Supplementary Information

In Situ Recrystallization of Lanthanide Coordination Polymer: From 1D Ladder Chain to 1D Linear Chain

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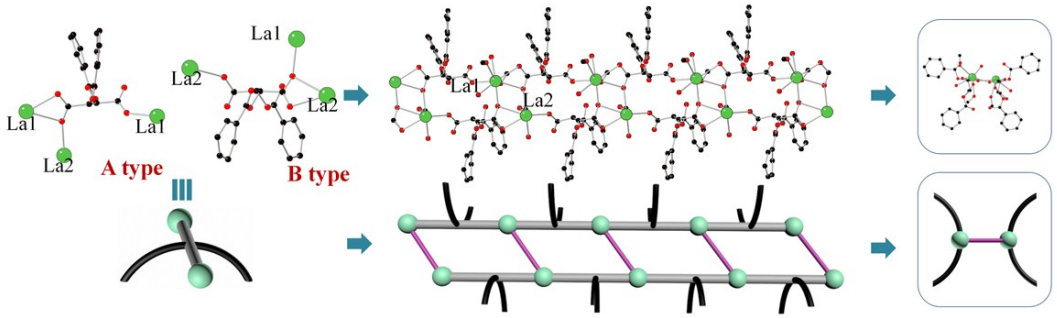

Figure S1. Combined ball/stick and cartoon representations of 1D ladder chain constructed by A-type, B-type ligands and La(III) cations (the insert pictures show the side view of 1D ladder chain) in **1a**

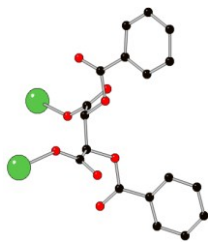

Figure S2. The coordination mode of L–DBTA^{2-} anions in complex **1**: (κ^1)-(κ^1)-μ_2

Table S1 Crystal Data and Structure Refinements for Complexes **1a**–**4a** and **1**–**6.**

Complexes	**1a**	**2a**	**3a**	**4a**	**1**
CCDC	855715	855716	855717	855718	723332
Empirical formula	$C_{58}H_{68}La_2O_{36}$	$C_{58}H_{62}Ce_2O_{33}$	$C_{58}H_{68}Pr_2O_{36}$	$C_{57}H_{60}Nd_2O_{33}$	$C_{44}H_{56}LaNO_{22}$
Formula weight	1618.94	1567.32	1622.94	1561.53	1089.81
Crystal system	Monoclinic				Orthorhombic
Space group	$P2_1$				$P2_12_12$
a (Å)	9.4321(19)	9.4048(19)	9.3330(9)	9.3238(19)	20.164(4)
b (Å)	23.555(5)	23.598(5)	23.444(2)	23.424(5)	16.345(5)
c (Å)	16.669(3)	16.683(3)	16.4638(15)	16.730(3)	16.679(5)
α (˚)	90				90
β (˚)	102.81(3)	102.47(3)	103.6280	102.70(3)	90
γ (˚)	90				90
V (Å^3)	3611.3(12)	3615.2(13)	3500.9(6)	3564.5(12)	5497(3)
F (000)	1636	1580	1644	1572	2240
Z	2				4
D_{cale} (g·cm^{-3})	1.489	1.440	1.540	1.455	1.317
μ (mm^{-1})	1.256	1.327	1.467	1.524	0.850
θ Range(˚)	3.05–27.48	3.04–27.48	2.46–28.29	3.04–27.48	3.21–25.00
Reflections collected	33350	34320	20200	34980	41258
Unique reflections	14914	16238	12976	15890	9558
R_{int}	0.0445	0.0599	0.0256	0.0577	0.0787
R_1[a], wR_2[b] ($I > 2\sigma(I)$)	0.0520, 0.1323	0.0628, 0.1505	0.0540, 0.1436	0.0577, 0.1580	0.0640, 0.1686
R_1[a], wR_2[b] (all data)	0.0731, 0.1568	0.1027, 0.1733	0.0632, 0.1536	0.1028, 0.2134	0.0962, 0.1903
GOF on F^2	1.031	0.964	1.065	1.093	1.047

[a] $R_1 = \Sigma||F_0|-|F_c||/\Sigma|F_0|$. [b] $wR_2 = \Sigma[w(F_0^2 - F_c^2)^2]/\Sigma[w(F_0^2)^2]^{1/2}$.

Table S1 continued.

Complexes	**2**	**3**	**4**	**5**	**6**
CCDC	859164	848922	859165	723336	723334
Empirical formula	$C_{44}H_{56}CeNO_{22}$	$C_{44}H_{56}PrNO_{22}$	$C_{44}H_{56}NdNO_{22}$	$C_{44}H_{56}GdNO_{22}$	$C_{44}H_{56}LuNO_{22}$
Formula weight	1091.02	1091.80	1095.14	1108.15	1125.87
Crystal system			Orthorhombic		
Space group			$P2_12_12$		
a (Å)	20.195(4)	20.285(4)	20.169(4)	20.140(4)	20.052(7)
b (Å)	16.765(3)	16.776(3)	16.722(3)	16.625(3)	16.350(4)
c (Å)	16.778(3)	16.805(3)	16.759(3)	16.701(3)	16.623(4)
α (°)			90		
β (°)			90		
γ (°)			90		
V (Å^3)	5680(2)	5719(2)	5652(2)	5592.0(19)	5450(3)
F (000)	2244	2244	2252	2268	2296
Z			4		
D_{cale} (g·cm^{-3})	1.276	1.267	1.287	1.316	1.372
μ (mm^{-1})	0.871	0.922	0.922	1.257	1.885
θ Range (°)	3.16–27.48	3.15–27.48	3.16–27.47	3.18–27.48	3.22–25.00
Reflections collected	56086	53660	55249	53532	38445
Unique reflections	13015	13073	12928	12723	9484
R_{int}	0.0436	0.1059	0.0459	0.0474	0.0756
R_1[a], wR_2[b] ($I > 2\sigma(I)$)	0.0510, 0.1687	0.0529, 0.1436	0.0512, 0.1632	0.0474, 0.1390	0.0554, 0.1415
R_1[a], wR_2[b] (all data)	0.0555, 0.1737	0.1107, 0.1623	0.0577, 0.1682	0.0586, 0.1464	0.0752, 0.1559
GOF on F^2	1.088	0.908	1.082	1.065	1.069

[a] $R_1 = \Sigma||F_0|-|F_c||/\Sigma|F_0|$. [b] $wR_2 = \Sigma[w(F_0^2 - F_c^2)^2]/\Sigma[w(F_0^2)^2]^{1/2}$.

Table S2 Selected bond lengths (Å) and angles (°) for complexes **1a**–**4a** and **1**–**6**

	1a	**2a**	**3a**	**4a**
O(3)–Ln(1)	2.623(6)	2.601(7)	2.574(6)	2.557(8)
O(4)–Ln(1)	2.754(5)	2.749(6)	2.697(6)	2.713(7)
O(11)–Ln(1)	2.430(8)	2.425(9)	2.419(8)	2.389(9)
O(22)–Ln(1)	2.484(5)	2.472(6)	2.447(5)	2.425(7)
O(25)–Ln(1)	2.548(9)	2.522(8)	2.500(7)	2.455(10)
O(26)–Ln(1)	2.578(8)	2.533(8)	2.544(7)	2.500(9)
O(27)–Ln(1)	2.668(8)	2.642(9)	2.668(8)	2.594(12)
O(31)–Ln(1)	2.542(9)	2.520(10)	2.520(7)	2.476(10)
O2(5)–Ln(1)	2.417(6)	2.425(7)	2.418(7)	2.392(8)
O(4)–Ln(2)	2.505(5)	2.485(6)	2.474(6)	2.449(6)
O(12)–Ln(2)	2.506(7)	2.487(7)	2.476(6)	2.430(8)
O(13)–Ln(2)	2.527(6)	2.496(7)	2.498(6)	2.474(8)
O(21)–Ln(2)	2.580(6)	2.571(6)	2.538(7)	2.551(7)
O(22)–Ln(2)	2.817(5)	2.813(6)	2.784(5)	2.780(6)
O(28)–Ln(2)	2.514(7)	2.505(9)	2.477(7)	2.434(9)
O(29)–Ln(2)	2.564(7)	2.548(7)	2.533(6)	2.508(8)
O(30) –Ln(2)	2.577(7)	2.560(8)	2.533(7)	2.543(10)
O1(19)–Ln(2)	2.445(6)	2.425(5)	2.387(5)	2.398(7)
O(3)–Ln(1)–O(4)	48.46(17)	48.4(2)	49.39(18)	49.0(2)
O(4)–Ln(1)–O(22)	66.96(16)	67.05(19)	67.01(18)	66.5(2)
O(4)–Ln(1)–O(11)	70.2(2)	69.9(2)	69.9(2)	69.9(3)
O(5)–Ln(1)–O(22)	84.8(2)	84.7(2)	84.9(2)	85.7(3)
O(4)–Ln(2)–O(22)	65.68(16)	65.85(19)	65.27(19)	65.1(2)
O(12)–Ln(2)–O(13)	66.60(18)	67.1(2)	67.0(2)	67.6(2)
O(12)–Ln(2)–O(22)	69.83(19)	69.2(2)	70.5(2)	69.9(3)
O(21)–Ln(2)–O(22)	47.82(17)	47.67(19)	48.61(18)	48.6(2)

Table S2 continued

	1	**2**	**3**	**4**	**5**	**6**
O(8)−Ln(1)	2.455(6)	2.450(3)	2.457(4)	2.426(3)	2.375(3)	2.330(6)
O(16)−Ln(1)	2.445(5)	2.418(3)	2.429(5)	2.394(3)	2.341(3)	2.294(5)
O(17)−Ln(1)	2.590(6)	2.559(3)	2.504(6)	2.521(3)	2.463(3)	2.394(5)
O(18)−Ln(1)	2.527(6)	2.516(3)	2.483(5)	2.484(3)	2.419(4)	2.342(6)
O(4)−Ln(2)	2.490(5)	2.461(3)	2.442(5)	2.437(3	2.391(3)	2.356(5)
O(12)−Ln(2)	2.446(5)	2.448(3)	2.401(5)	2.421(3)	2.384(3)	2.314(5)
O(19)−Ln(2)	2.529(6)	2.521(3)	2.556(6)	2.487(3)	2.428(4)	2.320(5)
O(20) −Ln(2)	2.530(6)	2.520(3)	2.483(5)	2.487(4)	2.428(3)	2.321(5)
O(16)−Ln(1)−O1(16)	83.4(3)	81.69(15)	76.7(3)	80.92(16)	79.59(17)	77.0(3)
O1(8)−Ln(1)−O(8)	81.3(3)	79.45(16)	76.3(2)	78.87(17)	76.94(19)	76.3(3)
O2(4)−Ln(2)−O3(4)	80.1(3)	77.20(14)	79.3(3)	76.77(15)	75.80(17)	74.4(3)
O1(12)−Ln(2)−O(12)	79.3(3)	77.77(15)	81.0(3)	76.75(15)	75.33(16)	74.6(2)

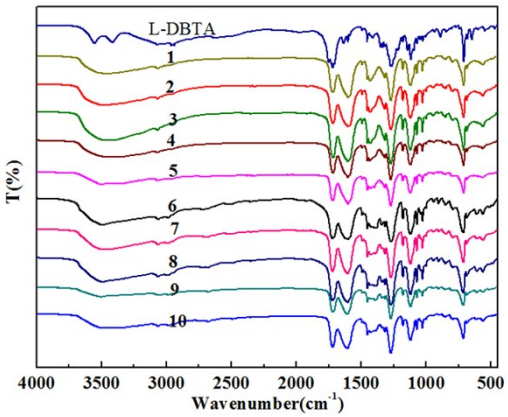

Figure S3. Infrared spectra of L–DBTA and complexes **1a**–**4a** and **1**–**6**

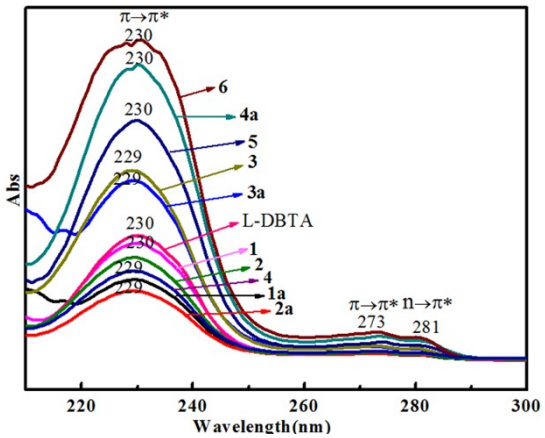

Figure S4. Ultraviolet spectra of L–DBTA and complexes **1a**–**4a** and **1**–**6**

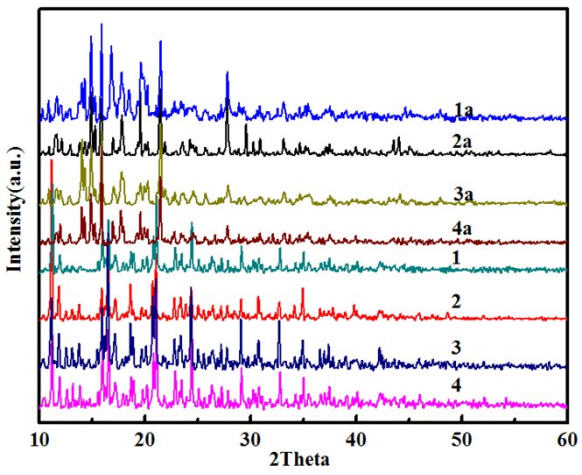

Figure S5. PXRD patterns of complexes **1a**–**4a** and **1**–**4**

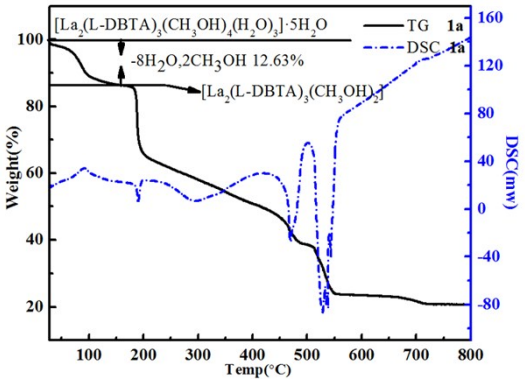

Figure S6. TG–DSC curves of complex **1a**

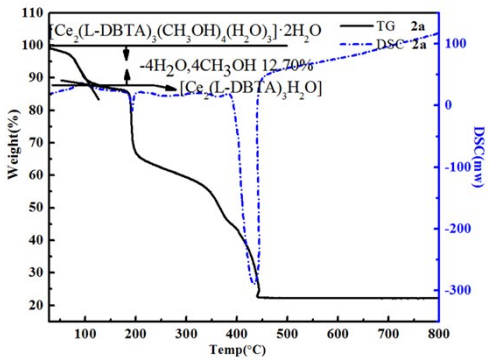

Figure S7. TG–DSC curves of complex **2a**

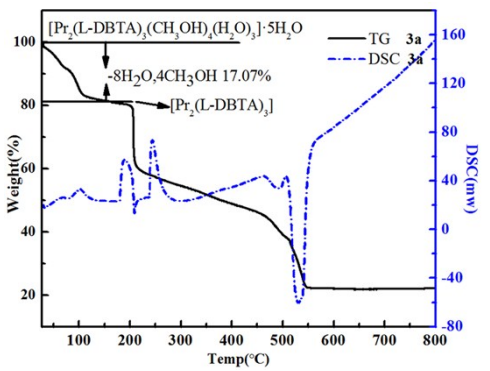

Figure S8. TG–DSC curves of complex **3a**

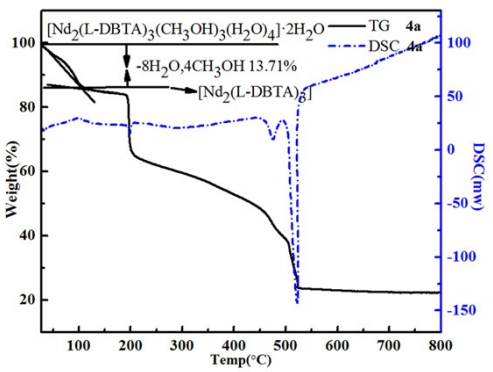

Figure S9. TG–DSC curves of complex **4a**

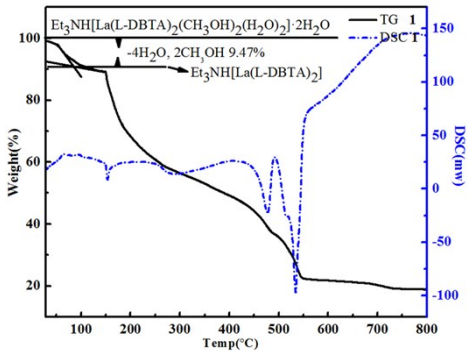

Figure S10. TG–DSC curves of complex **1**

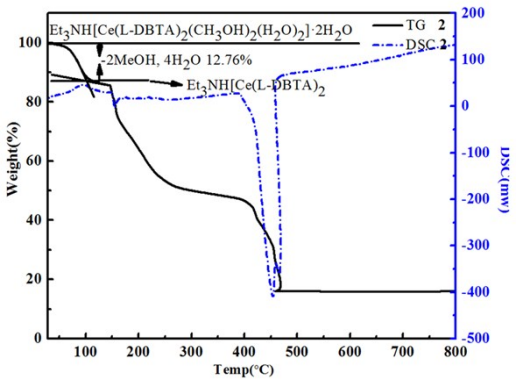

Figure S11. TG–DSC curves of complex **2**

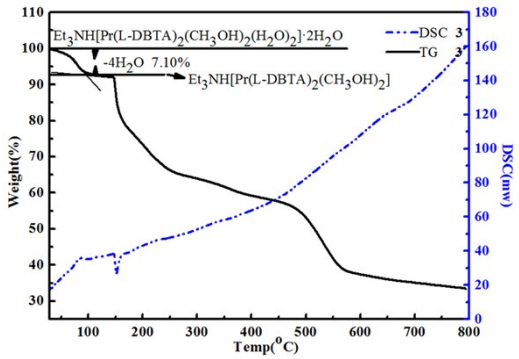

Figure S12. TG–DSC curves of complex **3**

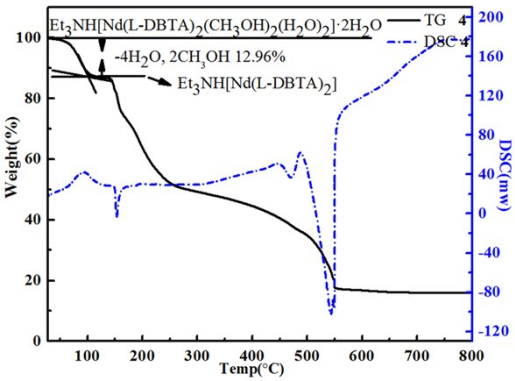

Figure S13. TG–DSC curves of complex **4**

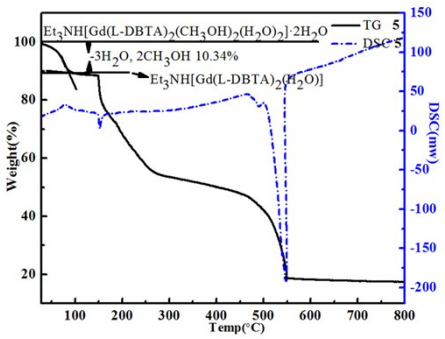

Figure S14. TG–DSC curves of complex **5**

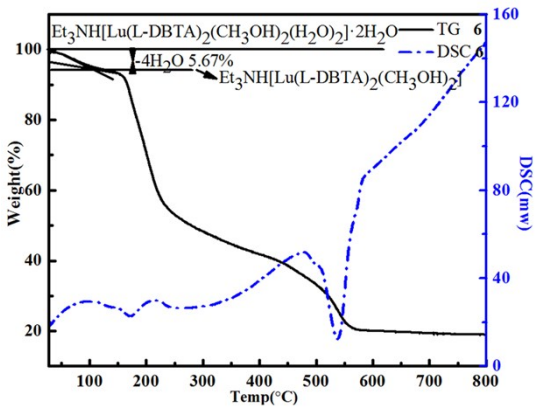

Figure S15. TG–DSC curves of complex **6**

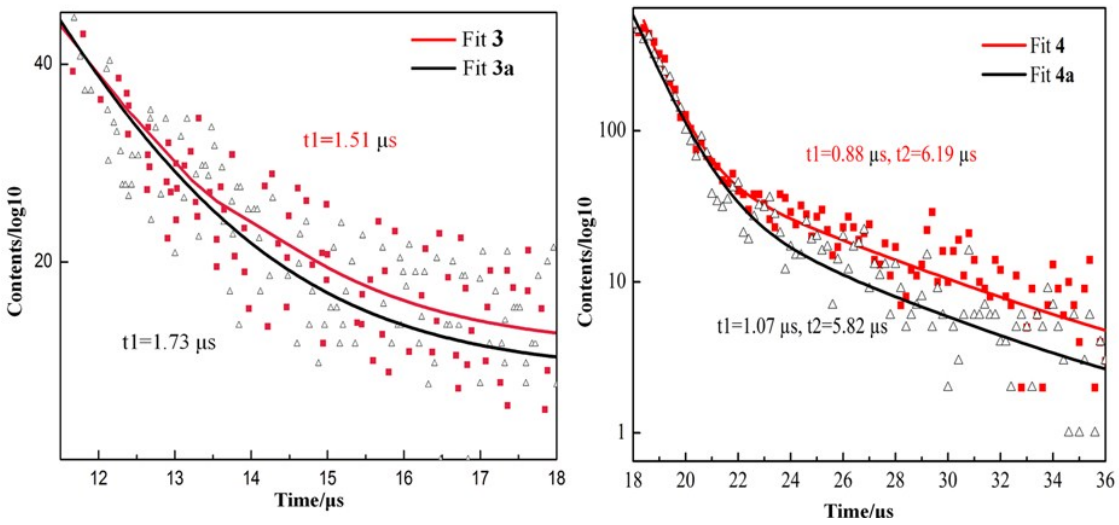

Figure S16. Room-temperature luminescence decay curves of complexes **3a**, **3**, **4a** and **4**