

# Aromaticity introduced by antiferromagnetic ligand mediated metal-metal interactions. Insights from the induced magnetic response in [Cu<sub>6</sub>(dmPz)<sub>6</sub>(OH)<sub>6</sub>]

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[trans-Cu( $\mu$ -OH)( $\mu$ -dmpz)]<sub>6</sub> (1) exhibits six Cu(II) centers effectively coupled through a ligand mediated mechanism leading to a diamagnetic ground state over a wide temperature range. Here we investigate further magneto-structural correlations based on the possible free electron precession along such a copper-based ring-like nanocoil mediated by bridging ligands. We find that in 1, mediated antiferromagnetic coupling leads to characteristics that induce aromatic ring behavior through evaluation of both induced currents and shielding of cones from a relativistic density functional theory level. According to our gauge calculations including magnetically induced current densities and an induced magnetic field, a sizable ring current strength susceptibility is obtained for the cyclic Cu-N-N-Cu and Cu-O-Cu pathways, allowing a magnetic exchange between the copper centers. Our study suggests that [Cu<sub>6</sub>(dmPz)<sub>6</sub>(OH)<sub>6</sub>] consisting of an aromatic ring structure displays aromaticity and superexchange along the Cu-O-Cu and Cu-N-N-Cu backbones, which accounts for 80% and 20% of the overall ring current strength susceptibility, respectively. This reveals the presence of particular aromatic ring characteristics in coordination compounds without a direct metal-metal bond, where several formally paramagnetic centers are antiferromagnetically-coupled through supporting ligands. We envisage that our findings can be extended to other examples depicting ligand-mediated interaction between metal centers. © 2017 the Partner Organisations.