

# Long-range magnetic response of toroidal boron structures: B16 and [Co@B16]<sup>-3-</sup> species

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A correlation between the long-range characteristics of the magnetic response of toroidal boron-based structures is given, involving the uncoordinated B16 cluster and the hypercoordinated [Co@B16]<sup>-3-</sup> counterparts. It is found that the perfectly symmetrical doubly aromatic systems share common features, involving a continuous shielding region for the orientation-averaged response (isotropic), and a long-ranged shielding cone under a perpendicularly oriented applied field ( $B_{zext}$ ). In contrast, the conflicting aromatic structure given by the slightly distorted species, exhibits an enhanced deshielding cone under  $B_{zext}$ , which dominates the isotropic character of the response. In addition, [Mn@B16]<sup>-</sup> and [Cu@B16]<sup>-</sup> clusters were evaluated, denoting the role of the coordinated metal atom in such property. This information is valuable to account for a global magnetic response driven by the bonding pattern acting in each respective compound, and for the possible characterization of intermolecular aggregates or extended structures via NMR experiments.

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