Electronic supplementary material for

New microporous lanthanide organic frameworks. Synthesis, structure, luminescence, sorption, and catalytic acylaton of 2-naphthol

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Content

1. Synthesis of the ligand 1,3,5-tris(4-carboxyphenyl)-2,4,6-trimethylbenzene (H_3L)

In a 250 mL three-necked Schlenk flask, K_2CO_3 (6.55 g, 47 mmol) was dissolved in 30 mL of H_2O. To this solution, under vigourous stirring, 4-carboxyphenylboronic acid (1.94 g, 11.7 mmol) and triiodomesitylene (1.49 g, 3 mmol) were added, followed by tetrakis(triphenylphosphine)-palladium(0) (0.45 g, 0.38 mmol) in dioxane (50 mL) and EtOH (30 mL). This mixture was degassed by bubbling N_2 for 30 min and then refluxed under N_2 for 72 h. After the desired reaction time, the mixture was filtered and the filtrate was neutralized with a solution of hydrochloric acid (1 mol/L) until a fine white precipitate was formed. The product was isolated by centrifugation, washed several times with water and recrystallized (Yield 50 %, colorless crystals).

Synthesis of compound $[LaL(H_2O)_2]_n$ **(1)**

$La(NO_3)_3{\cdot}6H_2O$ (0.036 g, 0.08 mmol) and H_3L (0.01 g, 0.02 mmol) were dissolved in ethanol and water (2.5 mL/0.5 mL) at room temperature. The solution was transferred into a 20 mL culture tube and kept under static conditions for 5 days at 80 °C. After cooling, the colorless crystalline product was collected by centrifugation and washed with ethanol. Finally, the crystals were dried at room temperature (0.008 g).

Synthesis of compound $[CeL(H_2O)_2]_n$ **(2)**

2 was prepared following the synthetic procedure for 1 using $Ce(NO_3)_3{\cdot}6H_2O$ (0.039 g, 0.08 mmol), H_3L (0.01 g, 0.02 mmol), deionized water (0.5 mL) and ethanol (2.5 mL). The colorless crystals were dried at room temperature (0.012 g).

Synthesis of compound $[NdL(H_2O)_2]{\cdot}1.33DMF{\cdot}2H_2O$ (3)

To a solution of H_3L (0.01 g, 0.02 mmol) in DMF (5.0 mL), in a 20 mL culture tube was added $Nd(NO_3)_3{\cdot}6H_2O$ (0.036 g, 0.08 mmol) dissolved in ethanol/water (2.5 mL/0.5 mL) at room temperature. The tube with clear solution was kept under static conditions for 1 day at 80 °C. After cooling, the violet crystalline product was collected by centrifugation and washed with DMF and ethanol. Finally, the crystals were dried at room temperature (0.0138g).

Synthesis of compound $[EuL(H_2O)_2]{\cdot}1.33DMF{\cdot}2H_2O$ (4)

$Eu(NO_3)_3{\cdot}6H_2O$ (0.04 g, 0.08 mmol) and H_3L (0.01 g, 0.02 mmol) were dissolved in DMF and ethanol (0.5 mL/2.5 mL) at room temperature. The solution was kept under static conditions for 4 days at 80 °C. After cooling, the colorless crystalline product was collected by centrifugation and washed with DMF and then with ethanol. Finally, the crystals were dried at room temperature (0.01 g).

Synthesis of compound $[GdL(H_2O)_2]{\cdot}2DMF{\cdot}2H_2O$ **(5)**

A solution containing H_3L (0.0298 g, 0.06 mmol), $Gd(NO_3)_3{\cdot}6H_2O$ (0.085 g, 0.24 mmol), DMF (1.5 mL), ethanol (4 mL) and water (1.5 mL) was transferred into a tube and kept under static conditions for 2 day at 80 °C. The white crystalline product was isolated and dried at room temperature (0.04 g).

Synthesis of compound $[DyL(H_2O)_2]{\cdot}$ **(6)**

6 was prepared following the synthetic procedure for 3 using: $Dy(NO_3)_3{\cdot}6H_2O$ (0.093 g, 0.26 mmol), H_3L (0.032 g, 0.06 mmol) in DMF/ethanol/water (1.5 mL/4 mL/0.75 mL). The tube

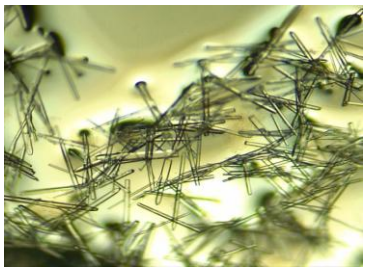
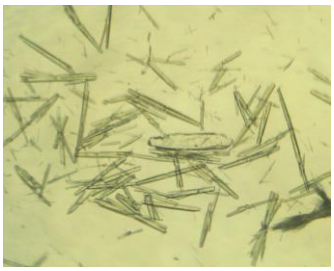
with clear solution was kept under static conditions for 3 day at 80 °C. The white crystals were dried at room temperature (0.03 g).

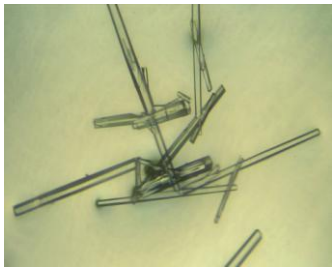
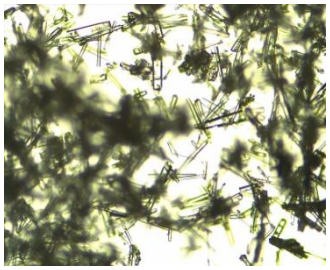
***Synthesis of compound [HoL(H$_2$O)$_2$]·1.33DMF·2H$_2$O* (7)**

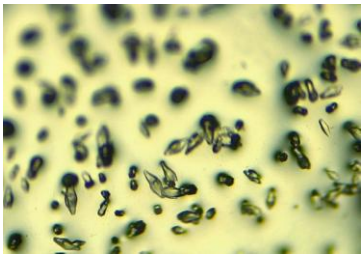
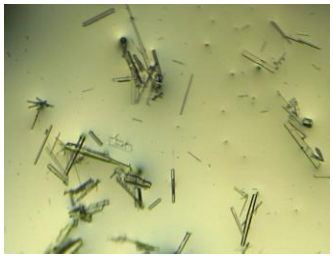
7 was prepared following the synthetic procedure for **3** using: Ho(NO$_3$)$_3$·5H$_2$O (0.09 g, 0.2 mmol), H$_3$L (0.032 g, 0.06 mmol) in DMF/ethanol/water (1.5 mL/4 mL/0.75 mL). The crystalline product was isolated and dried at room temperature (0.02 g).

Table S1. Overview of the experimental details for the synthesis of **1-7**.

Compound	DMF (mL)	EtOH (mL)	H_2O (mL)	Time (d)	T (°C)	Yield (%)
1	-	2.5	0.5	5	80	62
2	-	2.5	0.5	5	80	88
3	5	2.5	0.5	1	80	84
4	0.5	2.5	-	4	80	66
5	1.5	4	1.5	2	80	82
6	1.5	4	0.75	3	80	77
7	1.5	4	0.75	3	80	45

1  **2** 

3a  3b 

4  **5** 

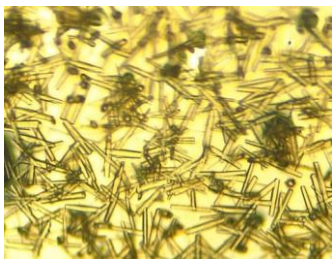
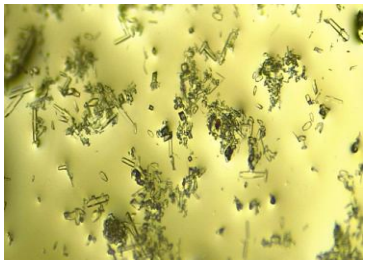
6  **7** 

Figure S1: Optical microscopy image of **1-7**, with Leica ICC50 W, 4x/0.10.

2. Infrared spectroscopy (ATR)

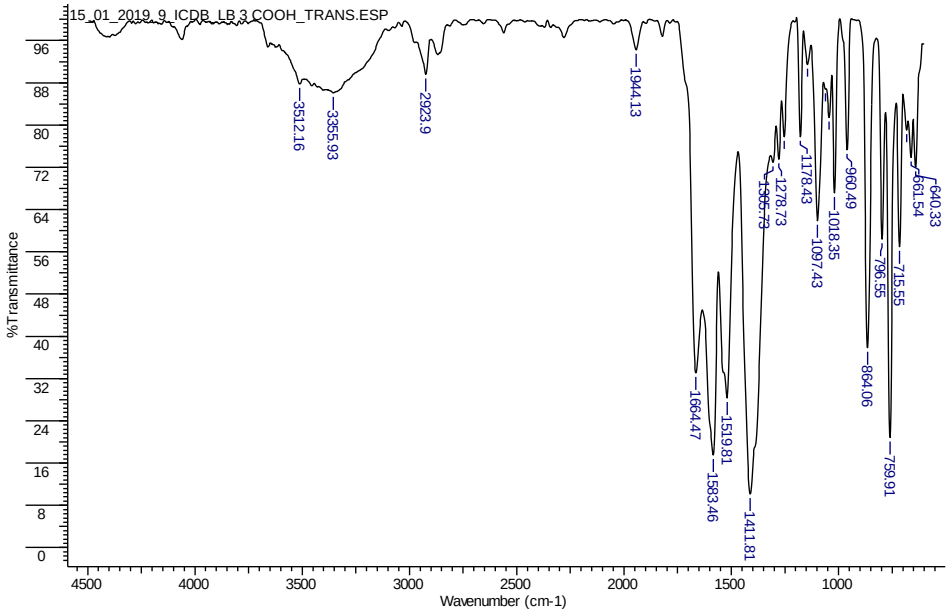


Figure S2. IR spectrum of ligand **H_3L.**

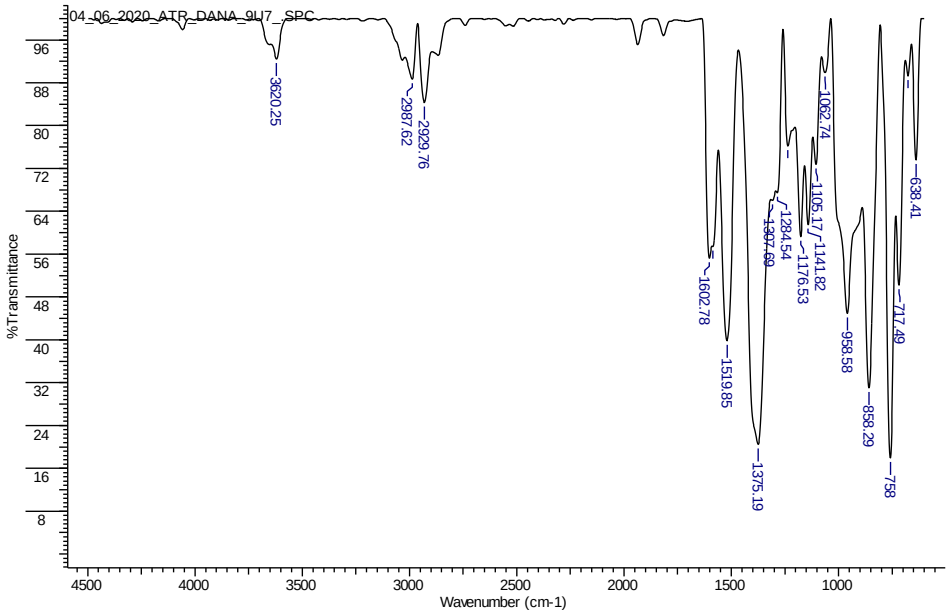


Figure S3. IR spectrum of compound $[LaL(H_2O)_2]_n$ **(1)**.

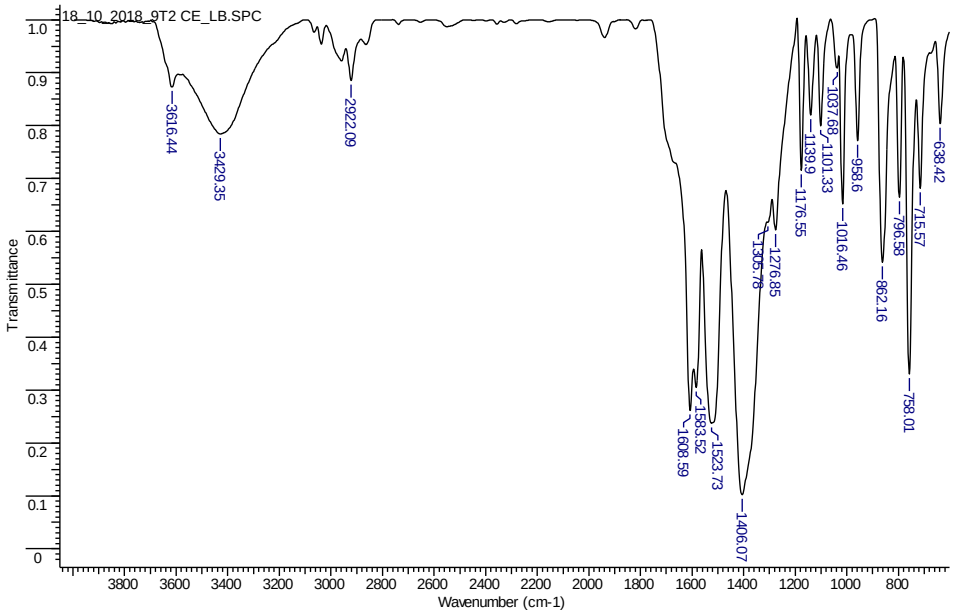


Figure S4. IR spectrum of compound $[CeL(H_2O)_2]_n$ **(2)**.

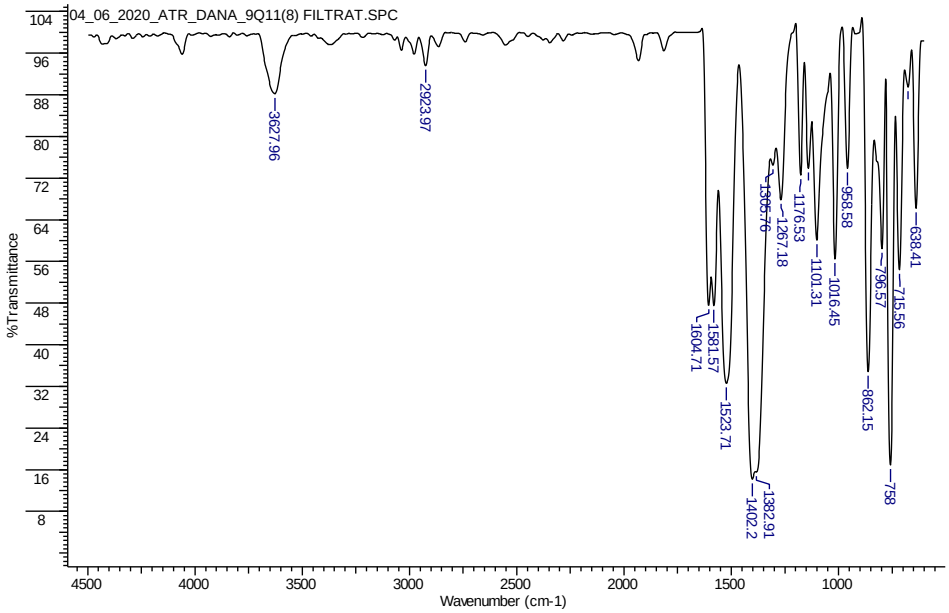


Figure S5. IR spectrum of compound $[NdL(H_2O)_2]_n \cdot 1.33DMF \cdot H_2O$ (**3**).

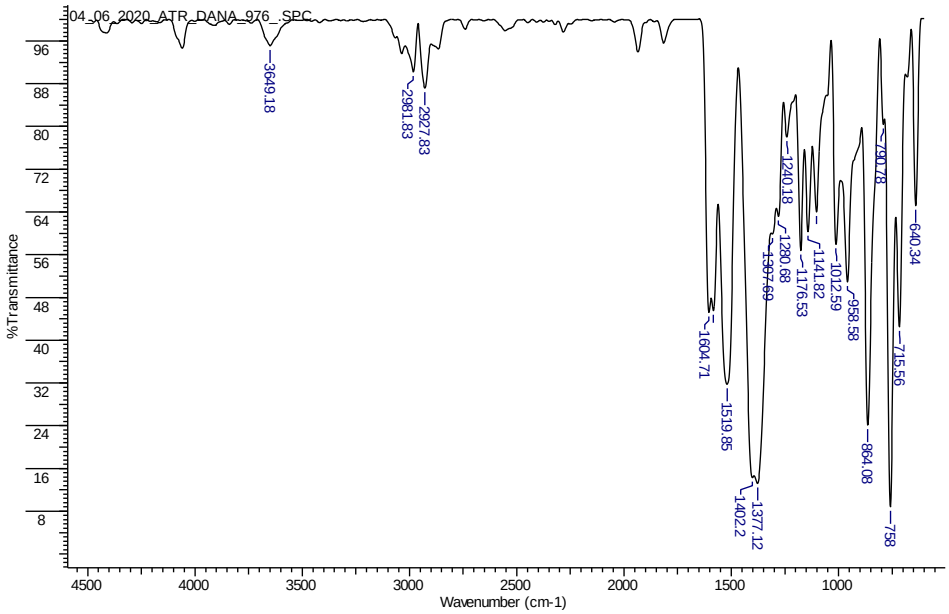


Figure S6. IR spectrum of compound $[EuL(H_2O)_2]_n \cdot 1.33DMF \cdot 2H_2O$ (**4**).

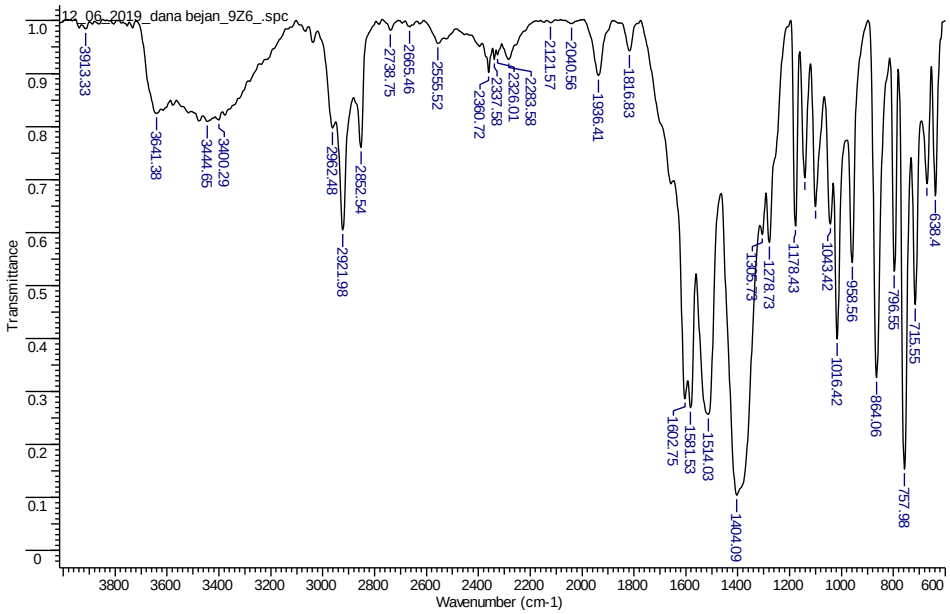


Figure S7. IR spectrum of compound $[GdL(H_2O)_2]_n \cdot 2DMF\ 2H_2O$(**5**).

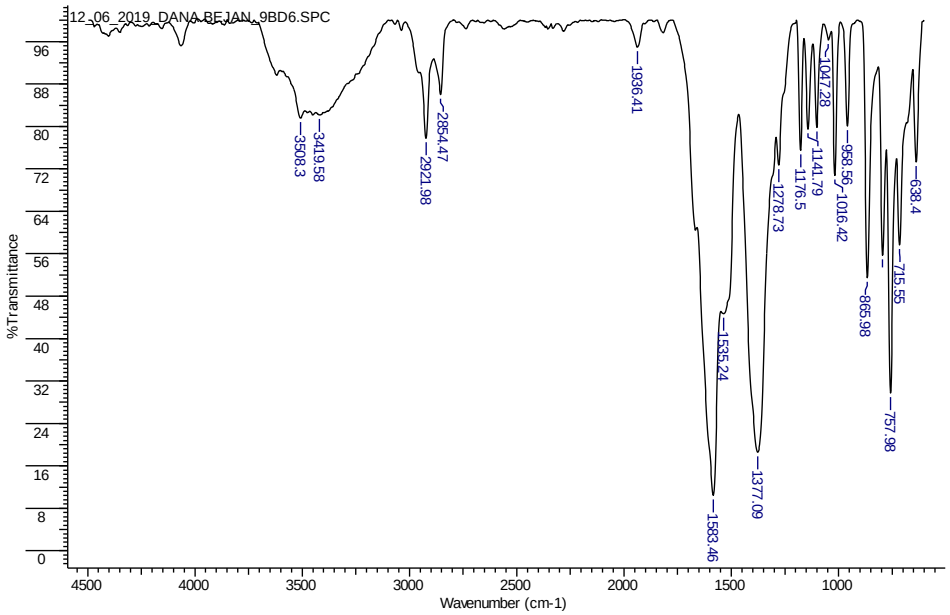


Figure S8. IR spectrum of compound $[DyL(H_2O)_2]_n$ (**6**).

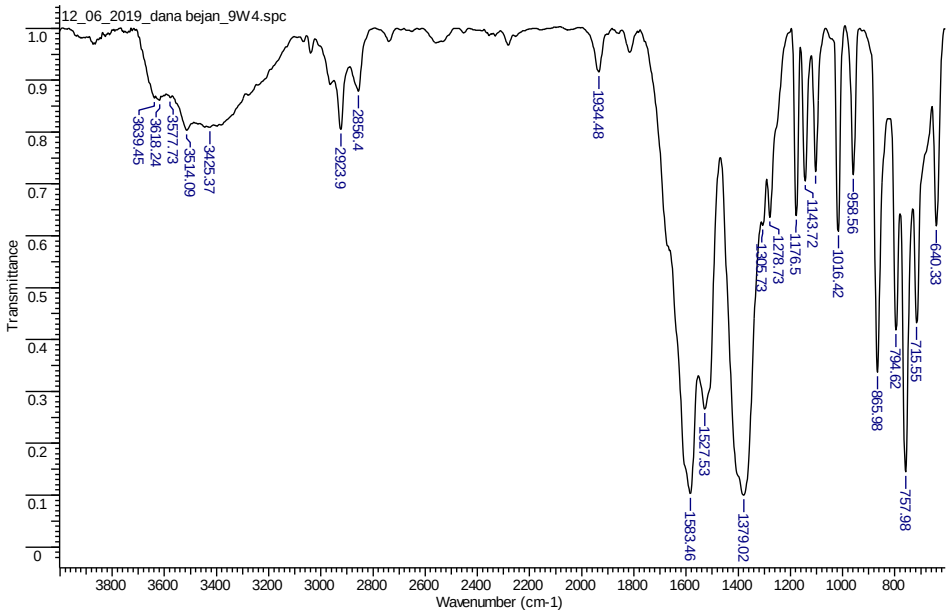


Figure S9. IR spectrum of compound $[HoL(H_2O)_2]_n \cdot 1.33DMF \cdot 2H_2O$ (**4**).

3. Powder X-ray Diffraction (PXRD)

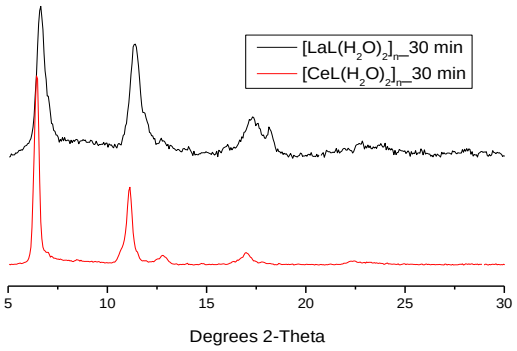


Figure S10. PXRD patterns of the two isostructural compounds $[LaL(H_2O)_2]_n$ (**1**) and $[CeL(H_2O)_2]_n$ (**2**) recorded at different time (6 min and 30 min).

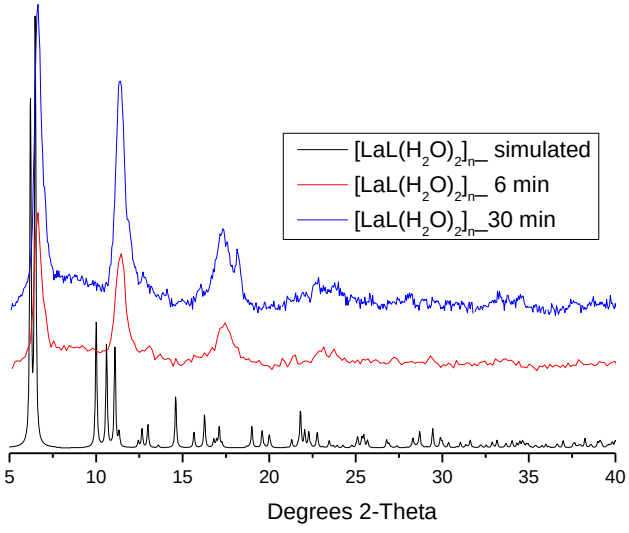


Figure S11. PXRD patterns of $[LaL(H_2O)_2]_n$ (**1)** recorded at different time. (6 min and 30 min).

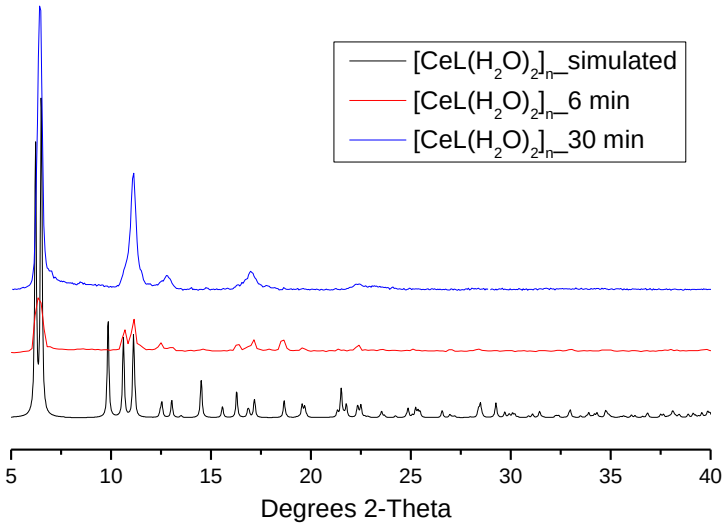


Figure S12. PXRD patterns of $[CeL(H_2O)_2]_n$ (**2)**.

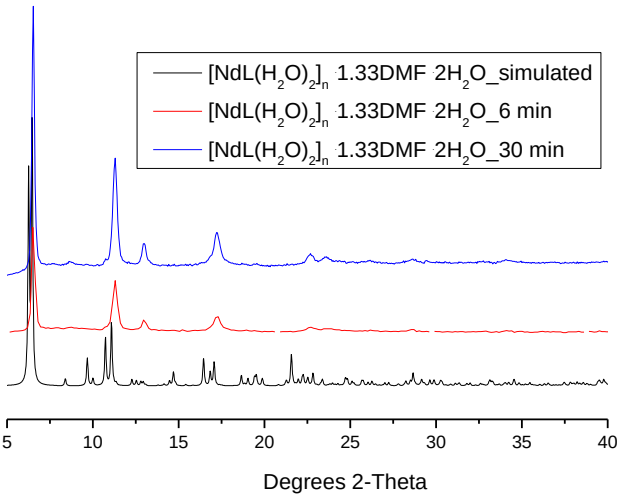


Figure S13. PXRD patterns of $[NdL(H_2O)_2]_n \cdot 1.33DMF \cdot H_2O$ (**3)**.

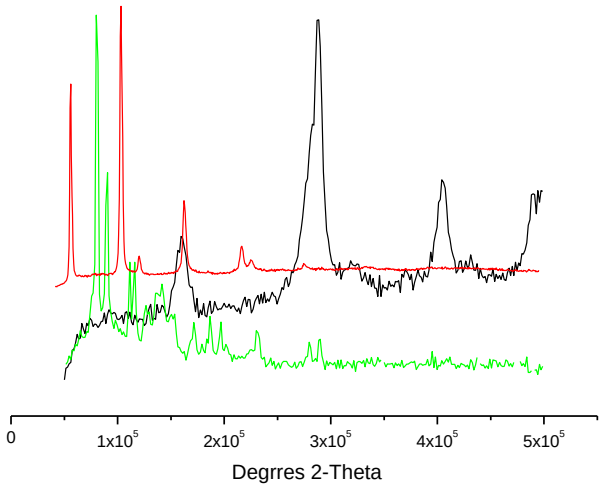


Figure S14. PXRD patterns of compound $[NdL(H_2O)_2]_n \cdot 1.33DMF \cdot H_2O$ (**3**)-red, compound **3** after basic condition- black; compound **3** after acidic condition- green.

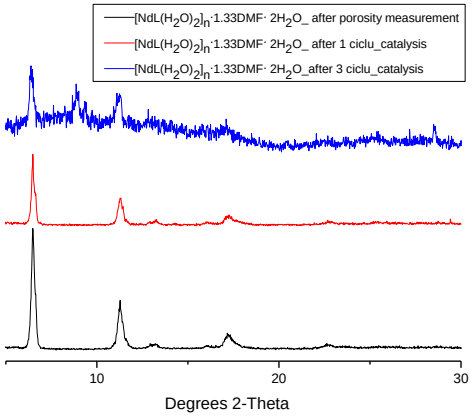


Figure S15. PXRD patterns of activated compound $[NdL(H_2O)_2]_n \cdot 1.33DMF \cdot H_2O$ (**3**) - black and compound (**3**) after catalytic reaction (first cycle) – red and (**3**) – blue, after third cycle in catalytic processes.

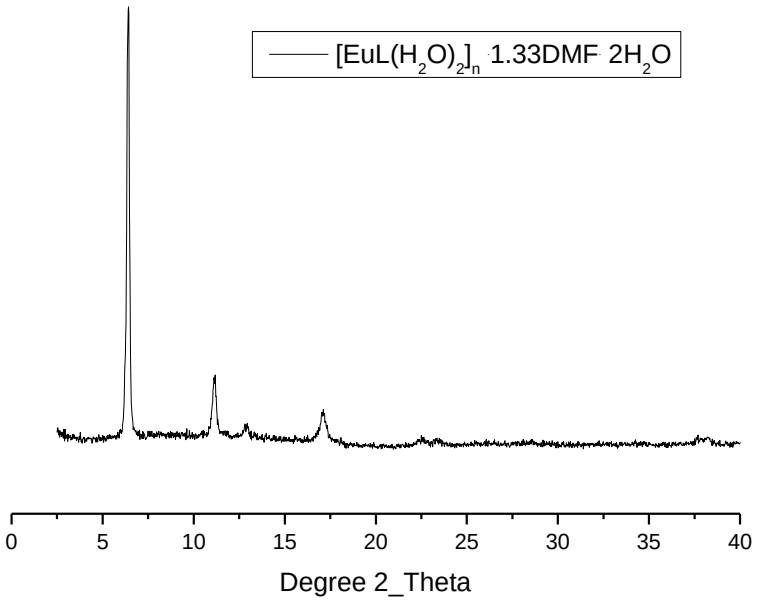


Figure S16. PXRD patterns of $[EuL(H_2O)_2]_n \cdot 1.33DMF \cdot 2H_2O$ (**4)**.

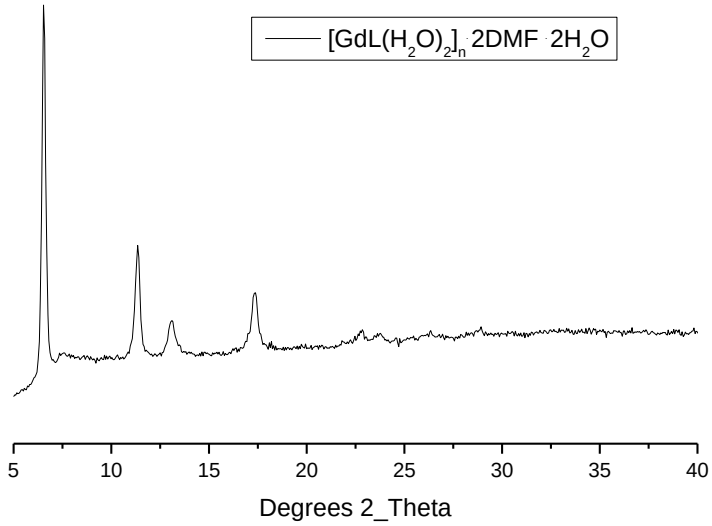


Figure S17. PXRD patterns of $[GdL(H_2O)_2]_n \cdot 2DMF\ 2H_2O$(**5)**.

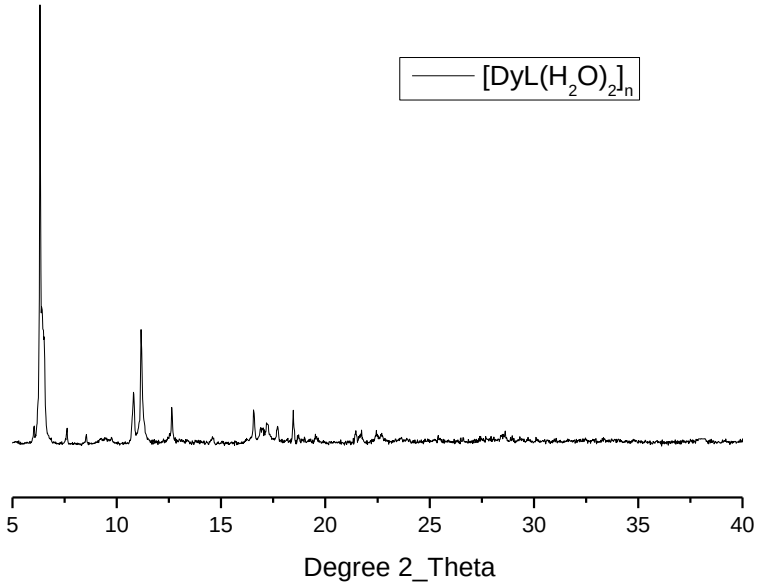


Figure S18. PXRD patterns of $[DyL(H_2O)_2]_n$ (**6**).

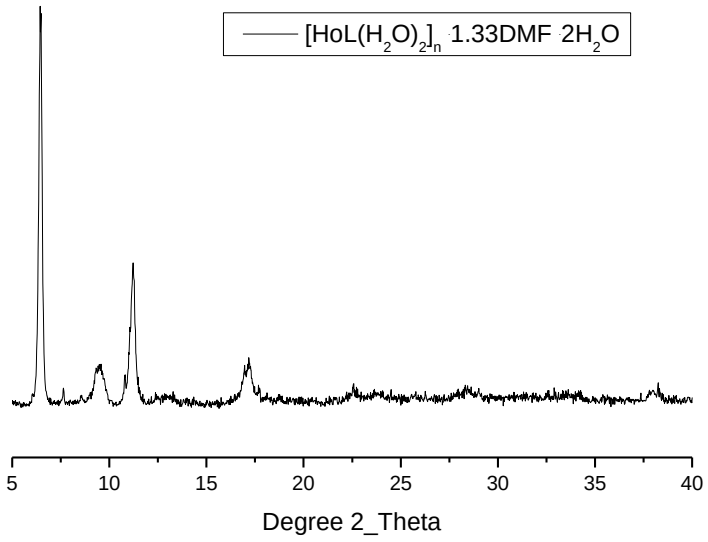


Figure S19. PXRD patterns of $[HoL(H_2O)_2]_n \cdot 1.33DMF \cdot H_2O$ (**7**).

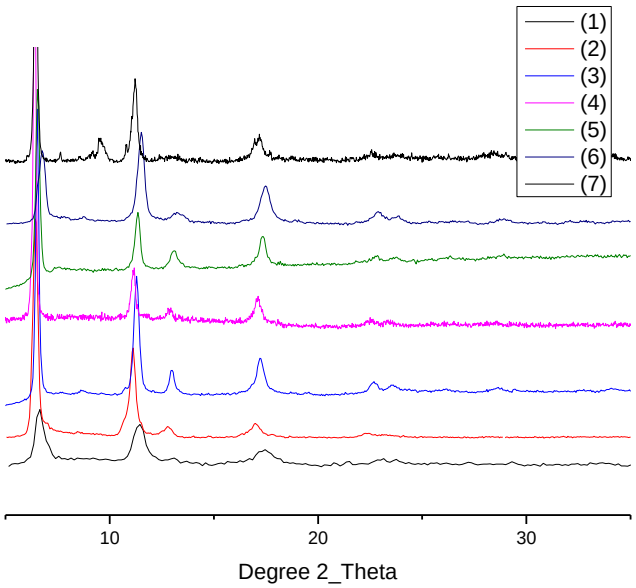


Figure S20. PXRD patterns of all compounds (**1-7**).

4. Thermal (TG/DTG) Analysis

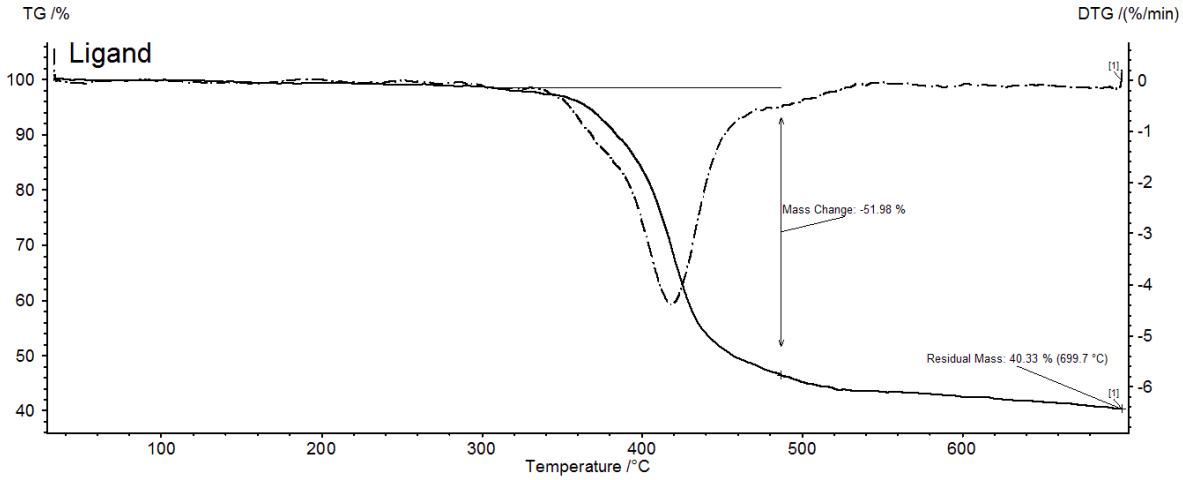


Figura S21. Thermogravimetric analysis of ligand **H_3L.**

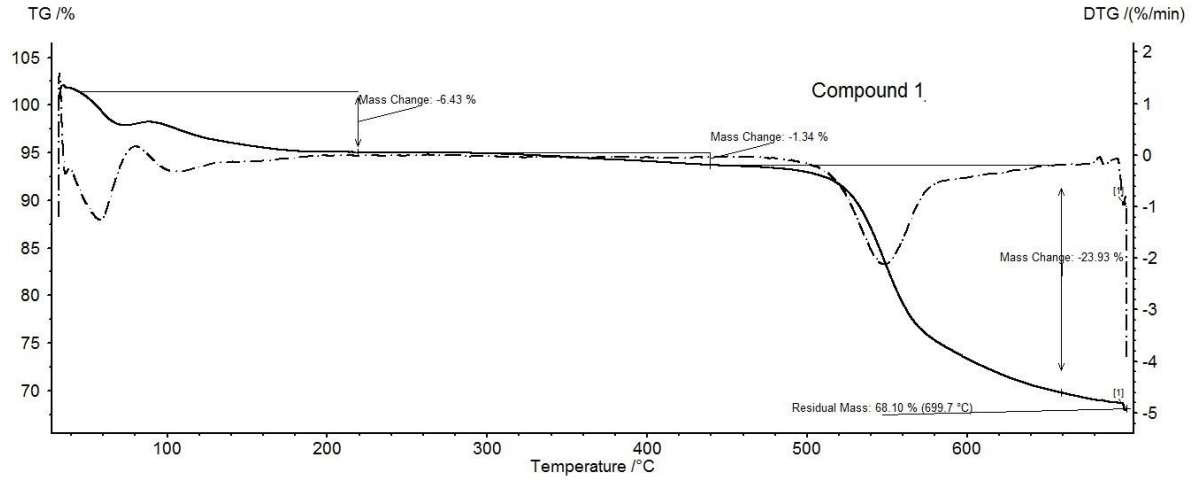


Figura S22. Thermogravimetric analysis of compound $[LaL(H_2O)_2]_n$ (**1**).

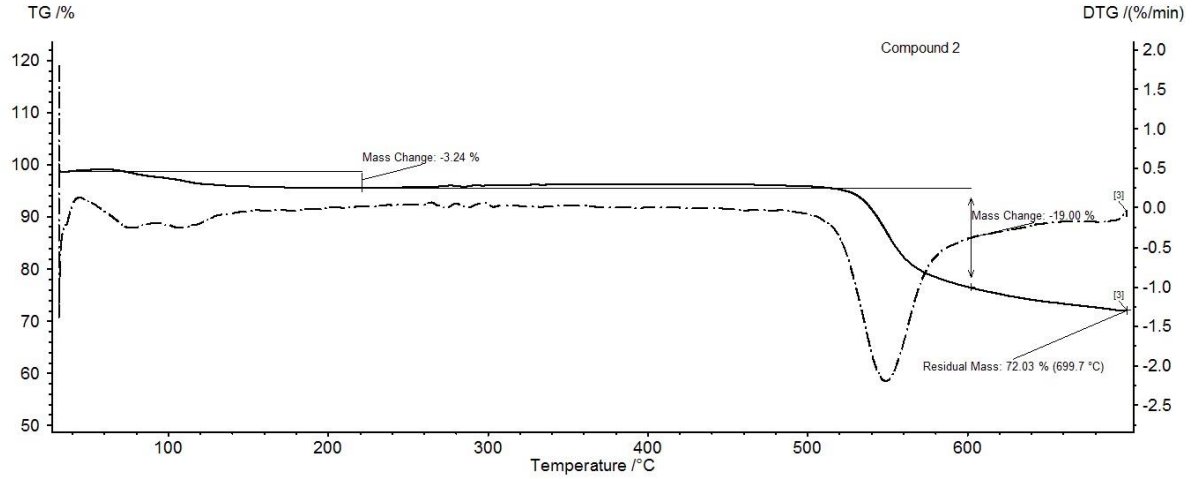


Figura S23. Thermogravimetric analysis of compound $[CeL(H_2O)_2]_n$ (**2**).

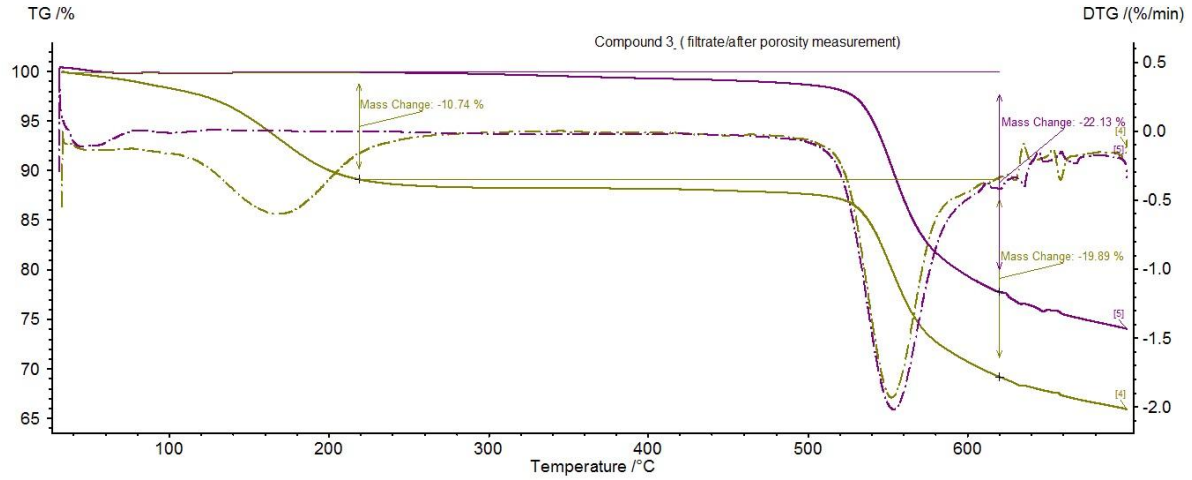


Figura S24. Thermogravimetric analysis of compound $[NdL(H_2O)_2]_n \cdot 1.33DMF \cdot H_2O$ (**3**).

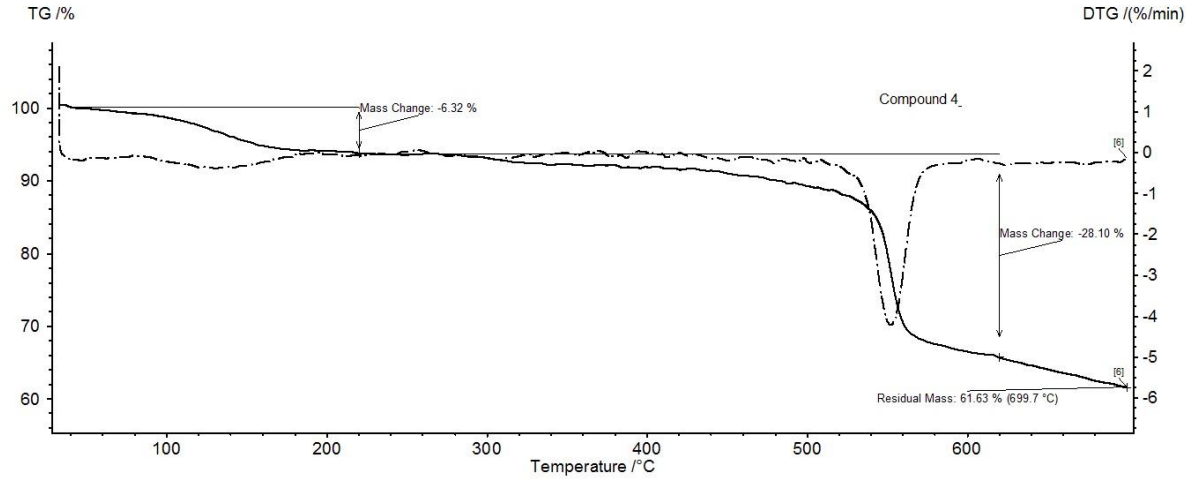


Figura S25. Thermogravimetric analysis of compound $[EuL(H_2O)_2]_n \cdot 1.33DMF \cdot 2H_2O$ (**4)**.

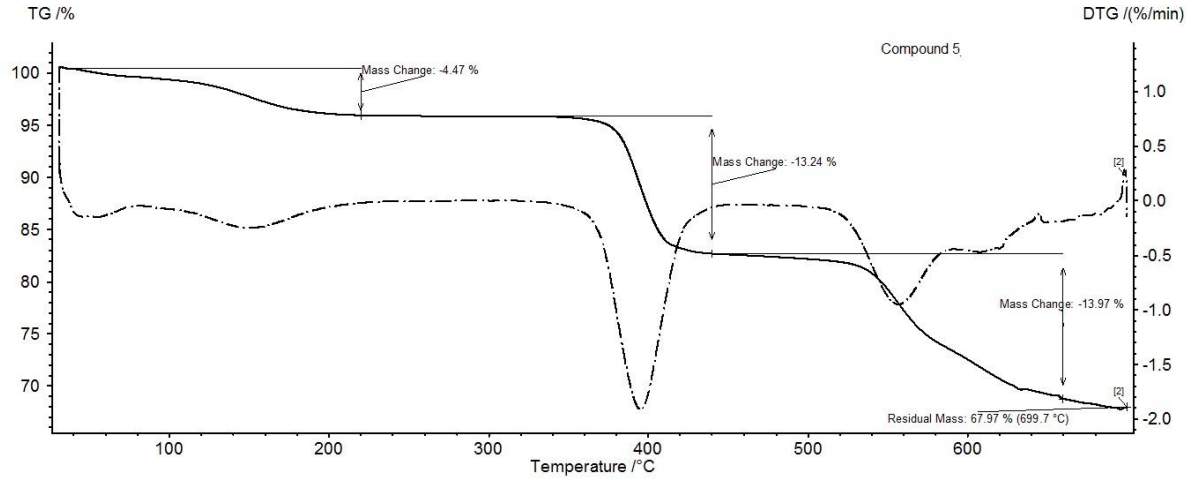


Figure S26. Thermogravimetric analysis of compound $[GdL(H_2O)_2]_n \cdot 2DMF\ 2H_2O$(**5)**.

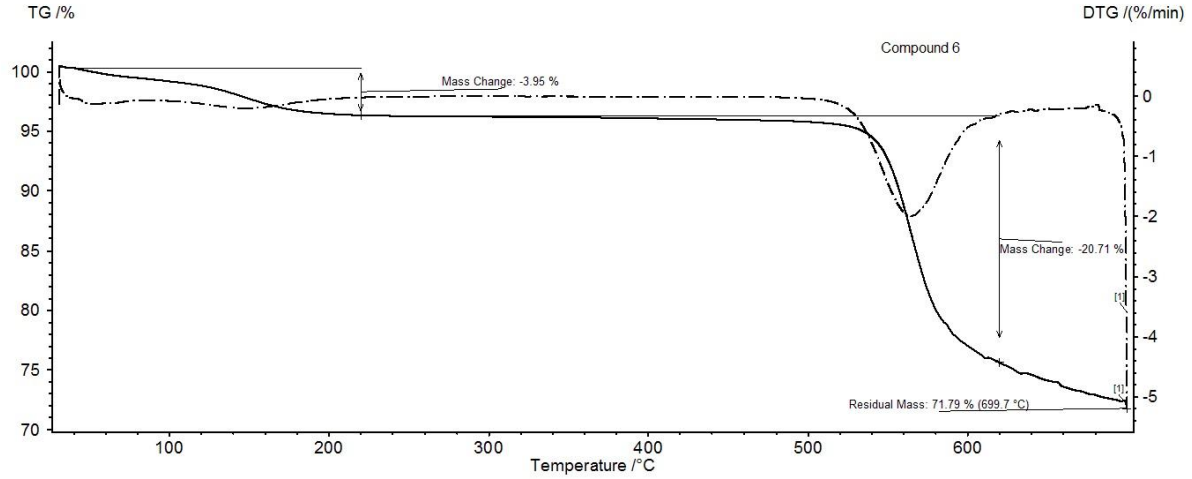


Figure S27. Thermogravimetric analysis of compound $[DyL(H_2O)_2]_n$ (**6)**.

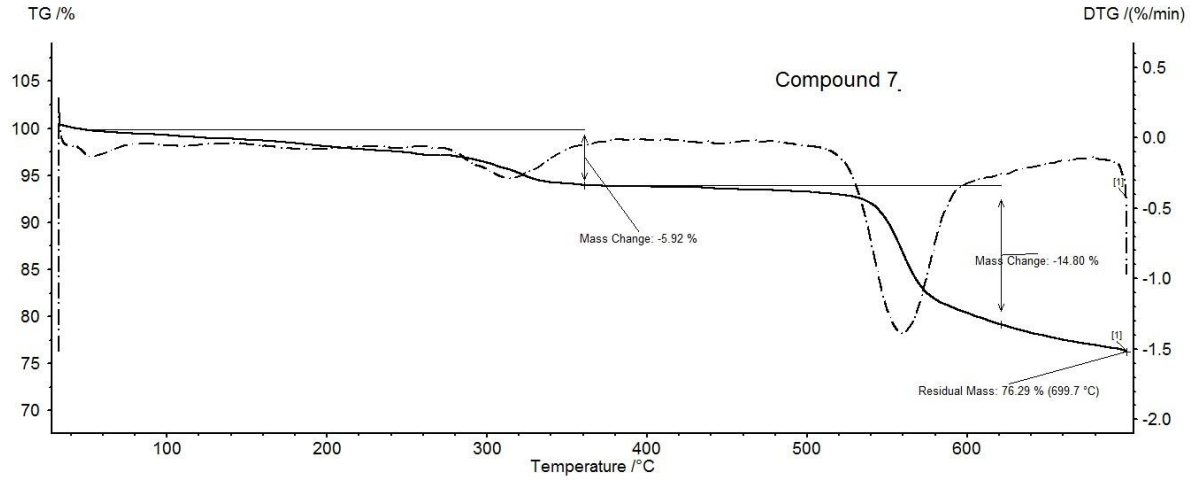


Figure S28 Thermogravimetric analysis of compound $[HoL(H_2O)_2]_n \cdot 1.33DMF \cdot H_2O$ **(7).**

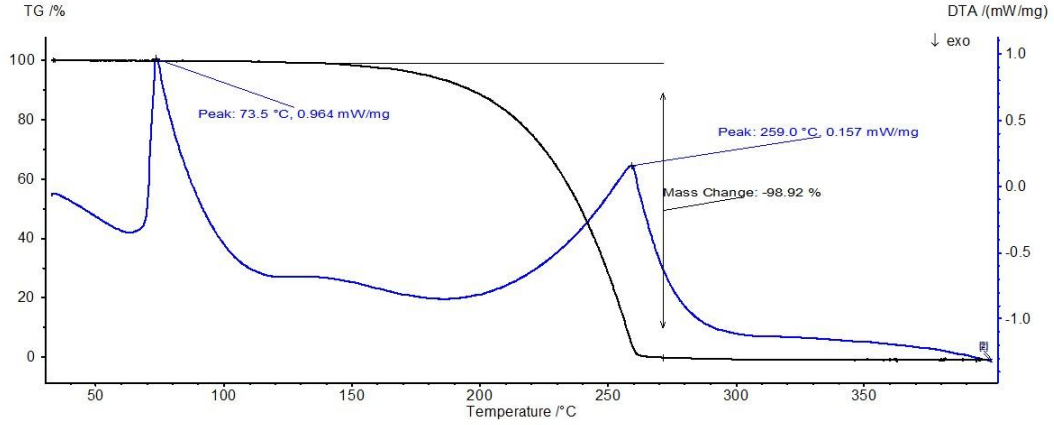


Figure S29. Thermogravimetric analysis of 2-naphyl acetate.

5. Gas sorption isotherms

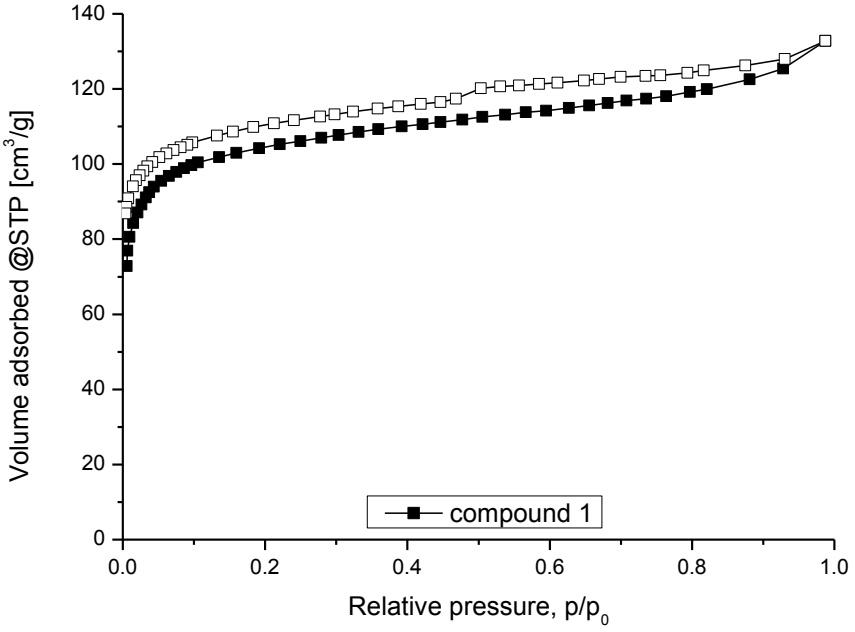


Figure S30. Nitrogen sorption isotherms of $[LaL(H_2O)_2]_n$ (**1**) recorded at 77 K. Filled symbols are for adsorption, empty symbols are for desorption (S_{BET} = 405 m^2/g).

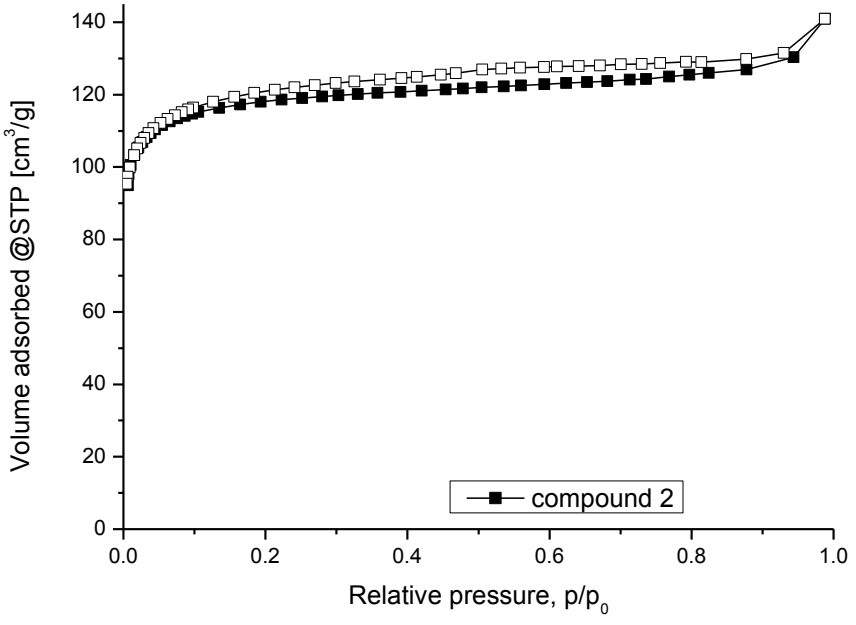


Figure S31. Nitrogen sorption isotherms of $[CeL(H_2O)_2]_n$ (**2**) recorded at 77 K. Filled symbols are for adsorption, empty symbols are for desorption (S_{BET} = 467 m^2/g).

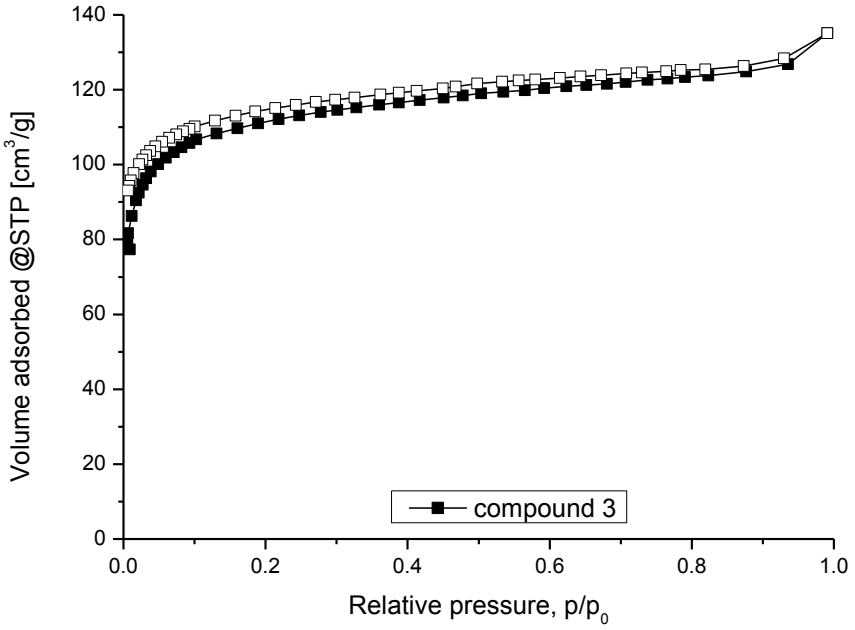


Figure S32. Nitrogen sorption isotherms of $[NdL(H_2O)_2]_n \cdot 1.33DMF \cdot H_2O$ (**3)** recorded at 77 K. Filled symbols are for adsorption, empty symbols are for desorption (S_{BET} = 426 m^2/g).

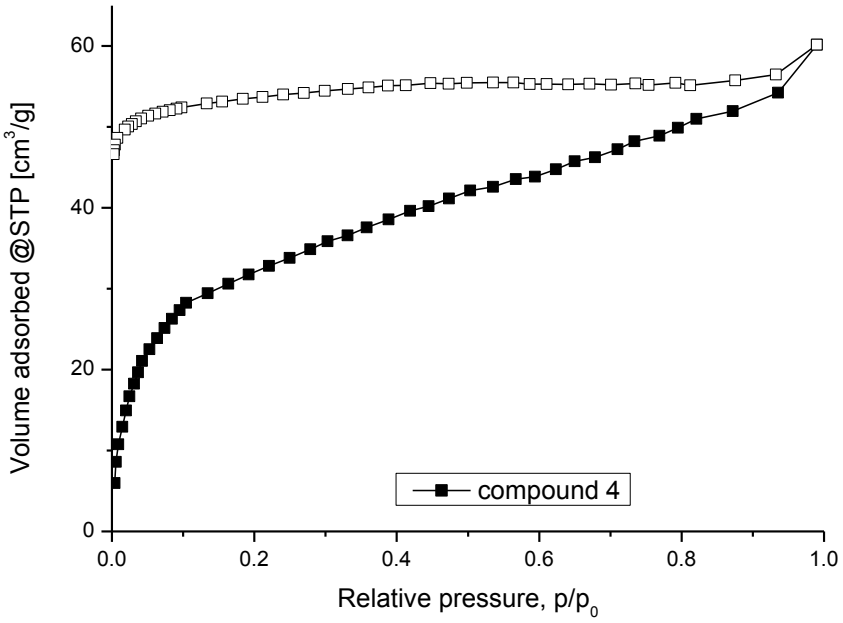


Figure S33. Nitrogen sorption isotherms of $[EuL(H_2O)_2]_n \cdot 1.33DMF \cdot 2H_2O$ (**4)** recorded at 77 K. Filled symbols are for adsorption, empty symbols are for desorption (S_{BET} = 114 m^2/g).

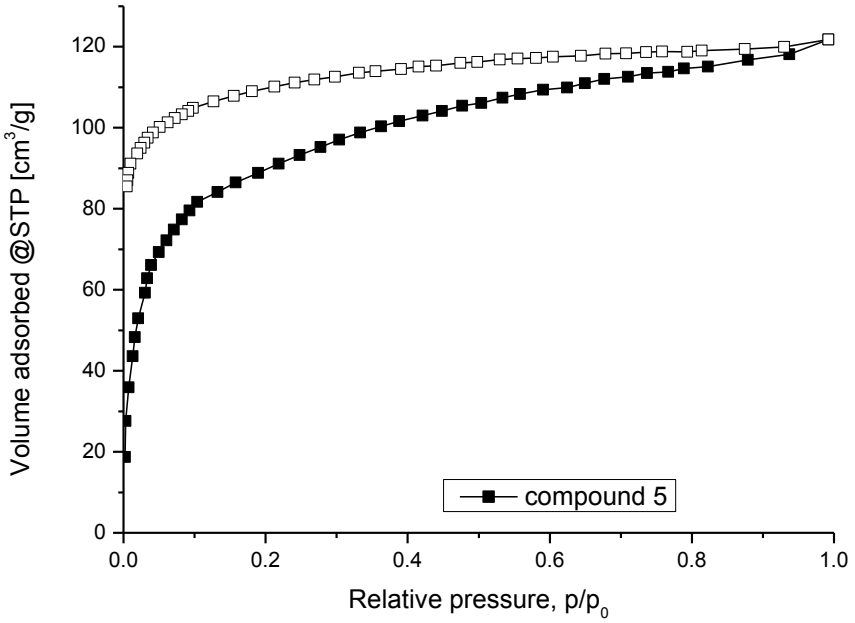


Figure S34 . Nitrogen sorption isotherms of $[GdL(H_2O)_2]_n \cdot 2DMF\ 2H_2O$(**5)** recorded at 77 K. Filled symbols are for adsorption, empty symbols are for desorption (S_{BET} = 348 m^2/g).

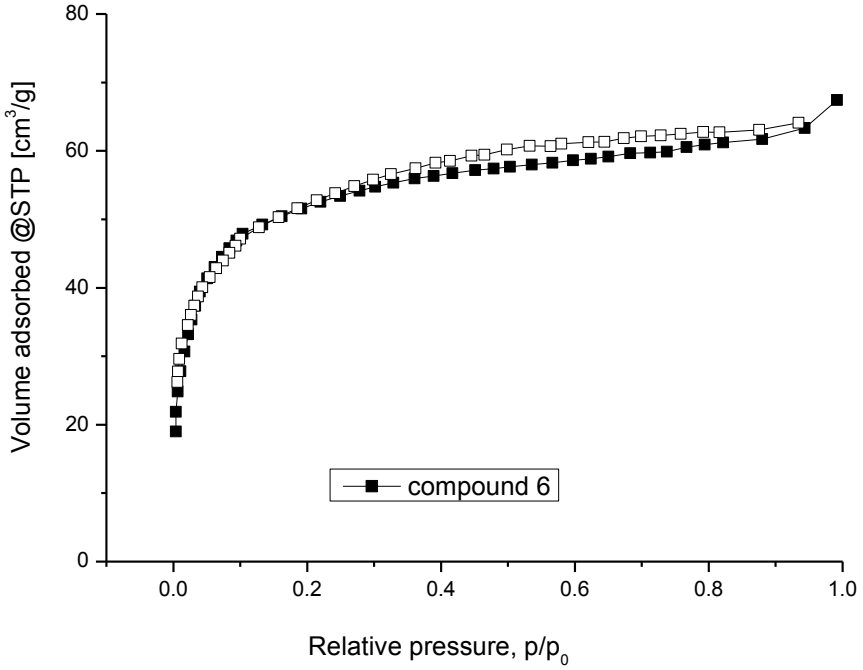


Figure S35a. Nitrogen sorption isotherms of $[DyL(H_2O)_2]_n$ (**6)** recorded at 77 K. Filled symbols are for adsorption, empty symbols are for desorption (S_{BET} = 202 m^2/g).

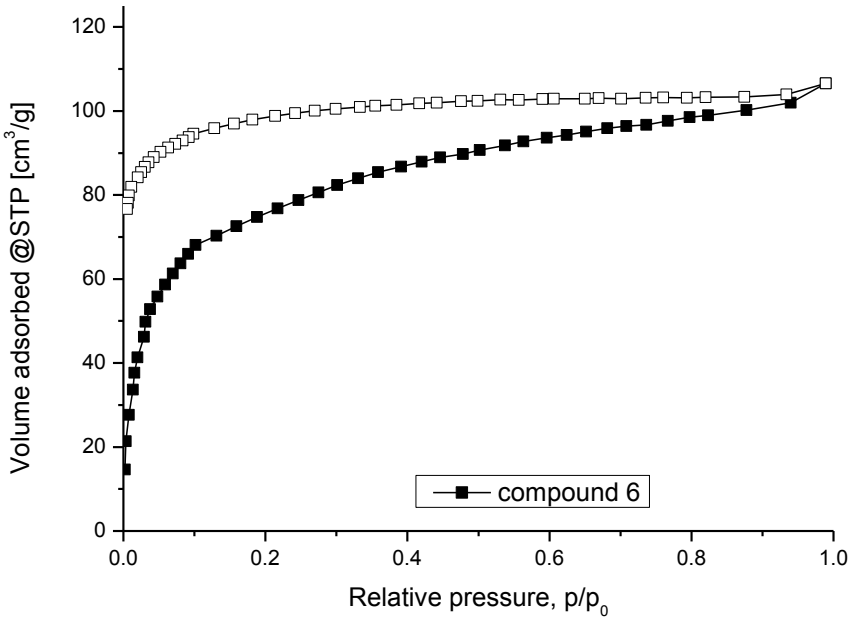


Figure S35b. Nitrogen sorption isotherms of $[DyL(H_2O)_2]_n$ (**6)** recorded at 77 K. (different synthesis, the same condition). Filled symbols are for adsorption, empty symbols are for desorption (S_{BET} = 298 m^2/g).

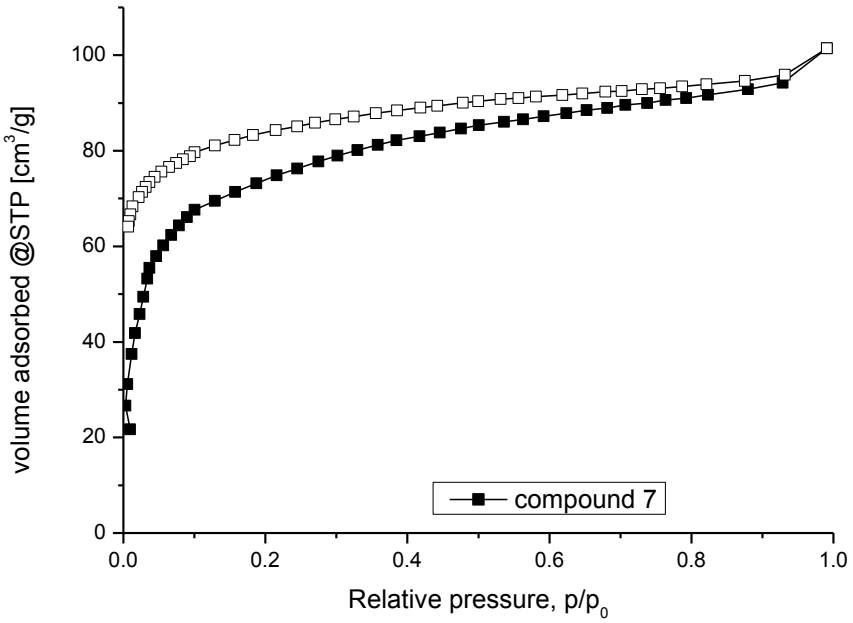
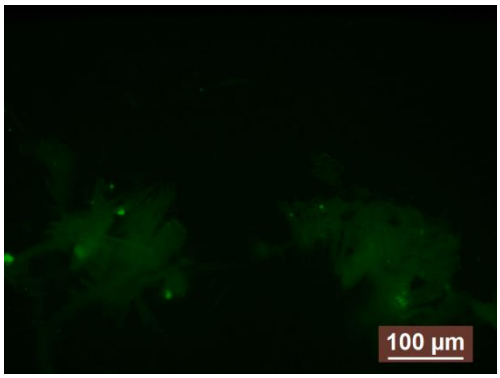
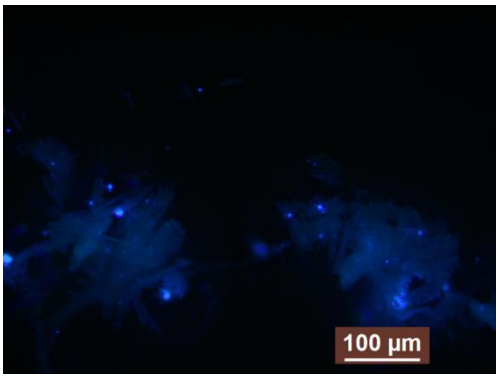


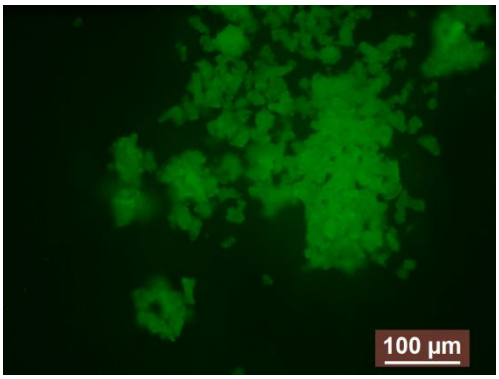
Figure S36. Nitrogen sorption isotherms of $[HoL(H_2O)_2]_n \cdot 1.33DMF \cdot H_2O$ (**7)** .Filled symbols are for adsorption, empty symbols are for desorption (S_{BET} = 286 m^2/g).

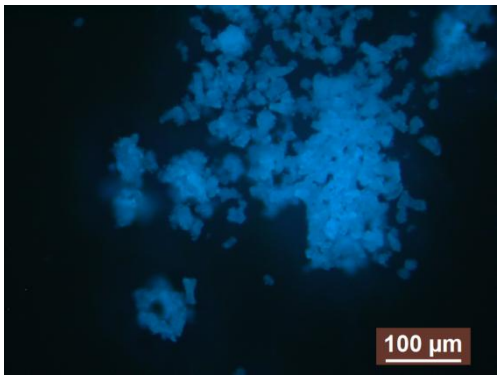
6. Fluorescence

Ligand 

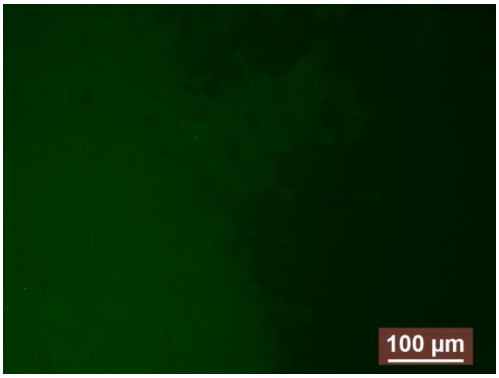


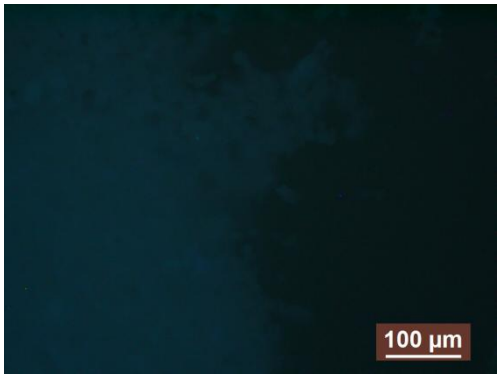
(b)

1 (a) 

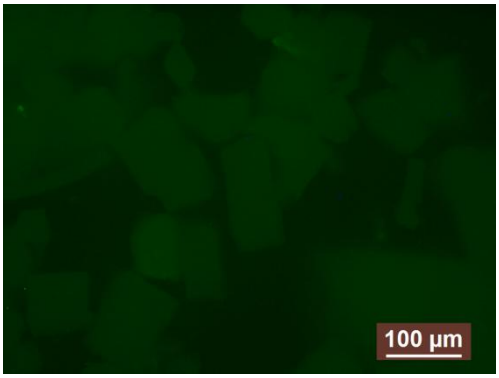


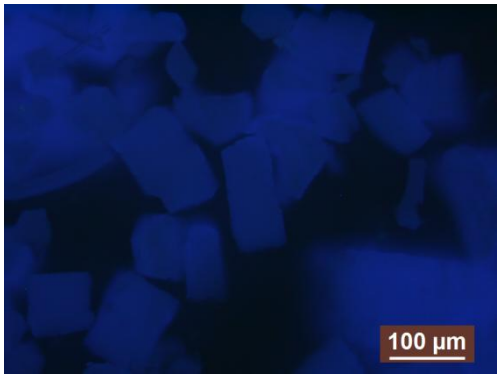
(b)

2 (a) 

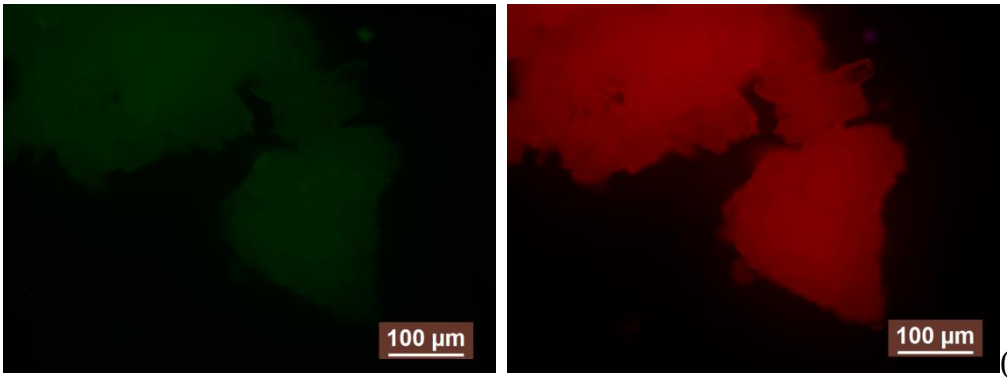


(b)

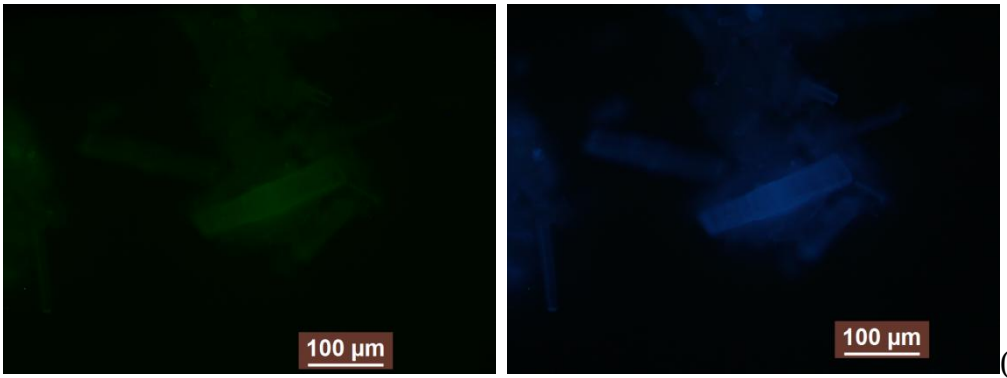
3 (a) 



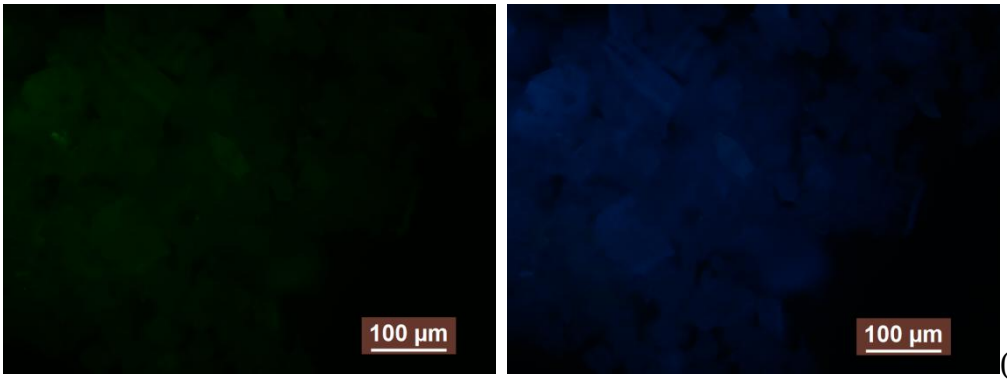
(b)



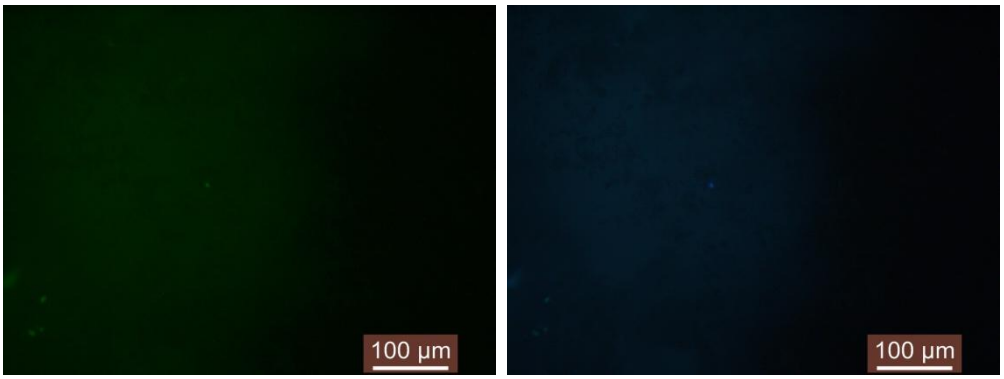
4 (a) (b)



5 (a) (b)



6 (a) (b)



7 (a) (b)

Figure S37. Fluorescence imaging of representative samples (Ligand; C1-7): a) green light (470 nm), or b). UV (365 nm), Objective 20x.

7. Catalytic experiments

The chemical reagents used in catalytic reaction were as follows: 2-naphthol (1 mmol), acetic anhydride (1.5 equiv.), catalyst (1 mmol%) and $CHCl_3$ (2 mL). The catalytic reaction was performed at room temperature for 24 hours. The catalyst was activated by exchange of the solvent with $CHCl_3$ (3·3 mL) at RT for 24 hours, followed by pore evacuation drying at 80 °C during of 20 hours.

Filtration test: After running the reaction for 5 hours, the catalyst material (**3**) was separated by centrifugation. The filtrate was separated and isolated (yield 65%). Then the reaction was repeated and after 5 hours the clear supernatant solution was filtered and the reaction was continued at room temperature for another 19 hours to a total run time of 24 h. The filtrate was isolated and analyzed and the yield of product had not increased to the yield of the separation after 5 h (both yields were 65%).

8. Crystallographic Data

Table S2. Bond distances (Å) and angles(°) for shI_3971_BeDa.

Ce1-O1[1]	2.461(4)	C3-C4	1.385(6)
Ce1-O1*w*	2.524(3)	C5-C6	1.371(7)
Ce1-O2	2.467(4)	C6-C7	1.415(7)
Ce1-O3[4]	2.574(3)	C8-C10	1.391(7)
O1-C1	1.256(6)	C10-C13	1.506(7)
O2-C1	1.252(6)	C11-C14	1.524(10)
O3-C18	1.270(4)	C14-C15	1.361(6)
C1-C2	1.493(7)	C15-C16	1.395(7)
C2-C3	1.383(7)	C16-C17	1.383(6)
C2-C7	1.371(7)	C17-C18	1.469(9)

[1)] – 1– *x*, – *y*, – 1 – *z*; [2)] ½ + *x*, + *y*, – 1– *z*; [3)] – ½ – *x*, – *y*, + *z*; [4)] – 1 – *x*, ½ + *y*, – ½ + *z*; [5)] ½ + *x*, – ½ – *y*, – ½ + z

C1-O1-Ce1[1]	165.0(3)	C10-C8-C9	120.7(5)
C1-O2-Ce1	113.9(4)	C8-C9-C8[3]	119.2(7)
C18-O3-Ce1[2]	95.2(4)	C8-C9-C12	120.4(3)
O1-C1-C2	120.0(5)	C8-C10-C11	118.6(6)
O2-C1-O1	123.2(5)	C8-C10-C13	120.6(5)

O2-C1-C2	116.7(5)	C11-C10-C13	120.7(6)
C3-C2-C1	120.7(5)	C10-C11-C10[3]	122.3(7)
C7-C2-C1	120.4(5)	C10-C11-C14	118.9(4)
C7-C2-C3	118.9(5)	C15-C14-C11	121.3(4)
C4-C3-C2	121.1(5)	C15[3]-C14-C15	117.4(7)
C3-C4-C5	120.9(5)	C14-C15-C16	122.6(6)
C4-C5-C8	119.7(5)	C17-C16-C15	119.0(6)
C6-C5-C4	117.5(5)	C16-C17-C16[3]	119.4(7)
C6-C5-C8	122.7(5)	C16-C17-C18	120.3(4)
C5-C6-C7	121.7(5)	O3-C18-Ce1[2]	59.6(3)
C2-C7-C6	119.7(5)	O3[3]-C18-O3	119.3(7)
C9-C8-C5	121.0(5)	O3-C18-C17	120.4(3)
C10-C8-C5	118.3(5)		

[1)] $-1-x,-y,-1-z$; [2)] $-\frac{1}{2}+x,-\frac{1}{2}-y,\frac{1}{2}+z$; [3)] $-3/2-x,-1-y,+z$

Table S3. Bond distances (Å) and angles(°) for shI_3972_BeDa.

Nd1-O1	2.558(6)	C10-C24	1.469(13)
Nd1-O1*w*	2.477(6)	C11-C12	1.405(12)
Nd1-O2	2.535(6)	C11-C16	1.514(11)
Nd1-O2*w*	2.515(6)	C12-C13	1.409(12)
Nd1-O3[1]	2.464(6)	C12-C17	1.505(12)
Nd1-O3[2]	2.947(6)	C13-C14	1.488(13)
Nd1-O42	2.454(6)	C17-C18	1.406(13)
Nd1-O5[3]	2.415(6)	C17-C22	1.350(13)
Nd1-O6[4]	2.395(6)	C18-C19	1.389(13)
Nd1-C1	2.928(8)	C19-C20	1.334(13)
O1-C1	1.291(11)	C20-C21	1.396(14)
O2-C1	1.252(10)	C20-C23	1.478(12)
O3-C23	1.246(11)	C21-C22	1.387(14)

O4-C23	1.268(10)	C24-C25	1.421(13)
O5-C30	1.247(10)	C24-C29	1.378(14)
O6-C30	1.260(11)	C25-C26	1.391(14)
C1-C2	1.472(11)	C26-C27	1.354(13)
C2-C3	1.392(13)	C27-C28	1.401(12)
C2-C7	1.387(13)	C27-C30	1.503(13)
C3-C4	1.399(13)	C28-C29	1.396(13)
C4-C5	1.402(14)	O7-C31	1.239(15)
C5-C6	1.358(13)	N1-C31	1.331(17)
C5-C8	1.509(11)	N1-C32	1.442(17)
C6-C7	1.379(12)	N1-C33	1.457(17)
C8-C9	1.442(13)	O8-C34	1.25(5)
C8-C13	1.392(12)	N2-C34	1.41(5)
C9-C10	1.388(12)	N2-C35	1.40(5)
C9-C15	1.524(13)	N2-C36	1.37(5)
C10-C11	1.421(12)		

[1)] ½ – *x*, ½ + *y*, 3/2 – *z*; [2)] – ½ + *x*, ½ – *y*, ½ + *z*; [3)] ½ + *x*, 3/2 – *y*, ½ + *z*; [4)] ½ – *x*, – ½ + *y*, 3/2 – *z*

C1-O1-Nd1	93.2(5)	C13-C12-C17	118.4(8)
C1-O2-Nd1	95.2(5)	C8-C13-C12	118.6(8)
$Nd1^{1}$-O3-$Nd1^{2}$	114.0(2)	C8-C13-C14	119.8(8)
C23-O3-$Nd1^{1}$	160.9(6)	C12-C13-C14	121.5(8)
C23-O3-$Nd1^{2}$	84.6(5)	C18-C17-C12	119.4(9)
C23-O4-$Nd1^{2}$	108.0(5)	C22-C17-C12	123.9(9)
C30-O5-$Nd1^{3}$	126.4(6)	C22-C17-C18	116.7(9)
C30-O6-$Nd1^{4}$	173.4(6)	C19-C18-C17	121.8(10)
O1-C1-Nd1	60.7(4)	C20-C19-C18	120.1(9)
O1-C1-C2	119.3(8)	C19-C20-C21	119.4(9)

O2-C1-Nd1	59.6(4)	C19-C20-C23	121.0(9)
O2-C1-O1	120.3(8)	C21-C20-C23	119.2(8)
O2-C1-C2	120.4(8)	C22-C21-C20	120.0(9)
C2-C1-Nd1	178.6(6)	C17-C22-C21	122.0(10)
C3-C2-C1	121.6(9)	O3-C23-O4	120.5(8)
C3-C2-C7	117.4(9)	O3-C23-C20	121.4(8)
C7-C2-C1	121.0(9)	O4-C23-C20	118.0(8)
C2-C3-C4	120.9(9)	C25-C24-C10	123.3(9)
C3-C4-C5	120.1(9)	C29-C24-C10	119.6(9)
C4-C5-C8	119.2(9)	C29-C24-C25	117.0(9)
C6-C5-C4	118.4(9)	C26-C25-C24	119.5(10)
C6-C5-C8	122.5(9)	C27-C26-C25	122.4(9)
C5-C6-C7	121.7(9)	C26-C27-C28	119.4(9)
C6-C7-C2	121.4(9)	C26-C27-C30	121.5(8)
C9-C8-C5	119.2(8)	C28-C27-C30	119.0(8)
C13-C8-C5	119.7(8)	C29-C28-C27	118.5(9)
C13-C8-C9	121.0(8)	C24-C29-C28	123.1(10)
C8-C9-C15	121.1(9)	O5-C30-O6	124.0(8)
C10-C9-C8	118.8(8)	O5-C30-C27	117.5(8)
C10-C9-C15	119.8(9)	O6-C30-C27	118.5(8)
C9-C10-C11	121.2(8)	C31-N1-C32	123.1(14)
C9-C10-C24	118.3(8)	C31-N1-C33	116.3(12)
C11-C10-C24	120.4(8)	C32-N1-C33	120.5(14)
C10-C11-C16	120.3(8)	O7-C31-N1	123.4(15)
C12-C11-C10	118.4(8)	C34-N2-C35	126(4)
C12-C11-C16	121.2(8)	C36-N2-C34	107(4)
C11-C12-C13	122.0(8)	C36-N2-C35	126(4)
C11-C12-C17	119.6(8)	O8-C34-N2	113(4)

[1)] ½ – *x*, – ½ + *y*, 3/2 – *z*; [2)] ½ + *x*, ½ – *y*, – ½ + *z*; [3)] – ½ + *x*, 3/2 – *y*, – ½ + *z*; [4)] ½ – *x*, ½ + *y*, 3/2 – *z*;

Table S4. Bond distances (Å) and angles(°) for shI_3984_BeDa

La1-O1	2.503(7)	C5-C8	1.487(11)
La1-O1[1]	3.017(7)	C6-C7	1.371(12)
La1-O1*w*	2.545(7)	C8-C9	1.396(10)
La1-O2[1]	2.497(7)	C8-C10	1.394(13)
La1-O3[2]	2.611(6)	C9-C12	1.52(2)
O1-C1	1.291(11)	C10-C11	1.414(11)
O2-C1	1.237(11)	C10-C13	1.513(12)
O3-C18	1.276(8)	C11-C14	1.506(19)
C1-C2	1.483(11)	C14-C15	1.379(12)
C2-C3	1.349(11)	C14-C15[3]	1.380(12)
C2-C7	1.427(12)	C15-C16	1.377(14)
C3-C4	1.385(12)	C16-C17	1.381(11)
C4-C5	1.381(13)	C17-C18	1.506(17)
C5-C6	1.388(13)		

[1)] ½ + *x*, + *y*, 1 – *z*; [2)] + *x*, ½ – *y*, ½ – *z*; [3)] 3/2 – *x*, – *y*, + *z*

La1-O1-La1[1]	116.0(2)	C10-C8-C5	117.6(7)
C1-O1-La1[1]	83.4(5)	C10-C8-C9	121.7(8)
C1-O1-La1	159.9(6)	C8-C9-C8[3]	118.7(11)
C1-O2-La1[1]	110.0(6)	C8[3]-C9-C12	120.6(6)
C18-O3-La1[2]	93.6(5)	C8-C10-C11	118.8(8)
O1-C1-C2	120.0(8)	C8-C10-C13	121.1(8)
O2-C1-O1	120.6(8)	C11-C10-C13	120.1(9)
O2-C1-C2	119.4(8)	C10-C11-C10[3]	120.4(12)
C3-C2-C1	123.8(8)	C10-C11-C14	119.8(6)
C3-C2-C7	117.6(7)	C10[3]-C11-C14	119.8(6)
C7-C2-C1	118.3(7)	C15-C14-C11	120.5(6)

C2-C3-C4	122.1(8)	C15[3]-C14-C15	119.1(12)
C5-C4-C3	121.0(9)	C14-C15-C16	120.5(10)
C4-C5-C6	117.5(8)	C17-C16-C15	120.6(10)
C4-C5-C8	120.3(9)	C16[3]-C17-C16	118.8(12)
C6-C5-C8	122.0(8)	C16-C17-C18	120.6(6)
C7-C6-C5	121.8(9)	O3-C18-La1[2]	61.0(5)
C6-C7-C2	119.9(8)	O3[3]-C18-O3	122.1(11)
C9-C8-C5	120.7(8)	O3-C18-C17	119.0(5)

[1)] 1 – *x*, 1 – *y*, 1 – *z*; [2)] 3/2 – *x*, – ½ + *y*, ½ – *z*; [3)] 3/2 – *x*, – *y*, + *z*