

A series of novel lanthanide carboxyphosphonates with a 3D framework structure using 1,4-benzenedicarboxylic acid as second metal linker: Synthesis, structure, and luminescent and magnetic properties

Kai Chen, Da-Peng Dong, Zhen-Gang Sun,* Cheng-Qi Jiao, Chao Li, Cheng-Lin Wang, Yan-Yu Zhu, Yan Zhao, Jiang Zhu, Shou-Hui Sun, Ming-Jing Zheng, Hui Tian, and Wei Chu

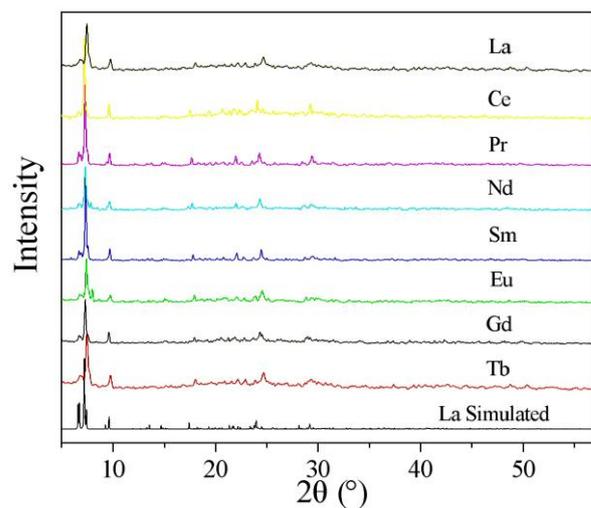


Fig. S1 The experimental powder XRD patterns of compounds **1–8** and the simulated XRD pattern of compound **1**.

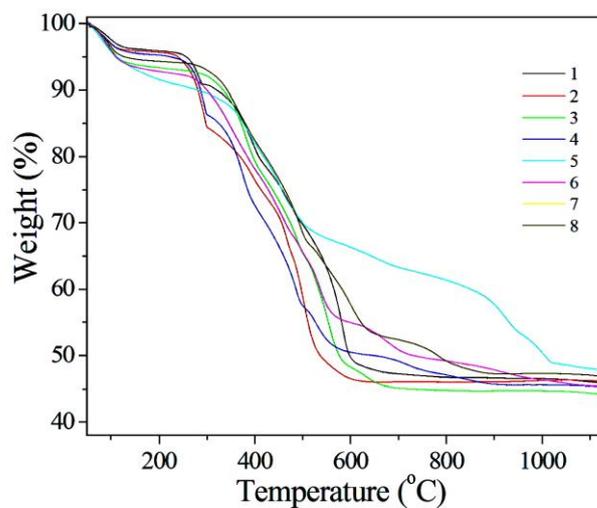


Fig. S2 The TGA curves of compounds **1–8**.

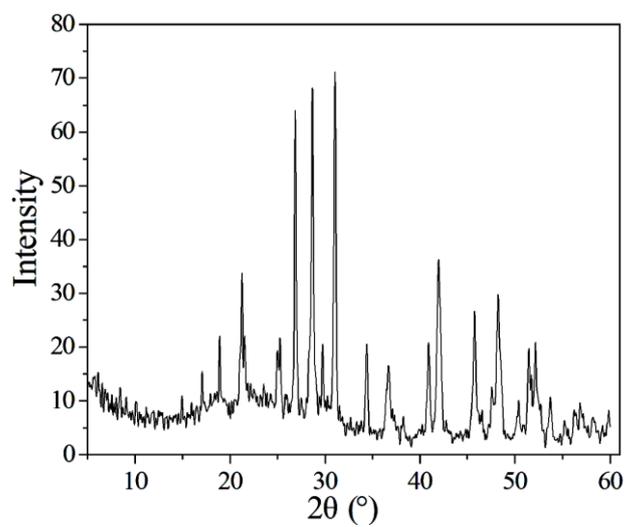


Fig. S3. The X-ray power diffraction patterns of the final product in the thermal decomposition for compound **1**.

The final product is LaPO_4 (JCPDS 01-084-0600)

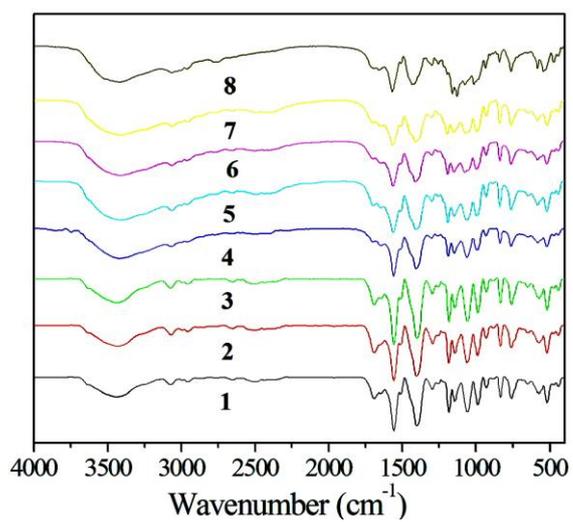


Fig. S4 The IR spectra of compounds **1–8**.

IR spectra

The IR spectra for compounds **1–8** are recorded in the region 4000–400 cm^{-1} (Fig. S4, ESI). The IR spectra of compounds **1–8** have many similar features corresponding to the common groups, thus only the spectrum of compound **1** will be discussed. The band is observed at 3442 cm^{-1} , which is due to the O–H stretching vibrations of the water molecules. The band centered at 3072 cm^{-1} corresponds to the stretching vibration of N–H. The C–H stretching vibrations are observed as sharp, weak bands close to 3000 cm^{-1} . There are two strong bands (1554 cm^{-1} and 1400 cm^{-1}) and two weak bands (1692 cm^{-1} and 1299 cm^{-1}), which are shifted from the expected value of uncoordinated carboxylic acids [$\nu(\text{C–O})$ typically around 1725–1700 cm^{-1}]. These shifts are due to the carboxylate function coordinated to the metal atom, and these bands are assigned to the asymmetric and symmetric stretching vibrations of C–O groups when present as COO^- moieties.¹ Strong bands between 1200 and 900 cm^{-1} is due to stretching vibrations of the tetrahedral $\{\text{CPO}_3\}$ groups, as expected.² Additional weak bands at low energy are found. These bands are probably due to bending vibrations of the tetrahedral $\{\text{CPO}_3\}$ groups.

Notes and references

- 1 A. Cabeza, M. A.-G. Aranda and S. Bruque, *J. Mater. Chem.*, 1998, **8**, 2479.
- 2 (a) A. Cabeza, X. Ouyang, C. V.-K. Sharma, M. A.-G. Aranda, S. Bruque and A. Clearfield, *Inorg. Chem.*, 2002, **41**, 2325. (b) Z.-M. Sun, J.-G. Mao, B.-P. Yang and S.-M. Ying, *Solid State Sci.*, 2004, **6**, 295.