Induced Magnetic Field of Fullerenes: Role of ?- And ?- Contributions to Spherical Aromatic, Nonaromatic, and Antiaromatic Character in C60q (q = +10, 0, -6, -12), and Related Alkali-Metal Decorated Building Blocks, Li12C60 and Na6C60

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The induced magnetic field of fullerenes is strongly dependent on the charge state, where C60 is depicted as a nonaromatic species, in contrast to C6010+ which exhibits a strong spherical aromatic character. Here, we account for the response of relevant charged stable building blocks for novel extended networks with variable applications, as observed in A12C60 and A6C60 phases (A = alkali metal), given by, Li12C60 and Na6C60, as well as four different charge states of C60q (q = +10, 0, -6, -12), to an external magnetic field is studied in detail, focusing on the contributions from the ? and ? systems to the induced magnetic field. C60, C606-, and C6012- accounts for the variation of their isolated species upon addition of charge, whereas C6010+ is a hypothetical highly aromatic counterpart. Our results show that each spherical shell and each canonical molecular orbital exhibit characteristic patterns, revealing the direct dependence of the magnetic response, and therefore of spherical aromatic character, with regard to electron configuration. In particular, low-lying S, P, D, and F ?-type shells exhibit identical strong and long-range shielding character among the four charge states. The G shell exhibits a weak shielding response, precluding the strong deshielding contribution from high-lying H and I shells. A similar analysis is given for ?-type orbitals. Thus, the aromatic, nonaromatic, and antiaromatic character of C60 among the different charge states is ruled by the population of the high-lying ?-shells, which is explained in terms of ? ? ?? excitations of high-lying canonical molecular orbitals. Hence, in spherical aromatic fullerenes, the formation of a shielding cone is given mainly by the ?-type shells, extending characteristic features from planar aromatics to three-dimensional structures, which is useful for further rationalization and characterization of spherical/nonaromatic and antiaromatic spherical structures.

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