

Poster Presentation

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Lanthanide Oxalates Under Pressure: Structural and Photoluminescence Properties

E. Spencer¹, K. Carter², C. Cahill², N. Ross¹

¹Virginia Tech, Department of Geosciences, Blacksburg, USA, ²George Washington University, Department of Chemistry, Washington, USA

Three dimensional lanthanide (Ln) framework compounds are renowned for their excellent photoluminescence properties, and there is growing interest in the development of this class of metal-organic framework (MOFs) materials for a diverse range of applications ranging from size-selective sensor technology to bio-imaging. Yet, although the physical and structural properties of Ln-MOFs under ambient conditions are well documented, there remains a distinct lack of information pertaining to the behaviour of these materials under non-ambient conditions. In this contribution we present both variable pressure (0–4 GPa) and temperature (100–300 K) single-crystal X-ray diffraction (XRD) studies of several Nd and Pr oxalate MOFs with different topologies (Fig. 1). Furthermore, these extensive XRD investigations have been complemented by variable pressure spectroscopic measurements that allow for evaluation of the influence of pressure on the photoluminescent emissions of these Ln-MOF compounds. This combined diffraction and spectroscopy study has enabled the structure-property relationships, which are so critical to the development of Ln-MOFs for practical usage, to be evaluated comprehensively. We will also show how the framework topology influences the structural behaviour of the Ln-MOF in response to pressure, resulting in the occurrence of unusual phenomena such as negative linear compression (NLC) in which one of the crystallographic axes expands, rather than contracts, with increasing pressure. Analysis of the high-pressure single-crystal XRD data has enabled the NLC mechanism to be elucidated and this will be presented.

[1] E.C. Spencer, J. Zhao, N. Ross, et al., *Solid State Chem.*, 202, 99-104 (2013), [2] M. Athar, A. M. Qureshi, G. Li, et al., *Chem.*, 51A, 708-713 (2012)

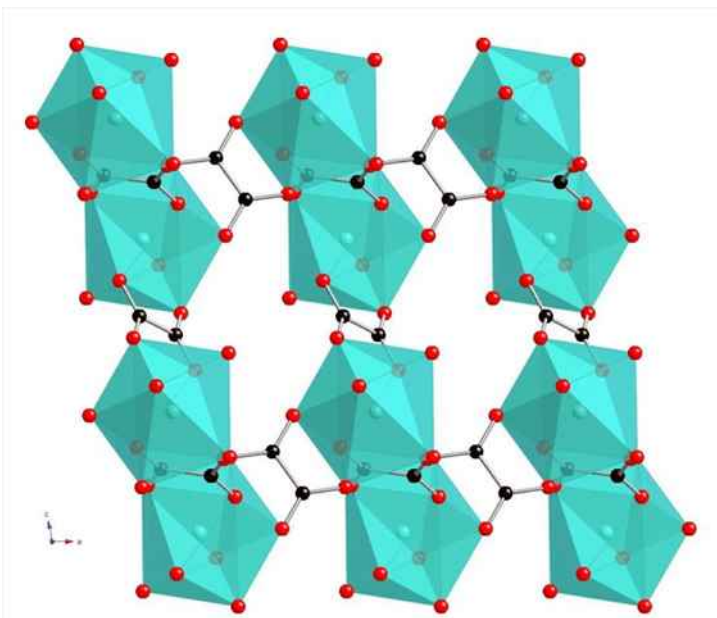


Figure 1. Nd-oxalate (triclincic form) as viewed along the [010] direction.

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