Formation of Spherical Aromatic Endohedral Metallic Fullerenes. Evaluation of Magnetic Properties of M@C28 (M = Ti, Zr, and Hf) from DFT calculations

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The small C28 cage has been shown experimentally to encapsulate titanium, zirconium, and hafnium (M), among other elements. Here, we explore computationally its magnetic response properties accounting for both global and local shielding tensors. Our results exhibit a continuous shielding region for M@C28 for an orientation-averaged applied field thereby differing from that observed for the hollow C28 structure. Moreover, under a specific orientation of the applied field a long-ranged shielding cone is obtained supporting the spherical aromatic behavior expected by the 2(N + 1)2 Hirsch rule for M@C28, standing for its particular abundance. The comparison between the hollow and endohedral C28 fullerenes exhibits a characteristic long-range behavior at the outside region of the structure. The particular shape of the local chemical shift anisotropy tensor at a representative carbon atom exhibits inherent patterns as a consequence of the spherical aromatic behavior. This shows the capabilities from NMR experiments to account for the nonaromatic - aromatic variation. We envisage that the current approach will be beneficial in comparative studies of aromatic and electronic structure properties, to gain a deeper understanding of the geometrical and electronic structure situation in other endohedral species beyond that available from the information provided by routine NMR measurements.