

RCMS & GTR Seminar

Electron and spin (de)localization in polynuclear complexes based on a triphenylene tris dioxolene bridge, experiment and theory



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A trinuclear (Ni_3) complex is assembled from the reaction of Ni(II) capped with a blocking tris-pyrazolyl borate tridentate ligand and deprotonated tris-catecholate hexahydroxytriphenylene (H_6HHTP).^{1,2} The crystal structure and the magnetic data are consistent with a three-electron oxidized bridge leading to the tris-semiquinone ([sq-sq-sq]) form with a single unpaired electron. The single unpaired electron is found to be mainly localized on one of the OCCO moieties of the tris-semiquinone. Upon one and two-electron reduction, the molecule switches to the [sq-sq-cat] (cat stands for catecholate) state and then to the [sq-cat-cat] one detected by EPR. Using a bidentate capping ligand allows the assembly of a hexanuclear (Ni_6) complex. The bridging ligands are in the semiquinone state. The electrochemical properties show two one-electron oxidation and reduction processes that can be rationalized as due to the interaction between the non-innocent bridging ligands as supported by wave function based theoretical calculations.



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