Poster Presentation

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Synthesis, magneto-structural features and thermal behavior of a new MOF

K. Aliouane[1], B. Benmerad[2], N. Rahahlia[1], H. Kherfi[1], A. Guehria-Laïdoudi[1], S. Dahaoui[3], C. Lecomte[3]

[1]University of Algiers, USTHB, Faculty of Chemistry, Algiers, Algeria, [2]University of Bejaia, Department of Chemistry, Bejaia, Algeria, [3]University of Henri Poincaré, CRM-UPRESA 7036, Nancy, France

By applying soft synthesis conditions, in presence of a mixture that contains malonic acid, (3 mmol), lanthanide salt CeCl3.7H2O (1 mmol), alkaline-earth hydroxide Ca(OH)2 (1 mmol), and at pH below 4, we have obtained single crystals of a novel rare-earth complex which includes the dianion [L2-], {[Ce2(C3H2O4)3(H2O)3].2H2O}.The given formula was deduced from the single crystal structure analysis. The asymmetric unit corresponds to chemical formula (Figure 1). This novel polymeric compound is a three-dimensional MOF, built up from cross-linked infinite chains of one-edge-shared CeO7(H2O)3 and CeO9 polyhedrons embedding solvent molecules. Each crystallographically different metal is connected to two neighbouring ones, through four m2-oxo bridges, to form repeat four-membered typical Ce/O/Ce/O rings. The three independant ligands show different conformations of their end functional groups: syn-syn, syn-anti, anti-anti, giving explanation for the concomitant magnetic interactions and interesting magneto-structural data. These studies are still in progress. The TG curve shows five successive weight losses. The material begins losing weight directly upon starting the thermal gravimetric experiments. It is one of the more unstable lanthanide malonates known. The correlative thermal behaviour data and X-Ray structural sub-features of the novel Ce(III)-based MOF obtained, brought out the great supramolecular effects: decarboxylation process, crystalline, and thermal stabilities are much more related to the specific infinite hydrogen patterns, than the size, shape, and embedding capability of voids accommodated in the 3D packing.

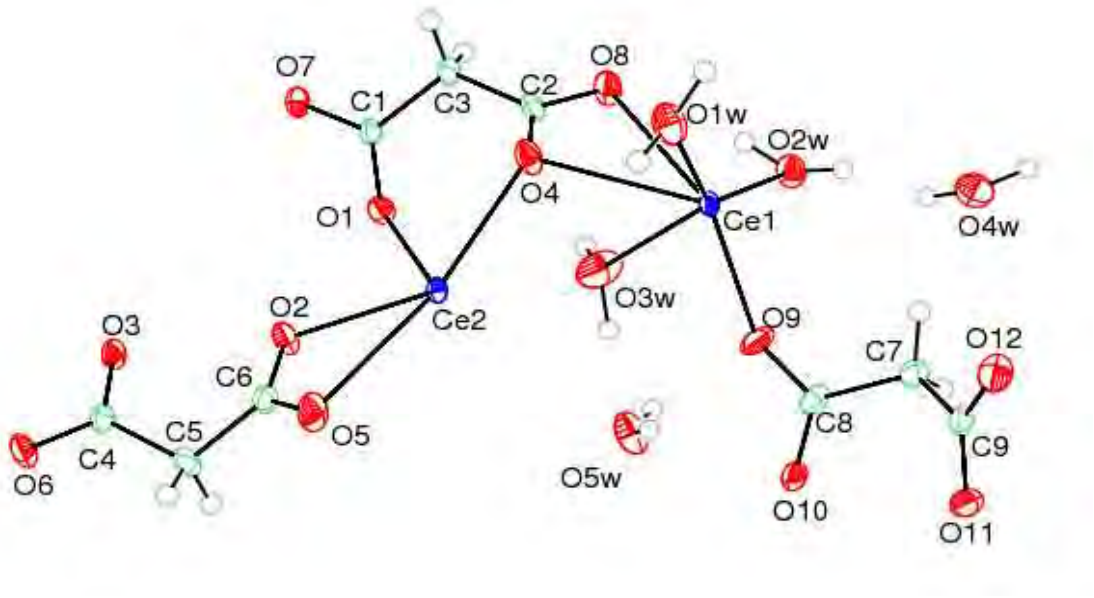

Fig.1: Asymmetric unit, including the labelling scheme at 50% probability displacement ellipsoids.

Keywords: coordination polymers, soft synthesis, thermal behavior