hückel's aromaticity and the aromaticity of complex and stable 3D systems that may be explored on the basis of magnetic response and bonding analysis. It also may open a way to novel findings in bottled clusters displaying aromatic behavior in multilayer structures, which are of great interest for inorganic nano- and material sciences due to their unprecedented stability.

aromaticity

cluster compounds

copper

density functional calculations

tin

Aromatic compounds

Binary alloys

Cluster computing

Copper

Copper alloys

Density functional theory

Isomers

Magnetism

Multilayers

Spheres

Tin

Tin alloys

Aromatic behavior

Aromaticities

Cluster compounds

Magnetic aromaticity

Magnetic response

Multi-layered structure

Multilayer structures

Structural characterization

Aromatization