

Supporting information

Homochiral 3D Lanthanide Camphorates with High Thermal Stability

Ming-Ling Sun,^a Xin Zhang,^a Yuan-Yuan Huang,^a Qi-Pu Lin,^a Ye-Yan Qin,^a and Yuan-Gen Yao^{*a}

^aKey Laboratory of Coal to Ethylene Glycol and Its Related Technology, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, 350002, People's Republic of China.

E-mail: yyg@fjirsm.ac.cn; Fax: +86-591-8371-4946; Tel: +86-591-8371-1523

Materials and Methods:

All reagents were purchased commercially and used without further purification. All syntheses were carried out in 23 mL poly(tetrafluoroethylene) lined stainless steel containers under autogenous pressure. Elemental analyses were performed on an EA1110 CHNS-0 CE elemental analyzer. FT-IR spectra were measured as KBr pellets on a Nicolet Magna 750 FT-IR spectrometer in the range of 400~4000 cm⁻¹. Thermal stability studies were carried out on a NETSCHZ STA-449C thermoanalyzer with a heating rate of 10 °C/min under nitrogen atmosphere. Powder X-ray diffraction (PXRD) analyses were recorded on a Rigaku Dmax2500 diffractometer with Cu K α radiation (λ = 1.54056 Å) with a step size of 0.05°. The temperature dependence of the magnetic susceptibilities were performed on a Quantum Design PPMS model 600 magnetometer in the temperature range 300 to 2 K with an applied field of 1 kOe. Single X-ray diffraction intensities of complexes **1**, **2** and **3** were collected on a Saturn 70 CCD diffractometer equipped with graphite monochromatic Mo-K α radiation (λ = 0.71073 Å) at 293(2) K. Empirical absorption corrections were applied to the data using the SADABS program.¹ The structures were solved by the direct method and refined by the full-matrix least-squares on F^2 using the SHELXTL-97 program.² All of the non-hydrogen atoms were refined anisotropically. Crystallographic data and

other pertinent information for **1**, **2** and **3** are summarized in CIFs. Due to somewhat flexibility of the D-cam and especially high thermal libration of its three terminal methyl groups, the restraints EADP, SIMU, DELU are applied for refinement in the cif of Er compound (**3**).

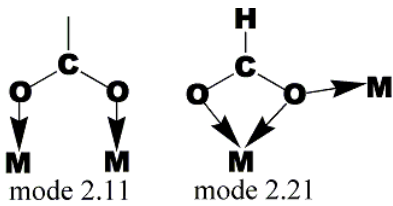
References

1. G. M. Sheldrick, *Program for Area Detector Adsorption Correction*, Institute for Inorganic Chemistry, University of Göttingen, Göttingen, Germany, 1996.
2. G. M. Sheldrick, *Program for Solution of Crystal Structures*, Institute for Inorganic Chemistry, University of Göttingen, Göttingen, Germany, 1997.

Table S1 Selected Bond Lengths (Å) for compounds **1-3**.

Bond	Dist.	Bond	Dist.	Bond	Dist.
Dy(1)-O(4)#1	2.226(5)	Ho(1)-O(4)#1	2.238(5)	Er(1)-O(4)#1	2.212(5)
Dy(1)-O(3)#2	2.245(5)	Ho(1)-O(2)#2	2.246(5)	Er(1)-O(3)#2	2.233(5)
Dy(1)-O(2)#3	2.245(4)	Ho(1)-O(3)#3	2.248(5)	Er(1)-O(2)#3	2.235(5)
Dy(1)-O(1)	2.249(4)	Ho(1)-O(1)	2.260(5)	Er(1)-O(1)	2.245(5)
Dy(1)-O(6)#3	2.337(4)	Ho(1)-O(6)#2	2.355(5)	Er(1)-O(6)#3	2.327(5)
Dy(1)-O(5)	2.416(5)	Ho(1)-O(5)	2.431(5)	Er(1)-O(5)	2.412(6)
Dy(1)-O(6)	2.462(4)	Ho(1)-O(6)	2.472(5)	Er(1)-O(6)	2.444(5)

Symmetry transformations used to generate equivalent atoms: for **1**: #1 -x,y+1/2,-z+1/2; #2: -x+1/2,-y+1,z-1/2; #3 x-1/2,-y+3/2,-z. for **2**: #1 -x+1, y-1/2, -z-1/2; #2 x+1/2, -y-3/2, -z-1; #3 -x+1/2,-y-1,z-1/2. for **3**: #1 -x-1, y-1/2, -z-3/2; #2 -x-1/2, -y-1, z+1/2; #3 x-1/2,-y-3/2,-z-1.



Scheme S1 coordination modes present in complex **1-3**. Mode 2.11 is for carboxylates of the D-cam ligand and mode 2.21 is for the formate group.

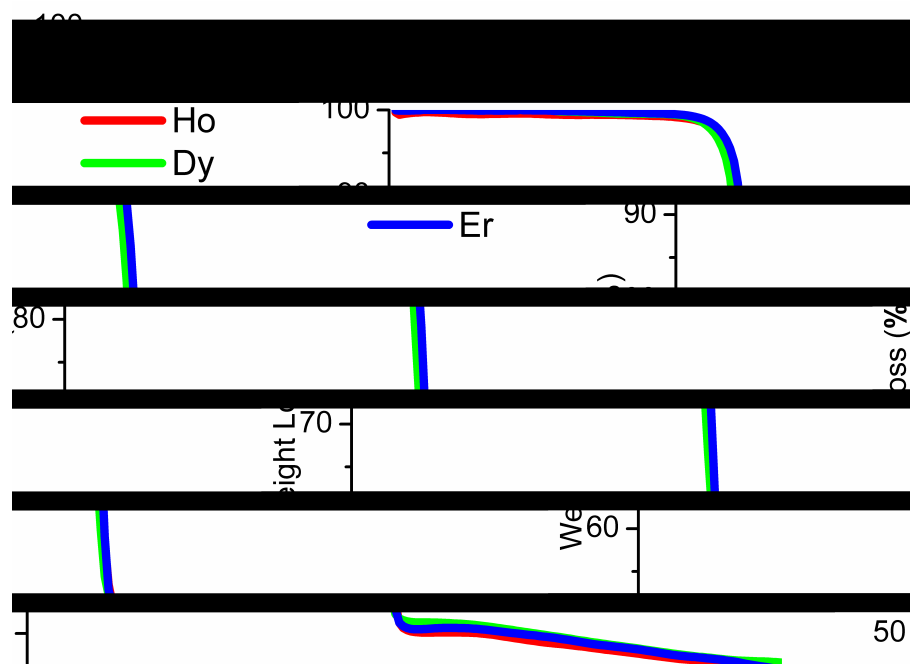


Fig. S1 TGA curves of 1-3. 1 (Dy); 2 (Ho); 3 (Er).

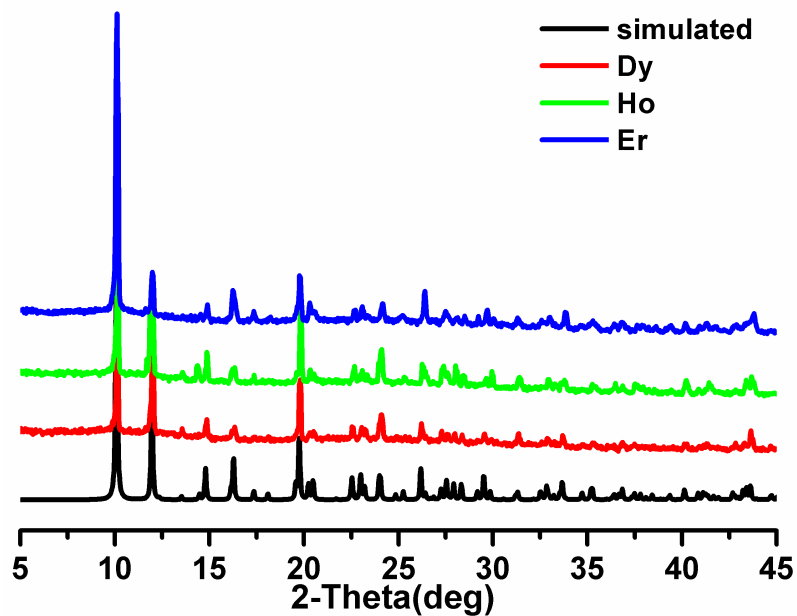


Fig. S2 Simulated and experimental PXRD patterns of 1-3 at 30 °C.

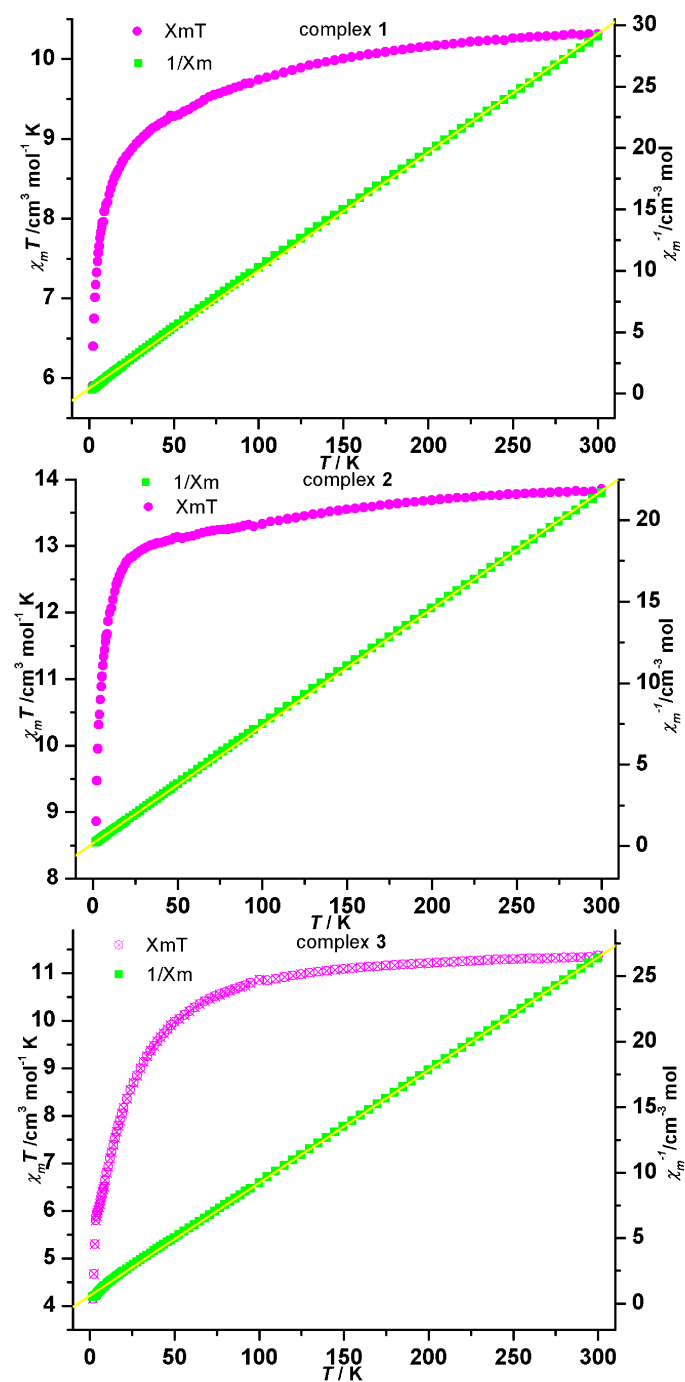


Fig.S3 Temperature dependence of $\chi_m T$ and χ_m^{-1} vs T for complexes 1-3. The solid yellow lines represent the best fit of the experimental data based on the theoretic model described Curie-Weiss law (for χ_m^{-1}).