Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

A series of three-dimensional (3D) chiral lanthanide coordination polymers generated by spontaneous resolution

Li-Min Zhang, Da-Yi Deng, Guo Peng, Lin Sun, Li Liang, Guo-Qiang Lan, Hong Deng*

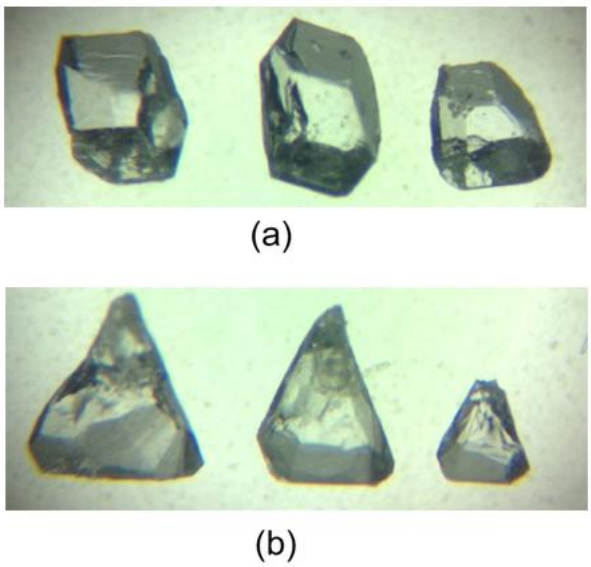

Fig. S1 Morphologies of the single crystals of **4a** (a) and **4b** (b).

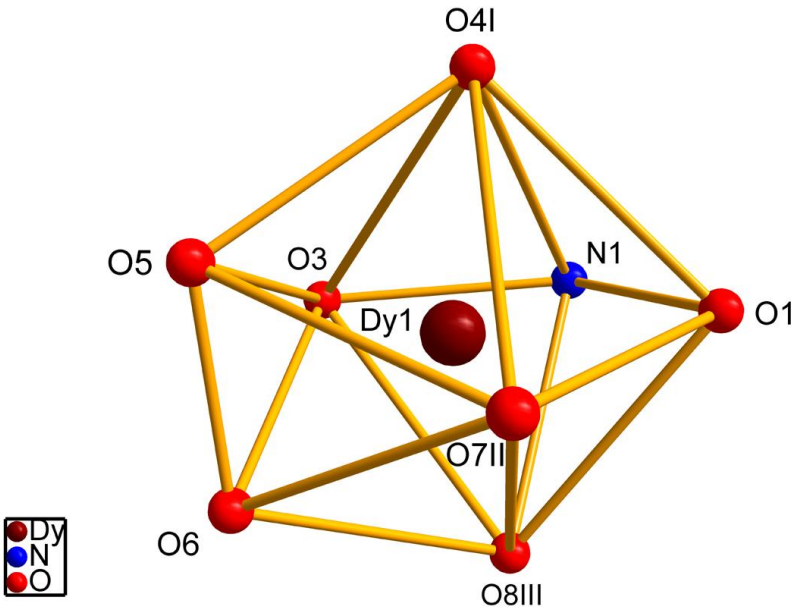

Fig. S2 The eight-coordinated dodecahedron geometry of Dy(III) center. Symmetry codes: I (0.5+*x*, 0.5-*y*, 2-*z*); II (1-*x*, 0.5+*y*, 1.5-*z*); III (1+*x*, *y*, *z*).

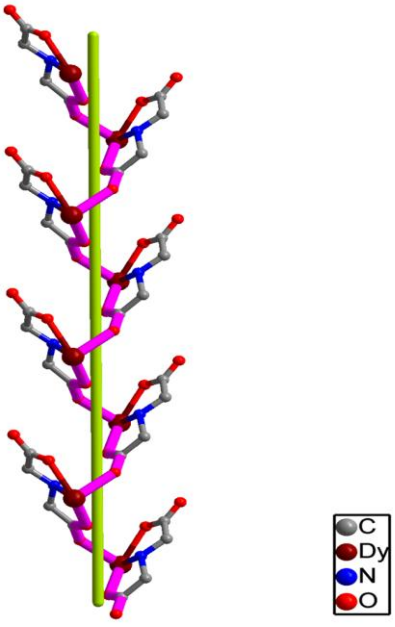

Fig. S3 The right-handed helix running parallel to *a*-axis in **4b.**

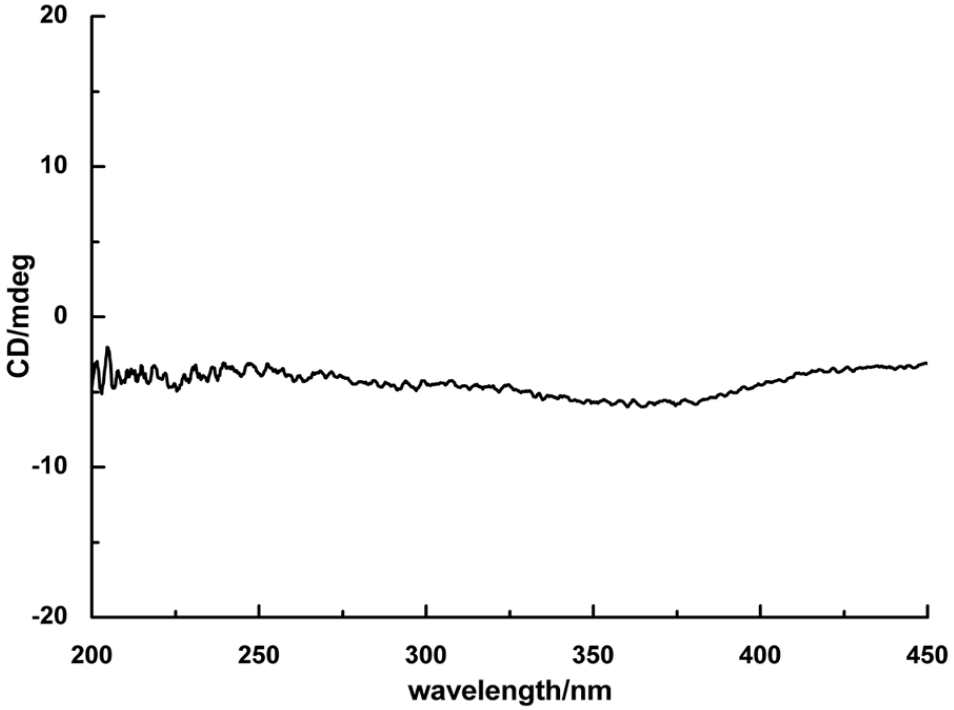

Fig. S4 The CD spectra of bulk sample of **4**.

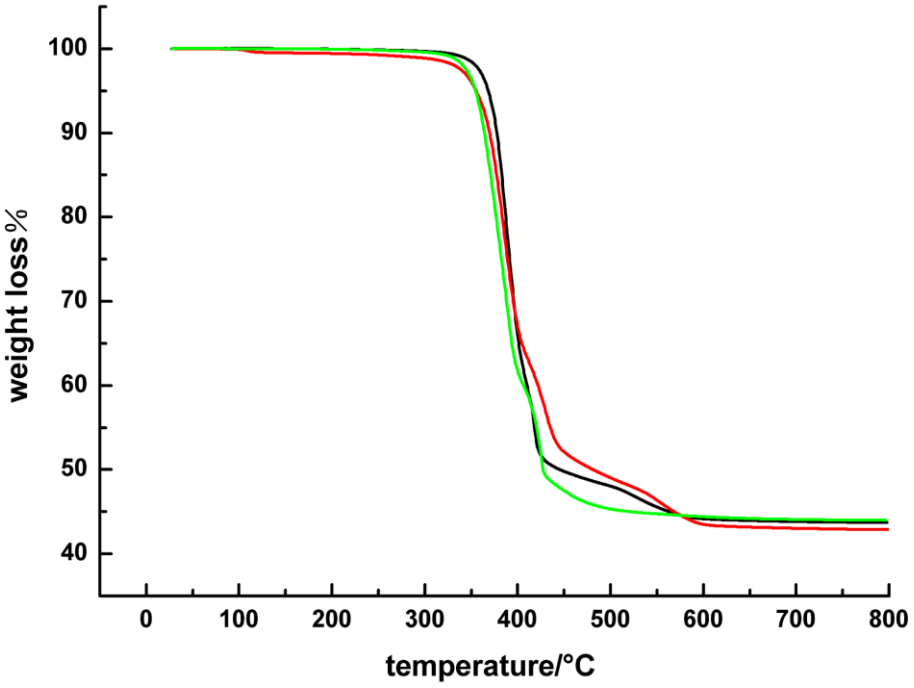

Fig. S5 The TG curve of **2** (red), **3** (green)**, 4** (black)**.**

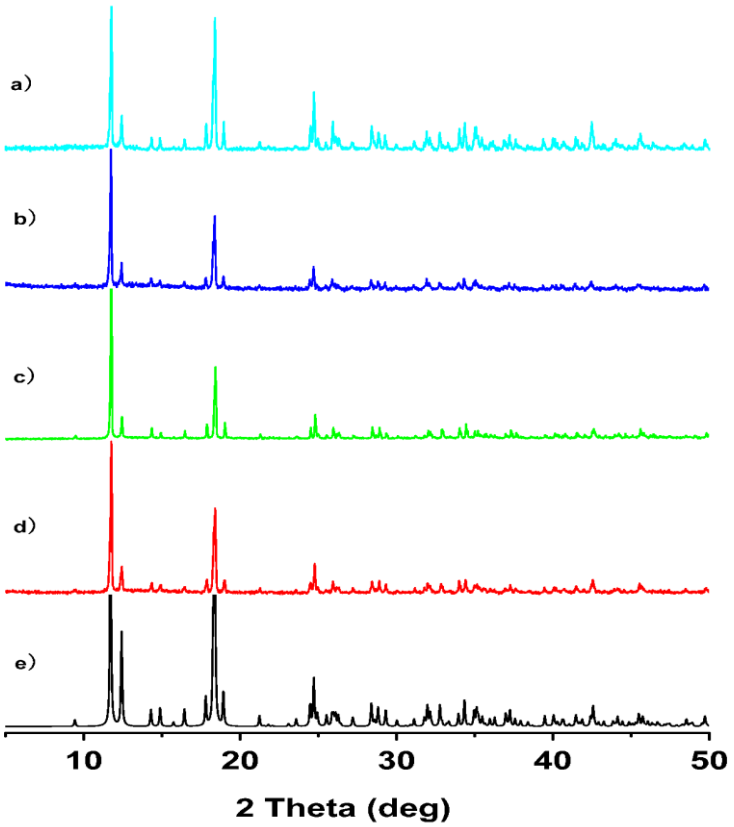

Fig. S6 PXRD patterns (a) for as-synthesized **1**, (b) for as-synthesized **2**, (c) for as-synthesized **3**, (d) for as-synthesized **4**, (e) stimulated based on the X-ray single-crystal diffraction data of **4**.

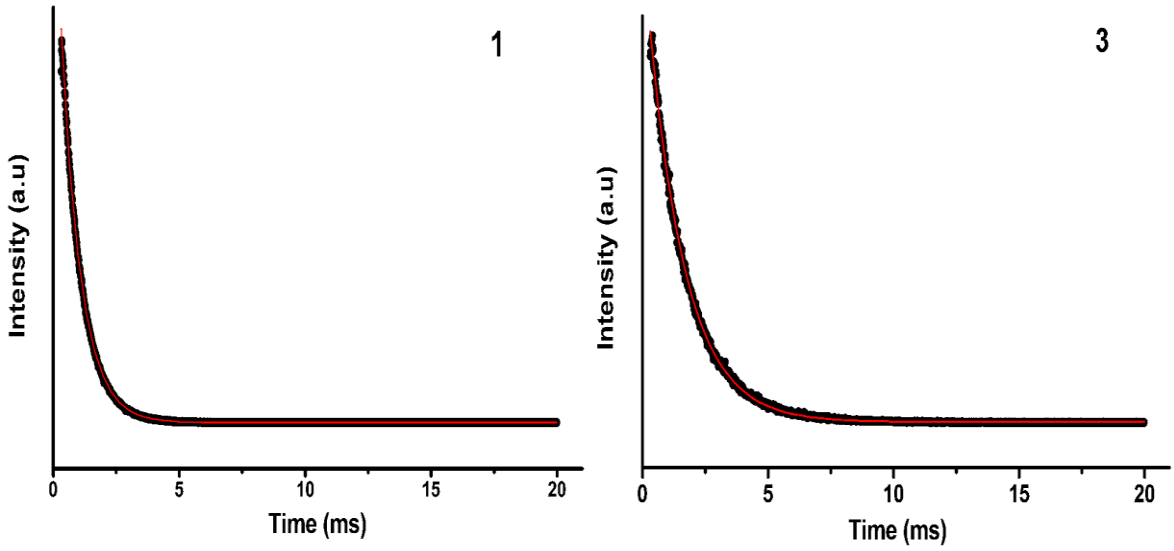

Fig. S7 View of the luminescent decay curves for compounds **1** and **3**. The red lines represent the fitting curves and the black lines are the raw

experimental curves.

Table S1 Selected Bond angels (°) for complexes **1**-**4**. Symmetry transformations used to generate equivalent atoms are given as footnotes.

Compound 1 [a]			
O(8)#2-Eu(1)-O(4)#3	160.44(16)	O(8)#2-Eu(1)-O(3)	89.74(16)
O(4)#3-Eu(1)-O(3)	94.05(18)	O(8)#2-Eu(1)-O(7)	93.39(16)
O(4)#3-Eu(1)-O(7)	91.29(18)	O(3)-Eu(1)-O(5)	80.62(17)
O(3)-Eu(1)-O(7)	154.86(16)	O(7)-Eu(1)-O(5)	77.11(18)
O(8)#2-Eu(1)-O(1)	82.79(17)	O(1)-Eu(1)-O(5)	141.85(18)
O(4)#3-Eu(1)-O(1)	80.08(17)	O(8)#2-Eu(1)-O(6)	72.68(15)
O(3)-Eu(1)-O(1)	129.94(15)	O(4)#3-Eu(1)-O(6)	126.87(16)
O(7)-Eu(1)-O(1)	75.19(15)	O(3)-Eu(1)-O(6)	79.92(15)
O(7)-Eu(1)-O(6)	77.25(16)	O(5)-Eu(1)-O(6)	52.05(15)
O(8)#2-Eu(1)-N(1)	78.22(17)	O(1)-Eu(1)-O(6)	141.60(14)
O(4)#3-Eu(1)-N(1)	86.03(16)	O(3)-Eu(1)-N(1)	64.91(15)
O(7)-Eu(1)-N(1)	140.07(17)	O(1)-Eu(1)-N(1)	65.10(15)
O(5)-Eu(1)-N(1)	139.20(16)	O(6)-Eu(1)-N(1)	133.98(16)
O(8)#2-Eu(1)-O(5)	124.72(15)	O(4)#3-Eu(1)-O(5)	74.84(15)
Compound 2 [b]			
O(7)#1-Gd(1)-O(2)#2	160.37(10)	O(3)-Gd(1)-O(5)	140.84(12)

O(7)#1-Gd(1)-O(1)	90.29(10)	O(1)-Gd(1)-O(6)	79.85(10)
O(2)#2-Gd(1)-O(1)	93.34(11)	O(8)#3-Gd(1)-O(6)	76.76(10)
O(7)#1-Gd(1)-O(8)#3	92.98(11)	O(3)-Gd(1)-O(6)	141.50(10)
O(2)#2-Gd(1)-O(8)#3	92.08(12)	O(5)-Gd(1)-O(6)	52.37(10)
O(1)-Gd(1)-O(8)#3	154.28(11)	O(7)#1-Gd(1)-N(1)	78.31(11)
O(7)#1-Gd(1)-O(3)	82.84(11)	O(2)#2-Gd(1)-N(1)	85.74(11)
O(2)#2-Gd(1)-O(3)	80.18(11)	O(1)-Gd(1)-N(1)	65.13(10)
O(1)-Gd(1)-O(3)	130.67(10)	O(8)#3-Gd(1)-N(1)	140.43(11)
O(8)#3-Gd(1)-O(3)	75.04(10)	O(3)-Gd(1)-N(1)	65.64(10)
O(7)#1-Gd(1)-O(5)	125.34(10)	O(5)-Gd(1)-N(1)	139.15(10)
O(2)#2-Gd(1)-O(5)	74.28(10)	O(6)-Gd(1)-N(1)	134.12(11)
O(1)-Gd(1)-O(5)	80.60(11)	O(7)#1-Gd(1)-O(6)	72.98(10)
O(8)#3-Gd(1)-O(5)	76.72(11)	O(2)#2-Gd(1)-O(6)	126.65(10)
Compound 3 [c]			
O(8)#2-Tb(1)-O(4)#3	160.00(16)	O(1)-Tb(1)-O(6)	141.58(16)
O(8)#2-Tb(1)-O(7)#4	92.81(18)	O(8)#2-Tb(1)-N(1)	78.28(18)
O(4)#3-Tb(1)-O(3)	93.23(19)	O(4)#3-Tb(1)-N(1)	85.28(18)
O(7)#4-Tb(1)-O(3)	153.61(18)	O(7)#4-Tb(1)-N(1)	140.53(19)
O(8)#2-Tb(1)-O(1)	82.69(17)	O(3)-Tb(1)-N(1)	65.66(17)
O(4)#3-Tb(1)-O(1)	80.19(17)	O(3)-Tb(1)-O(6)	79.22(17)
O(7)#4-Tb(1)-O(1)	75.08(17)	O(5)-Tb(1)-N(1)	138.72(17)
O(3)-Tb(1)-O(1)	131.29(16)	O(6)-Tb(1)-N(1)	134.17(18)
O(8)#2-Tb(1)-O(5)	125.98(17)	O(1)-Tb(1)-N(1)	65.71(16)
O(4)#3-Tb(1)-O(5)	74.01(17)	O(7)#4-Tb(1)-O(6)	76.64(18)
O(3)-Tb(1)-O(5)	80.03(17)	O(8)#2-Tb(1)-O(6)	73.25(16)
O(1)-Tb(1)-O(5)	140.63(19)	O(5)-Tb(1)-O(6)	52.74(17)
O(4)#3-Tb(1)-O(7)#4	92.71(19)	O(8)#2-Tb(1)-O(3)	90.31(17)
O(7)#4-Tb(1)-O(5)	76.96(19)	O(4)#3-Tb(1)-O(6)	126.75(17)
Compound 4a [d]			
O(7)#1-Dy(1)-O(4)#2	159.83(12)	O(6)-Dy(1)-N(1)	134.08(12)
O(7)#1-Dy(1)-O(3)	90.14(13)	O(1)-Dy(1)-N(1)	65.90(12)
O(4)#2-Dy(1)-O(3)	93.42(14)	O(8)#3-Dy(1)-N(1)	140.84(13)
O(7)#1-Dy(1)-O(8)#3	92.98(13)	O(3)-Dy(1)-N(1)	65.85(12)
O(4)#2-Dy(1)-O(8)#3	92.78(13)	O(4)#2-Dy(1)-N(1)	85.30(13)
O(3)-Dy(1)-O(8)#3	153.08(13)	O(7)#1-Dy(1)-N(1)	78.06(13)
O(7)#1-Dy(1)-O(1)	82.90(12)	O(6)-Dy(1)-O(5)	52.77(12)
O(4)#2-Dy(1)-O(1)	79.91(12)	O(1)-Dy(1)-O(5)	140.22(13)
O(3)-Dy(1)-O(1)	131.66(12)	O(8)#3-Dy(1)-O(5)	76.61(13)
O(8)#3-Dy(1)-O(1)	75.24(12)	O(3)-Dy(1)-O(5)	80.00(13)
O(7)#1-Dy(1)-O(6)	73.44(11)	O(4)#2-Dy(1)-O(5)	73.96(12)
O(4)#2-Dy(1)-O(6)	126.73(12)	O(7)#1-Dy(1)-O(5)	126.20(12)
O(3)-Dy(1)-O(6)	78.86(12)	O(1)-Dy(1)-O(6)	141.76(12)
O(8)#3-Dy(1)-O(6)	76.45(12)	O(5)-Dy(1)-N(1)	138.77(13)
Compound 4b [e]			

O(7)#1-Dy(1)-O(4)#2	160.1(3)	O(7)#1-Dy(1)-O(8)#3	92.6(3)
O(4)#2-Dy(1)-O(8)#3	92.7(3)	O(7)#1-Dy(1)-O(3)	90.5(3)
O(4)#2-Dy(1)-O(3)	93.4(3)	O(8)#3-Dy(1)-O(3)	153.3(3)
O(7)#1-Dy(1)-O(1)	82.8(3)	O(4)#2-Dy(1)-O(1)	80.1(3)
O(8)#3-Dy(1)-O(1)	74.7(3)	O(3)-Dy(1)-O(1)	131.9(2)
O(7)#1-Dy(1)-O(5)	126.0(3)	O(4)#2-Dy(1)-O(5)	73.9(3)
O(8)#3-Dy(1)-O(5)	76.6(3)	O(3)-Dy(1)-O(5)	80.2(3)
O(1)-Dy(1)-O(5)	139.9(3)	O(7)#1-Dy(1)-O(6)	73.1(2)
O(4)#2-Dy(1)-O(6)	126.8(3)	O(8)#3-Dy(1)-O(6)	76.4(3)
O(3)-Dy(1)-O(6)	79.2(3)	O(1)-Dy(1)-O(6)	141.2(2)
O(5)-Dy(1)-O(6)	52.9(3)	O(7)#1-Dy(1)-N(1)	78.4(3)
O(4)#2-Dy(1)-N(1)	85.3(3)	O(8)#3-Dy(1)-N(1)	140.6(3)
O(3)-Dy(1)-N(1)	65.8(2)	O(1)-Dy(1)-N(1)	66.1(2)
O(5)-Dy(1)-N(1)	138.9(3)	O(6)-Dy(1)-N(1)	134.3(3)

[a] #1: -x+1,y+1/2,-z+3/2; #2: x+1/2,-y+1/2,-z+2; #3: x+1,y,z; #4: x-1/2,-y+1/2,-z+2; #5: x-1,y,z; #6: -x+1,y-1/2,-z+3/2; [b] #1: -x+1,y+1/2,-z+1/2; #2: x-1/2,-y+3/2,-z; #3: x-1,y,z; #4: x+1/2,-y+3/2,-z; #5: -x+1,y-1/2,-z+1/2; #6: x+1,y,z; [c] #1: x-1/2,-y+1/2,-z; #2: -x,y-1/2,-z+1/2; #3: x+1/2,-y+1/2,-z; #4: x+1,y,z; #5: -x,y+1/2,-z+1/2; #6: x-1,y,z; [d] #1: -x+1,y+1/2,-z+3/2; #2: x+1/2,-y+1/2,-z+2; #3: x+1,y,z; #4: x-1/2,-y+1/2,-z+2; #5: -x+1,y-1/2,-z+3/2; #6: x-1,y,z; [e] #1: -x+1,y-1/2,-z+1/2; #2: x-1/2,-y+3/2,-z; #3: x-1,y,z; #4: x+1/2,-y+3/2,-z; #5: x+1,y,z; #6: -x+1,y+1/2,-z+1/2.