

Double aromaticity of the B₄₀ fullerene: Induced magnetic field analysis of π and σ delocalization in the boron cavernous structure

Charistos N.D.

Muñoz-Castro A.

The induced magnetic field of B₄₀ was dissected into contributions from π , σ and core electrons revealing the origins for the formation of the strong long range shielding response characterizing the spherical aromatic nature of the cavernous D_{2d} structure. Our analysis showed the complementary role of π and σ orbitals for the formation of the global shielding cone, with weak π contributions at a long range and strong σ contributions inside the cage, supporting the molecule as double aromatic with weak π and strong σ delocalization. Similar local variations of both π and σ magnetic responses were identified portraying peripheral diatropic and local paratropic currents. The weak π aromaticity is explained on the basis of symmetry rules pertaining to its electronic structure which forbid small gap paratropic rotational excitations. © 2019 the Owner Societies.