# Switchable magnetic properties under the action of a redox stimulus in a molecular complex

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This work deals with the rational design of Ni(II)-based qubits with the purpose of controlling the interaction between three qubits by using a redox active central ligand as some examples have been reported [1]. These systems are potential candidates as quantum logic gates.
One trinuclear complex based on the central hexahydroxytriphenylene (HHTP) redox active ligand is studied. Its redox states are characterized by spectroelectrochemical measurements and isolation of the first oxidized and first reduced states is reported.

In doing so and with the addition of EPR measurements [2], a switch is observed. It occurs from a paramagnetic state where a single electron is present on the central ligand (that magnetically couples the three metallic centers) to a state for which the diamagnetic central ligand isolates the magnetic centers.
Ab initio calculations on a toy model show interesting insights in the electronic structure of the studied species. More precisely, the properties of the HHTP ligand are investigated and allow to explain the experimentally observed properties of the complexes.

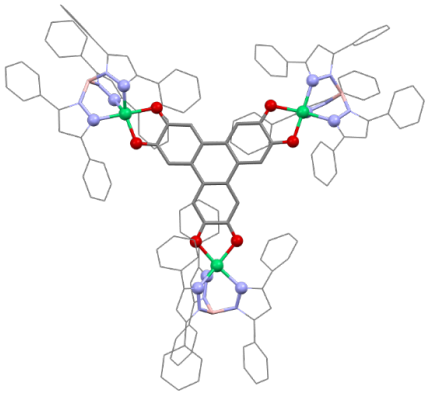

*Figure-1:Crystallographic structure of the trinuclear complex [Ni3(HHTP)(HBTp(Ph,Ph)3)3]*

**[1]** Ma, X., Suturina, E.A., Rouzières, M., Platunov, M., Wilhelm, F., Rogalev, A., Clérac, R., Dechambenoit, P., 2019. Using Redox-Active π Bridging Ligand as a Control Switch of Intramolecular Magnetic Interactions. J. Am. Chem. Soc. 141, 7721–7725. https://doi.org/10.1021/jacs.9b03044

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