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Cryomagnetic Studies of Isostructural Homometallic One-Dimensional Coordination Polymers Based on Lanthanide(III)-Oxamato complexes

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In the context of new technologies, it is essential to develop and explore new advanced multifunctional materials with magnetic properties to serve as potential candidates for assembling spin qubits in the field of quantum computing and spintronics.[1] Coordination polymers (CPs), which are compounds where the metal ions are coordinated to organic ligands as spacers, building extended structures of one (1D), bi- (2D), or three (3D) dimensionalities, can be potential candidates to materialize new advanced magnetic materials. Several ligands, such as cyanide, oxalate, and oxamate, for instance, can be used to design CPs and advanced inorganic materials.[2] This work concerns the synthesis and characterization of two new 1D coordination polymers containing the *N*-(4-methylphenyl)oxamate ligand[3] and neodymium (Nd^{3+}) and europium (Eu^{3+}) ions. They were characterized by infrared spectroscopy (IR), thermogravimetric analysis (TG), elemental analysis (C, H, N), and variable-temperature static (dc) and dynamic (ac) magnetic measurements. Single crystal X-ray diffraction was used to provide detailed insights into their crystalline structures, revealing that the Eu^{3+} and Nd^{3+} are isostructural homometallic isostructural zigzag chains. The Nd^{3+} derivative exhibits slow magnetic relaxation effects characteristic of field-induced SMMs below 15 K. Our results suggest that the complex containing Nd^{3+} ions can be considered a spin qubit candidate at low temperatures for quantum processing technologies.[3]

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References

[1] R. Marin, G. Brunet and M. Murugesu, *Angew. Chem. Int. Ed.*, **60**, 1728–1746 (2021).
[2] J. Ferrando-Soria, J. Vallejo, M. Castellano, J. Martínez-Lillo, E. Pardo, J. Cano, I. Castro, F. Lloret, F., R. Ruiz-García, M. Julve, *Coord. Chem. Rev.* **339**, 17–103 (2017).
[3] F. R. Fortea-Pérez, I. Schlegel, M. Julve, D. Armentano, G. De Munnob, S.-E. Stiriba, *J. Org. Chem.* **743,** 102–108 (2013).
[4] J. Wang, Y. Jing, M. Cui, Y. Lu, Z. Ouyang, C. Shao, Z. Wang, Y. Song, *Chem. Eur. J.* **29**, 66, e202301771 (2023).