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Structural Characterisation of Heavy Lanthanide Oxalates Synthesized by Homogeneous Precipitation

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Metal oxalates are salts of very low solubility allowing an easy precipitation of metal ions from the acidic aqueous solutions into crystalline material. Due to this property, oxalates have an important role in the technology of lanthanides and actinides. It is namely the separation of actinides from the spent nuclear fuel that is its application of interest. 4f-lanthanides are often used as 5f-actinides surrogates when optimizing or modeling the precipitation process.

A synthetic route for homogeneous precipitation of oxalates based on the thermal decomposition of oxamic acid was developed, as published recently [1]. Further investigation about the structure and morphology of products of this reaction using six heaviest lanthanides (Dy, Ho, Er, Tm, Yb, Lu) was carried out. The products, developed microcrystals, were studied by means of solid-state analysis (X-ray crystallography, X-ray powder diffraction, TGA). New, previously undescribed structures of $\text{Er}_2(\text{C}_2\text{O}_4)_3 \cdot 3.7\text{H}_2\text{O}$, $\text{Tm}_2(\text{C}_2\text{O}_4)_3 \cdot 3.7\text{H}_2\text{O}$, and $\text{Lu}_2(\text{C}_2\text{O}_4)_3 \cdot 3.7\text{H}_2\text{O}$ were obtained. According to our observations, the synthesized oxalates form 2D framework structures that are stacked in one direction and connected by hydrogen bonds to form a 3D supramolecular structure. Each lanthanide atom is coordinated by three bidentate oxalates, two water molecules and weakly by one water molecule residing in a cavity. The cavities observed in the structure increase in size with decreasing atomic number of lanthanoid and are of great interest for its possible applications.

[1] A. Alemayehu, A. Zakharanka, & V. Tyrpekl, Homogeneous Precipitation of Lanthanide Oxalates. 7 (2022) 12288–12295. <https://doi.org/10.1021/acsomega.2c00763>.

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