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Data Article

# Structural data of structure variation and luminescence of 3D, 2D and 1D lanthanide coordination polymers with 1,3-adamantanediacetic acid



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## ARTICLE INFO

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### ABSTRACT

In this data article, we report the structure, Fourier transform infrared spectroscopy(FT-IR), powder X-ray diffraction (PARD), luminescence decay, thermogravimetric analysis (TGA) and UV-vis data of three series Ln-MOFs. Detailed structure and luminescence properties were discussed in our previous study (Zhao et al., 2018) [1]. The data includes the structure patterns of ligand H<sub>2</sub>ADA, FT-IR, PXRD and thermostability of Ln-MOFs in the air, detailed structure information for these structures are listed in Table 1–7.

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# Specifications table

Subject areaChemistryMore specific subject areaSingle crystal data of lanthanide complexesType of dataTable, figure

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1454	CH. Zeng et al. / Data in Brief 20 (2018) 1453–1461
How data was acquired	Crystallography open data base and crystallographic tool – Diamond:
Data format	Crystallographic Information File Code: 1562086–1562091 1574790.cif
Experimental factors	Single crystal X-ray diffraction data was collected on a Bruker SMART 1000
<b>r</b>	CCD at 293 K, with Mo-Ka radiation (0.71073 Å). The structure was refined
	by full-matrix least-squares methods with SHELXL-97 module. The three
	series structures crystalize in orthorhombic space group $Pna2_1$ (no. 33),
	triclinic space group P-1 (no. 2) and monoclinic space group P2(1)/n.
Experimental features	Block colorless single crystals.
Data source location	Jiangxi Normal University, Nanchang, China.
Data accessibility	The data are with this article.
Related research article	Zhi-Peng Zhao, <sup>a</sup> Kai Zheng, <sup>a</sup> Hao-Ran Li, <sup>a</sup> Cheng-Hui Zeng, <sup>a,b,d*</sup>
	Shengliang Zhong, <sup><i>a</i>*</sup> Seik Weng Ng, <sup><i>d</i></sup> Yanqiong Zheng, <sup><i>d</i></sup> Yun Chen <sup><i>a</i></sup> ,
	Structure Variation and Luminescence of 3D, 2D and 1D Lanthanide
	Coordination Polymers with 1,3-Adamantanediacetic Acid, Inorganica
	Chimica Acta, revised.

# Value of the data

- This data would be valuable for other properties studies of lanthanide complexes that based on 1,3-Adamantanediacetic Acid.
- This data would be valuable for synthesizing lanthanide complexes that coordinated by dmp.
- This data provide a new strategy to control the structure of lanthanide complexes.

## 1. Data

Three series of lanthanide coordination polymers (Ln-CPs) [1], 3D Ln-CPs  $[Tb_2(ADA)_3]_n$  (1a, H<sub>2</sub>ADA = 1,3-Adamantane-diacetic Acid), 2D Ln-CPs  $[Ln_2(ADA)_3(dmp)_2]_n \cdot 2EtOH \cdot H_2O$ ,  $(Ln^{3+} = Eu^{3+}, 2a; Gd^{3+}, 2b; Tb^{3+}, 2c; dmp = 4,7-dimethyl-1,10-phenanthroline), and 1D Ln-CPs <math>[Ln(ADA)(HADA)(H_2O)]_n$  (Ln<sup>3+</sup> = Eu<sup>3+</sup>, 3a; Gd<sup>3+</sup>, 3b; Tb<sup>3+</sup>, 3c), by using the ligand H<sub>2</sub>ADA (Fig. 1). The Ln-CPs are characterized by single-crystal X-ray diffraction, FT-IR (Figs. 2 and 3), PXRD (Figs. 4 and 5), TGA (Fig. 6) and UV-vis (Fig. 7). Detailed information about selected bord lengths and angles for 1a, 2a–2c and 3a–3c are listed in Tables 1–7, they show that the bond lengths and angles are in the normal value as known lanthanide complexes [2–7].



Fig. 1. Structure of the ligand H<sub>2</sub>ADA.



Fig. 2. FT-IR spectra of the ligand and 2a-2c.



Fig. 3. FT-IR spectra of the ligand, 3a and 3c.



Fig. 4. Experimental and calculated PXRD of 2a, 2b and 2c indicate phase purity of the as-synthesized samples.



Fig. 5. PXRD patterns of bulk samples 3a, 3b and 3c compete well with their simulated results of 3a, 3b and 3c, indicating the high phase purity of bulk samples 3a, 3b and 3c.



Fig. 6. a) TGA of 2D Ln-CPs 2a, 2b and 2c in the air atmosphere; b) TGA of 1D Ln-CPs of 3a and 3c in the air atmosphere.



Fig. 7. UV-vis spectrum of solid state sample H<sub>2</sub>ADA at room temperature.

Table 1						
Selected bond	lengths	and	bond	angles	of	1a.

Tb(1)-O(1)	2.248(6)	Tb(2)-O(2)	2.301(5)
Tb(1)-O(3)	2.263(6)	Tb(2)-O(4)	2.283(6)
Tb(1)-O(5)	2.267(5)	Tb(2)O(6)	2.260(5)
Tb(1)-O(7)	2.325(4)	Tb(2)-O(7)	2.551(4)
Tb(1)-O(9)	2.331(5)	Tb(2)-O(8)	2.432(5)
Tb(1)-O(11)	2.562(5)	Tb(2)-O(9)	2.547(5)
Tb(1)-O(12)	2.389(4)	Tb(2)-O(10)	2.414(5)
Tb(1)-Tb(2)	3.9029(5)	Tb(2)-O(11)	2.344(5)
O(1)-Tb(1)-O(3)	173.8(2)	O(6)-Tb(2)-O(10)	127.94(18)
O(1)-Tb(1)-O(5)	91.9(2)	O(4)-Tb(2)-O(10)	84.07(19)
O(3)-Tb(1)-O(5)	93.2(2)	O(2)-Tb(2)-O(10)	75.9(2)
O(1)-Tb(1)-O(7)	86.05(19)	O(11)-Tb(2)-O(10)	75.76(16)
O(3)-Tb(1)-O(7)	91.0(2)	O(6)-Tb(2)-O(8)	76.07(19)
O(5)-Tb(1)-O(7)	82.02(18)	O(4)-Tb(2)-O(8)	74.86(19)
O(1)-Tb(1)-O(9)	91.4(2)	O(2)-Tb(2)-O(8)	127.2(2)
O(3)-Tb(1)-O(9)	93.0(2)	O(11)-Tb(2)-O(8)	87.63(18)
O(5)-Tb(1)-O(9)	81.18(18)	O(10)-Tb(2)-O(8)	151.56(18)
O(7)-Tb(1)-O(9)	162.91(15)	O(6)-Tb(2)-O(9)	78.02(17)
O(1)-Tb(1)-O(12)	90.1(2)	O(4)-Tb(2)-O(9)	79.77(19)
O(3)-Tb(1)-O(12)	86.6(2)	O(2)-Tb(2)-O(9)	80.38(19)
O(5)-Tb(1)-O(12)	158.2(2)	O(11)-Tb(2)-O(9)	127.76(15)
O(7)-Tb(1)-O(12)	119.83(18)	O(10)-Tb(2)-O(9)	52.00(14)
O(9)-Tb(1)-O(12)	77.02(18)	O(8)-Tb(2)-O(9)	138.53(17)
O(1)-Tb(1)-O(11)	89.3(2)	O(6)-Tb(2)-O(7)	83.50(17)
O(3)-Tb(1)-O(11)	84.5(2)	O(4)-Tb(2)-O(7)	123.67(18)
O(5)-Tb(1)-O(11)	149.43(18)	O(2)-Tb(2)-O(7)	78.08(19)
O(7)-Tb(1)-O(11)	67.58(16)	O(11)-Tb(2)-O(7)	67.51(15)
O(9)-Tb(1)-O(11)	129.35(15)	O(10)-Tb(2)-O(7)	135.23(16)
O(12)-Tb(1)-O(11)	52.33(17)	O(8)-Tb(2)-O(7)	51.96(16)
O(1)-Tb(1)-Tb(2)	70.94(16)	O(9)-Tb(2)-O(7)	153.07(15)
O(3)-Tb(1)-Tb(2)	103.41(19)	O(6)-Tb(2)-Tb(1)	112.78(15)
O(5)-Tb(1)-Tb(2)	117.52(14)	O(4)-Tb(2)-Tb(1)	129.17(17)
O(7)-Tb(1)-Tb(2)	38.86(11)	O(2)-Tb(2)-Tb(1)	65.19(16)
O(9)-Tb(1)-Tb(2)	153.79(11)	O(11)-Tb(2)-Tb(1)	39.29(12)
O(12)-Tb(1)-Tb(2)	83.62(15)	O(10)-Tb(2)-Tb(1)	100.58(12)
O(11)-Tb(1)-Tb(2)	35.39(10)	O(8)-Tb(2)-Tb(1)	79.19(13)
O(6)-Tb(2)-O(4)	102.3(2)	O(9)-Tb(2)-Tb(1)	141.34(11)
O(6)-Tb(2)-O(2)	83.1(2)	O(7)-Tb(2)-Tb(1)	34.87(10)
O(4)-Tb(2)-O(2)	157.8(2)	O(4)-Tb(2)-O(11)	96.3(2)
O(6)-Tb(2)-O(11)	150.87(19)	O(2)-Tb(2)-O(11)	88.1(2)

# Table 2

Selected bond lengths and bond angles of **2a**.

Eu(1)-O(8)#1 Eu(1)-O(12)#2 Eu(1)-O(11)#3 Eu(1)-O(10) Eu(1)-O(7) Eu(1)-N(4) Eu(1)-O(9) Eu(1)-N(3) O(8)#1-Eu(1)-O(12)#2 O(8)#1-Eu(1)-O(11)#3 O(8)#1-Eu(1)-O(11)#3 O(8)#1-Eu(1)-O(10) O(12)#2-Eu(1)-O(10) O(12)#2-Eu(1)-O(10) O(12)#2-Eu(1)-O(10) O(12)#2-Eu(1)-O(7) O(12)#2-Eu(1)-O(7) O(12)#2-Eu(1)-O(7) O(11)#3-Eu(1)-O(7) O(11)#3-Eu(1)-N(4) O(12)#2-Eu(1)-N(4)	2.358(3) 2.381(3) 2.379(3) 2.427(3) 2.510(3) 2.558(4) 2.564(3) 2.652(4) 77.01(10) 74.13(10) 137.39(9) 88.56(11) 128.82(10) 81.14(10) 124.75(9) 80.55(10) 90.85(10) 142.24(11) 144.91(11) 80.22(11)	Eu(2)-O(6)#4 Eu(2)-O(1) Eu(2)-O(2)#4 Eu(2)-O(3)#5 Eu(2)-O(3)#5 Eu(2)-O(4)#5 Eu(2)-N(2) Eu(2)-N(1) Eu(1)-Eu(1)#1 O(4)#5-Eu(2)-N(1) N(2)-Eu(2)-N(1) O(1)-Eu(2)-O(3)#5 O(5)-Eu(2)-O(3)#5 O(5)-Eu(2)-O(4)#5 O(1)-Eu(2)-O(4)#5 O(2)#4-Eu(2)-O(4)#5 O(5)-Eu(2)-O(4)#5 O(3)#5-Eu(2)-O(4)#5 O(3)#5-Eu(2)-O(4)#5 O(6)#4-Eu(2)-N(2) O(1)-Eu(2)-N(2)=N(2) O(1)-Eu(2)-N(2)=N(2) O(1)-Eu(2)-N(2)=N(2) O(1)-Eu(2)-N(2)=N(2)	$\begin{array}{c} 2.328(3)\\ 2.337(3)\\ 2.344(3)\\ 2.365(3)\\ 2.449(3)\\ 2.516(3)\\ 2.606(4)\\ 2.607(4)\\ 3.9343(4)\\ 71.36(11)\\ 61.85(11)78.29(11)\\ 144.66(10)\\ 134.71(10)\\ 136.07(10)\\ 80.20(11)\\ 145.06(10)\\ 85.99(10)\\ 52.32(10)\\ 83.57(11)\\ 144.79(11)\\ 72.67(11)\\ \end{array}$
O(8) #1-Eu(1)-N(4) O(12) #2-Eu(1)-N(4) O(11) #3-Eu(1)-N(4)	144.91(11) 80.23(11) 138.26(11)	O(6)#3-Eu(2)-O(4)#3 O(6)#4-Eu(2)-N(2) O(1)-Eu(2)-N(2) O(2)#4-Eu(2)-N(2)	144.79(11) 77.67(11) 136.36(11)
-()(-)(-)		-(=)====(=) (1(=)	

O(10)-Eu(1)-N(4)	85.25(11)	O(5)-Eu(2)-N(2)	142.67(9)
O(7)-Eu(1)-N(4)	76.45(11)	O(8)-Eu(1)-O(9)	145.73(11)
O(8)#1-Eu(1)-O(8)	73.92(10)	O(8)#1-Eu(1)-N(3)	137.23(11)
O(12)#2-Eu(1)-O(8)	70.60(9)	O(12)#2-Eu(1)-N(3)	75.83(11)
O(11)#3-Eu(1)-O(8)	71.70(9)	O(11)#3-Eu(1)-N(3)	70.79(12)
O(10)-Eu(1)-O(8)	150.73(10)	O(10)-Eu(1)-N(3)	71.47(11)
O(7)-Eu(1)-O(8)	51.02(9)	O(7)-Eu(1)-N(3)	62.43(12)
N(4)-Eu(1)-O(8)	122.43(10)	N(4)-Eu(1)-N(3)	111.47(10)
O(8)#1-Eu(1)-O(9)	80.38(10)	O(8)-Eu(1)-N(3)	105.06(11)
O(12)#2-Eu(1)-O(9)	77.63(9)	O(9)-Eu(1)-N(3)	78.91(11)
O(11)#3-Eu(1)-O(9)	126.33(9)	O(6)#4-Eu(2)-O(1)	76.54(10)
O(10)-Eu(1)-O(9)	51.45(10)	O(6)#4-Eu(2)-O(2)#4	126.31(11)
O(7)-Eu(1)-O(9)	141.46(10)	O(1)-Eu(2)-O(2)#4	125.92(11)
N(4)-Eu(1)-O(9)	68.83(11)	O(6)#4-Eu(2)-O(5)	77.74(11)
O(2)#4-Eu(2)-O(5)	79.43(10)	O(1)-Eu(2)-O(5)	
O(6)#4-Eu(2)-O(3)#5	85.68(11)		

#### Table 2 (continued)

Symmetry transformations used to generate equivalent atoms: #1 -x+2, -y, -z+1; #2 x+1, y, z; #3 -x+1, -y, -z+1; #4 -x+2, -y-1, -z; #5 -x+3, -y-1, -z; #6 x-1, y, z.

# Table 3Selected bond lengths and bond angles of 2b.

Gd(1)-O(8)#1	2.341(3)	Gd(1)-Gd(1)#1	3.9190(3)
Gd(1)-O(12)#2	2.367(3)	Gd(2)-O(6)#4	2.320(3)
Gd(1)-O(11)#3	2.372(3)	Gd(2)-O(1)	2.326(3)
Gd(1)-O(10)	2.418(3)	Gd(2)-O(2)#4	2.332(3)
Gd(1)-O(7)	2.494(3)	Gd(2)-O(5)	2.348(3)
Gd(1)-N(1)	2.546(3)	Gd(2)-O(3)#5	2.440(3)
Gd(1)-O(8)	2.560(2)	Gd(2)-O(4)#5	2.504(3)
Gd(1)-O(9)	2.584(3)	Gd(2)-N(4)	2.591(3)
Gd(1)-N(2)	2.641(4)	Gd(2)-N(3)	2.610(3)
O(8)#1-Gd(1)-O(12)#2	74.36(9)	O(6)#4-Gd(2)-O(1)	78.93(10)
O(8)#1-Gd(1)-O(11)#3	77.01(9)	O(6)#4-Gd(2)-O(2)#4	76.77(10)
O(12)#2-Gd(1)-O(11)#3	137.46(8)	O(1)-Gd(2)-O(2)#4	126.07(10)
O(8)#1-Gd(1)-O(10)	88.69(10)	O(6)#4-Gd(2)-O(5)	125.63(11)
O(12)#2-Gd(1)-O(10)	81.10(9)	O(1)-Gd(2)-O(5)	77.43(10)
O(11)#3-Gd(1)-O(10)	129.04(10)	O(2)#4-Gd(2)-O(5)	79.05(10)
O(8)#1-Gd(1)-O(7)	124.92(8)	O(6)#4-Gd(2)-O(3)#5	85.25(10)
O(12)#2-Gd(1)-O(7)	90.75(9)	O(1)-Gd(2)-O(3)#5	78.23(10)
O(11)#3-Gd(1)-O(7)	80.56(10)	O(2)#4-Gd(2)-O(3)#5	144.87(10)
O(10)-Gd(1)-O(7)	141.94(10)	O(5)-Gd(2)-O(3)#5	135.05(9)
O(8)#1-Gd(1)-N(1)	144.54(11)	O(6)#4-Gd(2)-O(4)#5	135.86(10)
O(12)#2-Gd(1)-N(1)	138.45(11)	O(1)-Gd(2)-O(4)#5	80.13(10)
O(11)#3-Gd(1)-N(1)	79.90(10)	O(2)#4-Gd(2)-O(4)#5	145.12(10)
O(10)-Gd(1)-N(1)	85.31(10)	O(5)-Gd(2)-O(4)#5	86.32(10)
O(7)-Gd(1)-N(1)	76.44(10)	O(3)#5-Gd(2)-O(4)#5	52.53(10)
O(8)#1-Gd(1)-O(8)	73.91(10)	O(6)#4-Gd(2)-N(4)	83.38(10)
O(12)#2-Gd(1)-O(8)	71.58(8)	O(1)-Gd(2)-N(4)	144.84(11)
O(11)#3-Gd(1)-O(8)	70.66(8)	O(2)#4-Gd(2)-N(4)	77.88(10)
O(10)-Gd(1)-O(8)	150.61(9)	O(5)-Gd(2)-N(4)	136.72(10)
O(7)-Gd(1)-O(8)	51.21(8)	O(3)#5-Gd(2)-N(4)	70.17(10)
N(1)-Gd(1)-O(8)	122.49(9)	O(4)#5-Gd(2)-N(4)	92.22(10)
O(8)#1-Gd(1)-O(9)	80.14(9)	O(6)#4-Gd(2)-N(3)	138.83(10)
O(12)#2-Gd(1)-O(9)	126.29(9)	O(1)-Gd(2)-N(3)	142.21(10)
O(11)#3-Gd(1)-O(9)	77.71(9)	O(2)#4-Gd(2)-N(3)	74.53(10)
O(10)-Gd(1)-O(9)	51.55(9)	O(5)-Gd(2)-N(3)	76.55(10)
O(7)-Gd(1)-O(9)	141.57(9)	O(3)#5-Gd(2)-N(3)	102.01(10)
N(1)-Gd(1)-O(9)	68.83(10)	O(4)#5-Gd(2)-N(3)	71.31(10)
O(8)-Gd(1)-O(9)	142.65(9)	N(4)-Gd(2)-N(3)	62.23(10)
O(8)#1-Gd(1)-N(2)	146.01(10)	O(7)-Gd(1)-N(2)	71.20(10)
O(12)#2-Gd(1)-N(2)	75.87(10)	N(1)-Gd(1)-N(2)	62.57(11)
O(11)#3-Gd(1)-N(2)	136.95(10)	O(8)-Gd(1)-N(2)	111.41(10)

Symmetry transformations used to generate equivalent atoms: #1 - x + 1, -y + 2, -z; #2 - x + 2, -y + 2, -z; #3 x - 1, y, z; #4 - x + 1, -y + 3, -z + 1; #5 - x, -y + 3, -z + 1; #6 x + 1, y, z.

Table 4				
Selected bond ler	ngths and	bond	angles	of 2c.

Tb(1)-O(2)#1	2.335(2)	Tb(1)-Tb(1)#1	3.9023(3)
Tb(1)-O(6)#1	2.352(2)	Tb(2)-O(3)	2.300(3)
Tb(1)-O(5)	2.354(2)	Tb(2)-O(10)	2.310(3)
Tb(1)-O(7)#2	2.400(3)	Tb(2)-O(9)#3	2.313(2)
Tb(1)-O(1)	2.484(3)	Tb(2)-O(4)#3	2.337(3)
Tb(1)-N(1)	2.525(3)	Tb(2)-O(11)#4	2.425(3)
Tb(1)-O(2)	2.550(2)	Tb(2)-O(12)#4	2.492(3)
Tb(1)-O(8)#2	2.587(3)	Tb(2)-N(3)	2.583(3)
Tb(1)-N(2)	2.624(3)	Tb(2)-N(4)	2.590(3)
O(2)#1-Tb(1)-O(6)#1	74.52(9)	O(3)-Tb(2)-O(10)	79.03(10)
O(2)#1-Tb(1)-O(5)	77.01(9)	O(3)-Tb(2)-O(9)#3	77.05(9)
O(6)#1-Tb(1)-O(5)	137.73(8)	O(10)-Tb(2)-O(9)#3	125.97(10)
O(2)#1-Tb(1)-O(7)#2	88.32(10)	O(3)-Tb(2)-O(4)#3	125.84(10)
O(6)#1-Tb(1)-O(7)#2	80.97(9)	O(10)-Tb(2)-O(4)#3	77.41(10)
O(5)-Tb(1)-O(7)#2	128.74(9)	O(9)#3-Tb(2)-O(4)#3	78.78(9)
O(2)#1-Tb(1)-O(1)	125.17(8)	O(3)-Tb(2)-O(11)#4	84.63(10)
O(6)#1-Tb(1)-O(1)	91.05(9)	O(10)-Tb(2)-O(11)#4	78.30(10)
O(5)-Tb(1)-O(1)	80.51(9)	O(9)#3-Tb(2)-O(11)#4	144.78(9
O(7)#2-Tb(1)-O(1)	142.22(10)	O(4)#3-Tb(2)-O(11)#4	135.47(9)
O(2)#1-Tb(1)-N(1)	144.25(10)	O(3)-Tb(2)-O(12)#4	135.52(9)
O(6)#1-Tb(1)-N(1)	138.48(10)	O(10)-Tb(2)-O(12)#4	80.05(10)
O(5)-Tb(1)-N(1)	79.71(10)	O(9)#3-Tb(2)-O(12)#4	145.18(9)
O(7)#2-Tb(1)-N(1)	85.47(10)	O(4)#3-Tb(2)-O(12)#4	86.50(10)
O(1)-Tb(1)-N(1)	76.33(9)	O(11)#4-Tb(2)-O(12)#4	52.79(9)
O(2)#1-Tb(1)-O(2)	74.05(9)	O(3)-Tb(2)-N(3)	82.85(10)
O(6)#1-Tb(1)-O(2)	71.62(8)	O(10)-Tb(2)-N(3)	144.69(10)
O(5)-Tb(1)-O(2)	70.91(8)	O(9)#3-Tb(2)-N(3)	77.99(10)
O(7)#2-Tb(1)-O(2)	150.42(9)	O(4)#3-Tb(2)-N(3)	136.97(9)
O(1)-Tb(1)-O(2)	51.36(8)	O(11)#4-Tb(2)-N(3)	70.00(9)
N(1)-Tb(1)-O(2)	122.59(9)	O(12)#4-Tb(2)-N(3)	92.45(10)
O(2)#1-Tb(1)-O(8)#2	79.78(8)	O(3)-Tb(2)-N(4)	138.85(10)
O(6)#1-Tb(1)-O(8)#2	126.31(9)	O(10)-Tb(2)-N(4)	142.10(10)
O(5)-Tb(1)-O(8)#2	77.30(8)	O(9)#3-Tb(2)-N(4)	74.65(9)
O(7)#2-Tb(1)-O(8)#2	51.67(9)	O(4)#3-Tb(2)-N(4)	76.60(10)
O(1)-Tb(1)-O(8)#2	141.32(8)	O(11)#4-Tb(2)-N(4)	102.10(10)
N(1)-Tb(1)-O(8)#2	68.84(10)	O(12)#4-Tb(2)-N(4)	71.29(9)
O(2)-Tb(1)-O(8)#2	142.41(8)	N(3)-Tb(2)-N(4)	62.54(10)
O(2)#1-Tb(1)-N(2)	145.73(10)	N(1)-Tb(1)-N(2)	63.07(11)
O(6)#1-Tb(1)-N(2)	75.42(10)	O(2)-Tb(1)-N(2)	111.19(9)
O(5)-Tb(1)-N(2)	137.23(10)	O(8)#2-Tb(1)-N(2)	105.68(10)

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+2, -z; #2 x+1, y, z; #3 -x+1, -y+3, -z+1; #4 -x+2, -y+3, -z+1; #5 x-1, y, z.

#### 2. Experimental design, materials, and methods

Synthesis of **1a**: In a 250 mL Teflon-lined stainless-steel autoclave, 0.396 mmol  $H_2ADA$ , 0.594 mmol  $Tb(NO_3)_3 \cdot 6H_2O$  and 0.396 mmol 1,10-phenanthroline (phen) were mixed, then 100 mL  $H_2O$  added, and mixed by a magnetic stirrer. The reactants were sealed in the Teflon-lined stainless-steel autoclave and heated at 418 K for 6 days.

Synthesis of **2a–2c**: In a 50 mL beaker, 0.396 mmol H<sub>2</sub>ADA and 20 mL H<sub>2</sub>O were mixed, and the pH adjusted to 6 with 0.1 M NaOH solution. Then the solution was mixed with 20 mL MeOH solution containing 0.27 mmol Ln(NO<sub>3</sub>)<sub>3</sub> · 6H<sub>2</sub>O. After that, 0.269 mmol dmp dissolved in 20 mL EtOH solution was added to the mixture. Then it was transferred to a bottle and sealed, allowing the reaction to proceed at 333 K for 72 h.

Synthesis of **3a-3c**: In a 100 mL bottle, 0.396 mmol H<sub>2</sub>ADA was mixed with 0.13 mmol Ln  $(NO_3)_3 \cdot 6H_2O$ . 10 mL DMF and 50 mL H<sub>2</sub>O was added and stirred for 10 min. Then the bottle was sealed and reacted at 333 K for 72 h.

Table 5							
Selected	bond	lengths	and	bond	angles	of 3	a

Eu(1)-O(6)#1	2.296(3)	Eu(1)-O(2)	2.610(2)
Eu(1)-O(5)	2.370(2)	Eu(1)-Eu(1)#2	4.1260(3)
Eu(1)-O(2)#2	2.377(2)	Eu(1)-O(4)#1	2.488(2)
Eu(1)-O(9)	2.377(2)	Eu(1)-O(1)	2.421(2)
Eu(1)-O(3)#1	2.415(2)		
O(6)#1-Eu(1)-O(5)	98.94(9)	O(3)#1-Eu(1)-O(1)	155.20(8)
O(6)#1-Eu(1)-O(2)#2	165.00(9)	O(6)#1-Eu(1)-O(4)#1	78.02(9)
O(5)-Eu(1)-O(2)#2	80.39(8)	O(5)-Eu(1)-O(4)#1	134.42(8)
O(6)#1-Eu(1)-O(9)	108.01(9)	O(2)#2-Eu(1)-O(4)#1	91.69(8)
O(5)-Eu(1)-O(9)	145.34(8)	O(9)-Eu(1)-O(4)#1	73.82(7)
O(2)#2-Eu(1)-O(9)	78.98(8)	O(3)#1-Eu(1)-O(4)#1	53.17(8)
O(6)#1-Eu(1)-O(3)#1	84.76(9)	O(1)-Eu(1)-O(4)#1	133.18(8)
O(5)-Eu(1)-O(3)#1	81.27(8)	O(6)#1-Eu(1)-O(2)	125.99(8)
O(2)#2-Eu(1)-O(3)#1	80.32(8)	O(5)-Eu(1)-O(2)	73.93(7)
O(9)-Eu(1)-O(3)#1	121.82(8)	O(2)#2-Eu(1)-O(2)	68.44(8)
O(6)#1-Eu(1)-O(1)	75.15(9)	O(9)-Eu(1)-O(2)	72.69(7)
O(5)-Eu(1)-O(1)	87.55(8)	O(3)#1-Eu(1)-O(2)	142.62(8)
O(2)#2-Eu(1)-O(1)	119.66(8)	O(1)-Eu(1)-O(2)	51.47(7)
O(9)-Eu(1)-O(1)	78.96(8)	O(4)#1-Eu(1)-O(2)	143.66(7)

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

### Table 6

Selected bond lengths and bond angles of 3b.

Gd(1)-O(6)#1	2.2839(19)	Gd(1)-O(3)#1	2.409(2)
Gd(1)-O(5)	2.3557(18)	Gd(1)-O(2)	2.4734(19)
Gd(1)-O(4)#2	2.3658(17)	Gd(1)-O(4)#1	2.5959(18)
Gd(1)-O(1W)	2.3641(18)	Gd(1)-O(1)	2.4069(19)
O(6)#1-Gd(1)-O(5)	98.54(7)	O(1)-Gd(1)-O(3)#1	154.83(7)
O(6)#1-Gd(1)-O(4)#2	164.99(7)	O(6)#1-Gd(1)-O(2)	77.98(7)
O(5)-Gd(1)-O(4)#2	80.77(6)	O(5)-Gd(1)-O(2)	134.30(6)
O(6)#1-Gd(1)-O(1W)	108.48(7)	O(4)#2-Gd(1)-O(2)	91.70(7)
O(5)-Gd(1)-O(1W)	145.49(6)	O(1W)-Gd(1)-O(2)	73.75(6)
O(4)#2-Gd(1)-O(1W)	78.44(7)	O(1)-Gd(1)-O(2)	53.36(6)
O(6)#1-Gd(1)-O(1)	84.59(7)	O(3)#1-Gd(1)-O(2)	133.25(7)
O(5)-Gd(1)-O(1)	80.96(7)	O(6)#1-Gd(1)-O(4)#1	126.04(6)
O(4)#2-Gd(1)-O(1)	80.48(6)	O(5)-Gd(1)-O(4)#1	74.01(6)
O(1W)-Gd(1)-O(1)	121.79(7)	O(4)#2-Gd(1)-O(4)#1	68.38(7)
O(6)#1-Gd(1)-O(3)#1	75.13(7)	O(1W)-Gd(1)-O(4)#1	72.83(6)
O(5)-Gd(1)-O(3)#1	87.38(7)	O(1)-Gd(1)-O(4)#1	142.47(6)
O(4)#2-Gd(1)-O(3)#1	119.69(6)	O(3)#1-Gd(1)-O(4)#1	51.55(6)
O(1W)-Gd(1)-O(3)#1	79.49(7)	O(2)-Gd(1)-O(4)#1	143.82(6)

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

The lanthanide salts were obtained by the procedures as our previous work [8–13].  $H_2ADA$  (97.0%) was purchased from Innochem (Beijing, China) and used without any purification. Other chemicals (A.R.) are commercially available and were used as received.

Single crystal X-ray diffraction data was collected on a Bruker SMART 1000 CCD, with Mo-Ka radiation (Wavelength = 0.71073 Å) at room temperature. The structure was refined by full-matrix least-squares methods with SHELXL-97 module. FT-IR was obtained in KBr pellets and recorded on a Nicolet 330 FT-IR spectrometer. TGA was recorded on a Netzsch-Bruker TG-209 unit in the air atmosphere. Luminescence spectra and lifetimes were recorded on an Edinburgh FLS980 at room temperature. Phase purity of bulk sample was determined on a DMAX2200VPC diffractometer, at 30 kV and 30 mA.

Tb(1)-O(2)#1	2.266(2)	Tb(1)-O(6)#3	2.394(2)
Tb(1)-O(0AA)	2.3371(19)	Tb(1)-O(8)#2	2.461(2)
Tb(1)-O(5)	2.3472(19)	Tb(1)-O(5)#3	2.597(2)
Tb(1)-O(1W)	2.3457(19)	Tb(1)-O(7)#2	2.390(2)
O(2)#1-Tb(1)-O(0AA)	98.14(8)	O(1W)-Tb(1)-O(6)#3	79.64(8)
O(2)#1-Tb(1)-O(5)	164.70(8)	O(7)#2-Tb(1)-O(6)#3	154.51(7)
O(0AA)-Tb(1)-O(5)	80.94(7)	O(2)#1-Tb(1)-O(8)#2	78.02(8)
O(2)#1-Tb(1)-O(1W)	108.68(8)	O(0AA)-Tb(1)-O(8)#2	134.32(7)
O(0AA)-Tb(1)-O(1W)	145.71(7)	O(5)-Tb(1)-O(8)#2	91.64(7)
O(5)-Tb(1)-O(1W)	78.56(7)	O(1W)-Tb(1)-O(8)#2	73.65(7)
O(2)#1-Tb(1)-O(7)#2	84.43(8)	O(7)#2-Tb(1)-O(8)#2	53.75(7)
O(0AA)-Tb(1)-O(7)#2	80.60(7)	O(6)#3-Tb(1)-O(8)#2	133.26(7)
O(5)-Tb(1)-O(7)#2	80.35(7)	O(2)#1-Tb(1)-O(5)#3	126.18(7)
O(1W)-Tb(1)-O(7)#2	122.08(7)	O(0AA)-Tb(1)-O(5)#3	74.32(6)
O(2)#1-Tb(1)-O(6)#3	75.17(8)	O(5)-Tb(1)-O(5)#3	68.47(8)
O(0AA)-Tb(1)-O(6)#3	87.23(7)	O(1W)-Tb(1)-O(5)#3	72.69(7)
O(5)-Tb(1)-O(6)#3	119.88(7)	O(7)#2-Tb(1)-O(5)#3	142.37(7)

Table 7 Selected bond lengths and bond angles of 3c.

Symmetry transformations used to generate equivalent atoms: #1 - x + 1, -y + 1, -z; #2 x + 1, y, z; #3 - x, -y + 1, -z; #4 x - 1, y, z.

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#### **Transparency document.** Supplementary material

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