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Non-Collinearity in Small Cobalt-Benzene Molecular Clusters
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Cobalt clusters covered with benzene in the form of bowl-like structures have recently been synthesized using laser ablation. Here, we investigate the types of magnetic order such clusters have, and whether they retain any magnetic order at all. We use different density functional theory (DFT) methods to study three cobalt atoms surrounded by benzene rings since, in addition to its inherent simplicity, this cluster is more stable. We found that the benzene rings induce a ground state with non-collinear magnetization, with the magnetic moments localized on the cobalt centers and lying on the plane formed by the three cobalt atoms. This is surprising because nanostructures and small clusters based on pure cobalt typically have a predominantly ferromagnetic order, and additional organic ligands such as benzene tend to remove the magnetization. We analyze the magnetism of such a cluster using an anisotropic Heisenberg model where the involved parameters are obtained by a comparison with the DFT results. Moreover, we propose electron paramagnetic resonance as an experimental tool to study the anisotropic response.

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