

$C_2B_9H_{9.91}]^-$  anion in salt **1** presented in Figure 1. The dicarbollide ligands are mutually rotated by  $180^\circ$  producing *transoid* conformation.

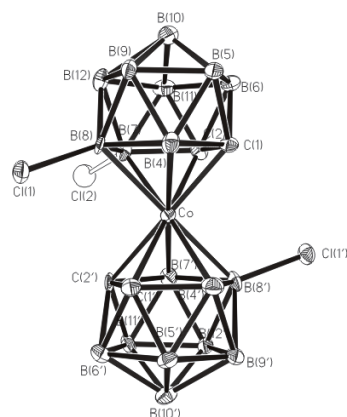


Fig. 1. The anion in (**1**). Hydrogen atoms omitted for clarity.

All radical cation salts prepared were found to be semiconductors, the room temperature conductivities are 2,  $10^{-5}$ ,  $0.5 \Omega^{-1}cm^{-1}$ , respectively.

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**Keywords:** molecular conductors, X-ray study, materials

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### Solvent-tuned Magnetic Behaviors of Manganese(III) Corroles

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Mn(tpfc) (tpfc = the trianion of 5,10,15-tri(pentafluorophenyl)corrole) is a good magnetic anisotropy motif. Compared to intense efforts on its catalytic performance [1, 2], rare research concentrates on its magnetic behaviors. We get three Mn(tpfc) solvates from methanol (**1**), ethyl acetate (**2**) and ethanol (**3**), respectively. Though they share the same magnetic repeating unit, they show quite different magnetic behaviors due to solvent-tuned different packing in crystal lattices. **1** and **2** are supramolecular 1D chains while **3** forms dimers. **1** with slow relaxation of magnetization below 2 K and magnetization hysteresis loop at 0.5 K is the first spin canted supramolecular single-chain magnet stemming from intermolecular  $\pi-\pi$  interaction. **2** is an antiferromagnetic chain without ordering or slow magnetization relaxation down to 0.5 K while **3** shows field-induced single-molecule magnet-like behaviors below 2.5 K.

Such control of solvent on magnetic behaviors comes from different relative orientations of magnetic anisotropy axes induced by solvents and shows clear magneto-structural correlation.

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[1] Z. Gross, G. Golubkov, L. Simkhovich *Angew. Chem. Int. Ed.* **2000**, *39*, 4045-4047. [2] M.J. Zdilla, M.M. Abu-Omar *J. Am. Chem. Soc.* **2006**, *128*, 16971-16979.

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### Multifunctional Gd<sup>III</sup><sub>5</sub>-core nanoparticles directed by alkylnitrosopyrazolones

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The area of gadolinium(III) labelled nanoparticles for use as MRI contrast agents is rapidly increasing. They are usually envisaged as an inorganic nanoparticulate core of a Gd-containing species (i.e. Gd<sub>2</sub>O<sub>3</sub>) coated with a polymeric shell.[1] Our strategy consists in developing Gd(III) coordination clusters where specific organic molecules act as chelating and coating agent simultaneously. For this function we have selected a pyrazolone-derivative.

Pyrazolones constitute a wide family of organic heterocyclic compounds that are very relevant because of chemical, biological and medicinal points of view. The tautomerism that they exhibit, their use in dyes, as derivatizing agents in carbohydrate analysis and also as chelating ligands are among the most appealing chemical points of these heterocycles. Concerning their biological/medicinal aspects, two illustrative examples are the analgesic antipyrine still in use in several countries and Edaravone<sup>®</sup>, a radical quencher that is used to treat brain ischemia.

Here we report the synthesis, crystal structure and magnetic properties of the complex [Gd<sub>5</sub>L<sub>11</sub>(μ<sub>3</sub>-O)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]-H<sub>2</sub>O where L = 1-hexyl-3-phenyl-4-nitroso-5-pyrazolone. This compound is formed by nanoparticles of ca. 3.5 nm diameter that are stable in solution, a situation that has been confirmed by AFM studies. The luminescence of the nanoparticles has also been characterized.

[1] M. Bottrill, L. Kwok, N.J. Long, *Chem. Soc. Rev.* **2006**, *35*, 557-571. [2] (a) J.S. Casas, M.S. García-Tasende, A. Sánchez, J. Sordo, A. Touceda, *Coord. Chem. Rev.* **2007**, *251*, 1561. (b) Y. Higashi, D. Jitsuiki, K. Chayama, M. Yoshizumi, *Recent Pat. Cardiovasc. Drug Discovery*, **2006**, *1*, 85. (c) H. Hammouda, *Arch. Pharm. Res.*, **1992**, *15*, 1.

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### Synthesis and structural characterization of [H<sub>3</sub>N(CH<sub>2</sub>)<sub>4</sub>NH<sub>3</sub>][Y(hedpH)][hedpH<sub>2</sub>]

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We have recently reported the synthesis and crystal structure of a family of [H<sub>3</sub>N(CH<sub>2</sub>)<sub>4</sub>NH<sub>3</sub>]<sub>n</sub>[Ln(hedpH)][hedpH<sub>2</sub>], with Ln = La, Pr, Sm, Eu, Gd, Tb and Er [1, 2].

These phosphonates are based on 1-hydroxyethane-1,1-diphosphonic acid [hedpH<sub>4</sub>, H<sub>2</sub>O<sub>3</sub>PC(OH)(CH<sub>3</sub>)PO<sub>3</sub>H<sub>2</sub>], which has been widely used as a strong chelating agent in the preparation of functional