Electronic supplementary information (ESI)

Synthesis, structure and adsorption property of lanthanide-organic frameworks with pyridine-3,5-bis(phenyl-4-carboxylate)

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Synthetic procedure of solvent exchanged sample. The as-synthesized samples were immersed in methanol, acetone, 1,4-dioxane, cyclohexane (CYH) and hexane, respectively. The solvents were decanted every 8 h and the fresh solvents were added. After 3 days, the samples were removed from the solvents and dried in air. In order to find the optimal solvent, the activated samples were studied by PXRD measurements. In this experiment, we found CYHis the optimal solvent as confirmed by PXRD. After soaked in CYH for 3 days, in order to find the optimal activating temperature, the samples were activated under a dynamic vacuum at different temperature for 10 h. Then, the samples were studied by PXRD and TGA. In this experiment, we found that 80 ℃ is the optimal temperature. As a result, the as-synthesized samples were soaked in CYH for 3 days. The exchange of DMF by CYH was confirmed by elemental analyses: $\{[Er_4(L)_3(\mu_3\text{-}OH)_4(H_2O)_4]\ (NO_3)_2 \cdot 1.5CYH \cdot 2H_2O\}_n$. Anal. Calcd for $C_{66}H_{67}N_5O_{28}Er_4$: C, 38.72; H, 3.30; N, 3.42%. Found: C, 37.73; H, 3.50; N, 3.72%.

As shown in Fig. S6a, before 150 ℃, the weight loss of 7.61% (calcd 7.91%) corresponds to the release of free CYH and water molecules. $\{[Yb_4(L)_3(\mu_3\text{-}OH)_4(H_2O)_4]\cdot(NO_3)_2\cdot 1.5CYH\cdot 3.5H_2O\}_n$. Anal. Calcd for $C_{66}H_{70}N_5O_{29.5}Yb_4$: C, 37.79; H, 3.36; N, 3.34%. Found: C, 37.32; H, 3.51; N, 3.31%. As shown in Fig. S6b, before 150 ℃, the weight loss of 9.01% (calcd 8.81%) corresponds to the release of free CYH and water molecules. $\{[Lu_4(L)_3(\mu_3\text{-}OH)_4(H_2O)_4]\cdot(NO_3)_2\cdot 1.5CYH\cdot 3H_2O\}_n$. Anal. Calcd for $C_{66}H_{69}N_5O_{29}Lu_4$: C, 37.82; H, 3.32; N, 3.34%. Found: C, 37.46; H, 3.20; N, 3.24%. As shown in Fig. S6c, before 150 ℃, the weight loss of 8.34% (calcd 8.59%) corresponds to the release of free CYH and water molecules. Then, the samples were activated under a dynamic vacuum at 80 ℃ for 10 hours to generate the desolvated form.

Table S1. Selected bond lengths (Å) and angles (°) for **1 - 3**.

Compound **1**			
Er(1)-O(3)#1	2.255(3)	Er(1)-O(6)#2	2.292(2)
Er(1)-O(2)	2.294(3)	Er(1)-O(4)#3	2.333(3)
Er(1)-O(7)	2.3559(17)	Er(1)-O(6)	2.397(2)
Er(1)-O(8)	2.437(3)	Er(2)-O(1)	2.277(4)
Er(2)-O(6)	2.366(2)	Er(2)-O(5)	2.427(7)
O(3)#1-Er(1)-O(6)#2	149.19(9)	O(3)#1-Er(1)-O(2)	106.99(14)
O(6)#2-Er(1)-O(2)	87.64(12)	O(3)#1-Er(1)-O(4)#3	103.69(13)
O(6)#2-Er(1)-O(4)#3	86.48(10)	O(2)-Er(1)-O(4)#3	128.48(13)
O(3)#1-Er(1)-O(7)	81.16(10)	O(6)#2-Er(1)-O(7)	72.34(9)
O(2)-Er(1)-O(7)	145.94(13)	O(4)#3-Er(1)-O(7)	78.61(10)
O(3)#1-Er(1)-O(6)	84.50(10)	O(6)#2-Er(1)-O(6)	72.19(11)
O(2)-Er(1)-O(6)	77.32(11)	O(4)#3-Er(1)-O(6)	146.48(9)
O(7)-Er(1)-O(6)	70.51(9)	O(3)#1-Er(1)-O(8)	79.27(15)
O(6)#2-Er(1)-O(8)	131.43(14)	O(2)-Er(1)-O(8)	73.64(13)
O(4)#3-Er(1)-O(8)	72.70(12)	O(7)-Er(1)-O(8)	140.01 (14)
O(6)-Er(1)-O(8)	140.63(10)	O(1)#2-Er(2)-O(1)	111.00(10)
O(1)#2-Er(2)-O(6)#2	82.50(13)	O(6)#2-Er(2)-O(6)#4	71.45(8)
O(1)#2-Er(2)-O(6)	150.13(11)	O(1)#4-Er(2)-O(6)	86.81(15)
O(1)-Er(2)-O(5)	72.10(10)	O(6)#2-Er(2)-O(5)	137.61(5)
Symmetry codes: #1 -y+1/2, -z, x-1/2; #2 z, x, y; #3 x-1/2, -y+1/2, -z; #4 y, z, x.			
Compound **2**			
Yb(1)-O(3)	2.195(5)	Yb(1)-O(2)#1	2.203(6)
Yb(1)-O(6)#2	2.234(4)	Yb(1)-O(4)#2	2.282(5)

Yb(1)-O(7)	2.309(3)	Yb(1)-O(6)	2.327(4)
Yb(1)-O(8)	2.372(7)	Yb(2)-O(1)#5	2.226(7)
Yb(2)-O(6)#7	2.310(4)	Yb(2)-O(5)	2.413(11)
O(3)-Yb(1)-O(2)#1	110.3(2)	O(3)-Yb(1)-O(6)#2	149.80(18)
O(2)#1-Yb(1)-O(6)#2	85.2(2)	O(3)-Yb(1)-O(4)#2	104.1(2)
O(2)#1-Yb(1)-O(4)#2	123.7(2)	O(6)#2-Yb(1)-O(4)#2	86.58(19)
O(3)-Yb(1)-O(7)	81.55(18)	O(2)#1-Yb(1)-O(7)	147.1(2)
O(6)#2-Yb(1)-O(7)	72.57(17)	O(4)#2-Yb(1)-O(7)	79.72(17)
O(3)-Yb(1)-O(6)	85.02(18)	O(2)#1-Yb(1)-O(6)	79.44(19)
O(6)#2-Yb(1)-O(6)	72.2(2)	O(4)#2-Yb(1)-O(6)	147.66(17)
O(7)-Yb(1)-O(6)	70.91(16)	O(3)-Yb(1)-O(8)	79.1(3)
O(2)#1-Yb(1)-O(8)	73.4(2)	O(6)#2-Yb(1)-O(8)	131.0(3)
O(4)#2-Yb(1)-O(8)	71.1(2)	O(7)-Yb(1)-O(8)	139.5(2)
O(6)-Yb(1)-O(8)	141.1(2)	O(1)#5-Yb(2)-O(1)	111.0(2)
O(1)#5-Yb(2)-O(6)#7	83.1(3)	O(1)-Yb(2)-O(6)#7	86.4(3)
O(1)#6-Yb(2)-O(6)#7	150.0(3)	O(6)#7-Yb(2)-O(6)#8	71.14(16)
O(1)#5-Yb(2)-O(5)	72.1(2)	O(6)#7-Yb(2)-O(5)	137.80(10)

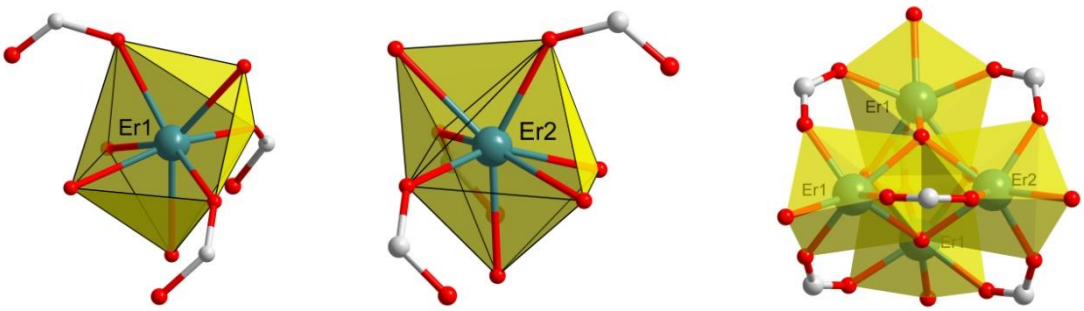
Symmetry codes: #1 -z+1, x+1/2, -y+3/2; #2 z-1, x, y+1; #5 -z+1/2, -x, y+1/2; #6 -y, z-1/2, -x+1/2; #7 x-1/2, -y+1/2, -z+2; #8 y-1/2, -z+3/2, -x+1.

Compound **3**

Lu(1)-O(3)#1	2.218(3)	Lu(1)-O(6)	2.256(2)
Lu(1)-O(2)	2.257(4)	Lu(1)-O(4)	2.297(3)
Lu(1)-O(7)	2.3176(18)	Lu(1)-O(6)#1	2.356(2)
Lu(1)-O(8)	2.397(3)	Lu(2)-O(1)	2.243(4)
Lu(2)-O(6)	2.327(2)	Lu(2)-O(5)	2.391(7)

O(3)#1-Lu(1)-O(6)	149.09(10)	O(3)#1-Lu(1)-O(2)	107.06(15)
O(6)-Lu(1)-O(2)	87.64(13)	O(3)#1-Lu(1)-O(4)	103.69(13)
O(6)-Lu(1)-O(4)	86.42(11)	O(2)-Lu(1)-O(4)	128.55(14)
O(3)#1-Lu(1)-O(7)	81.10(10)	O(6)-Lu(1)-O(7)	72.30(10)
O(2)-Lu(1)-O(7)	145.94(14)	O(4)-Lu(1)-O(7)	78.50(10)
O(3)#1-Lu(1)-O(6)#1	84.53(10)	O(6)-Lu(1)-O(6)#1	72.12(11)
O(2)-Lu(1)-O(6)#1	77.30(11)	O(4)-Lu(1)-O(6)#1	146.36(10)
O(7)-Lu(1)-O(6)#1	70.54(9)	O(3)#1-Lu(1)-O(8)	78.94(16)
O(6)-Lu(1)-O(8)	131.85(15)	O(2)-Lu(1)-O(8)	73.72(14)
O(4)-Lu(1)-O(8)	72.99(13)	O(7)-Lu(1)-O(8)	139.88(14)
O(6)#1-Lu(1)-O(8)	140.43(11)	O(1)#1-Lu(2)-O(1)#2	111.12(10)
O(1)#1-Lu(2)-O(6)	149.94(12)	O(1)#2-Lu(2)-O(6)	82.21(13)
O(1)-Lu(2)-O(6)	86.91(16)	O(6)-Lu(2)-O(6)#1	71.42(8)
O(1)#1-Lu(2)-O(5)	72.23(11)	O(6)-Lu(2)-O(5)	137.62(5)

Symmetry codes: #1 -y+1, z-1/2, -x+3/2; #2 -z+3/2, -x+1, y+1/2.



(a) (b) (c)

Fig. S1. Polyhedral view of the coordination geometry around Er1 (a), Er2 (b) and the SBU (c).

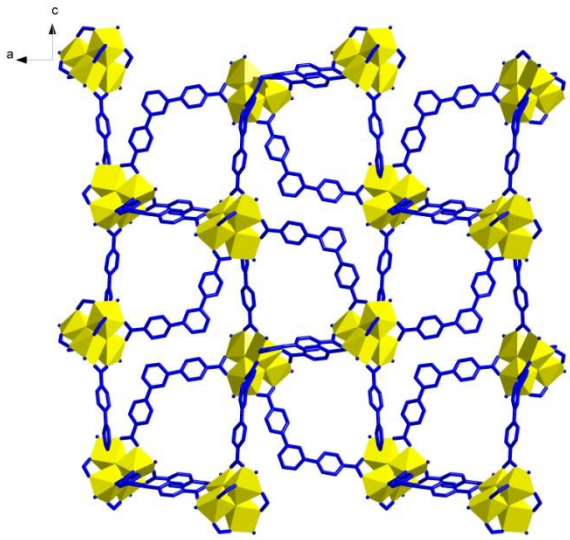


Fig. S2. The 3D structure of **1** formed by L^{2-} and SBUs along the *b* axis.

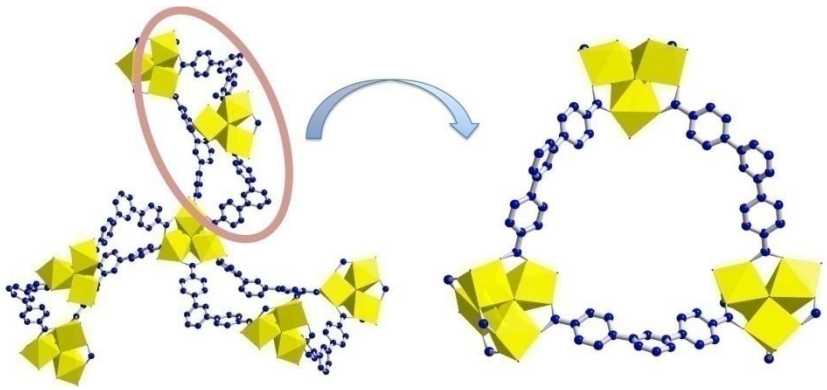


Fig. S3. The $[Er_4(COO)_6(\mu_3\text{-}OH)_4(H_2O)_4]$ SBU and the macrocyclic ring formed by three L^{2-} and three SBUs with a diameter of 15.2 Å in **1**.

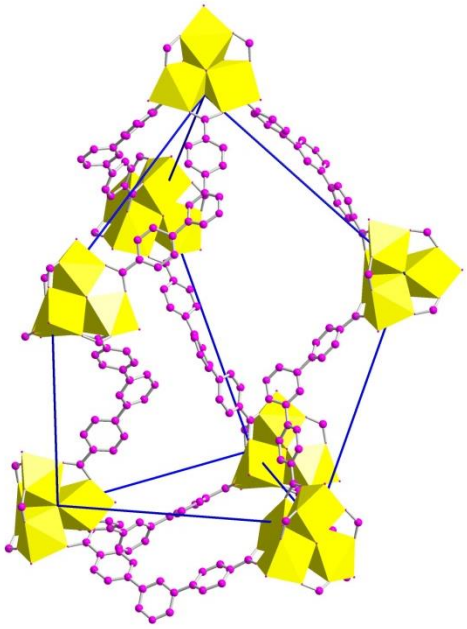


Fig. S4. The cage formed by nine L^{2-} ligands and seven SBUs in **1**.

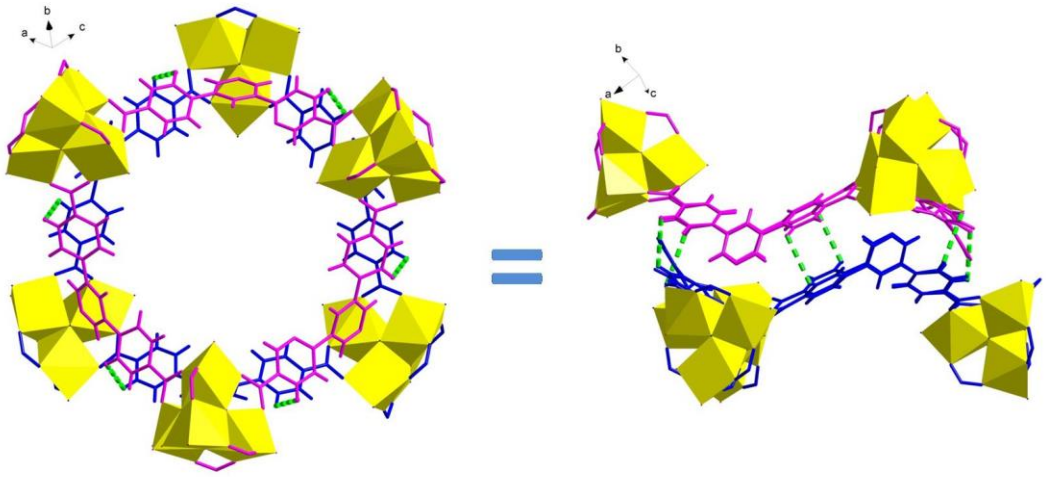
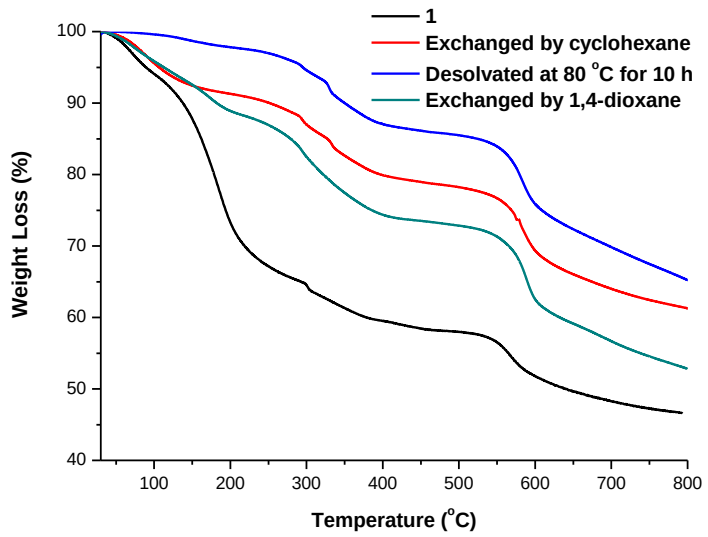
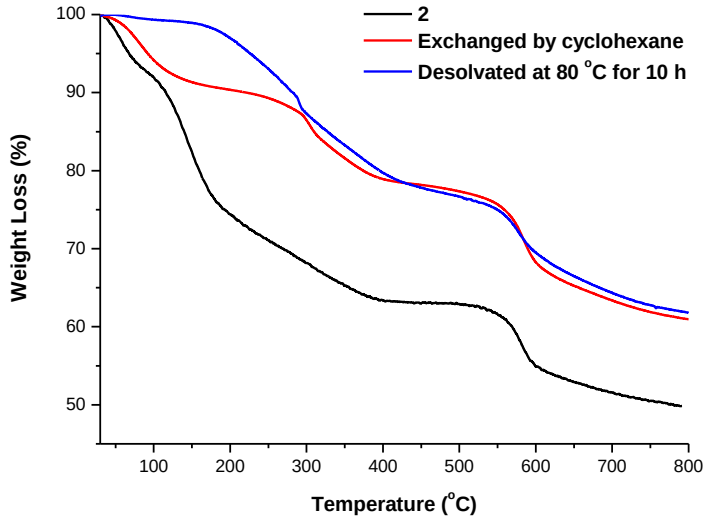


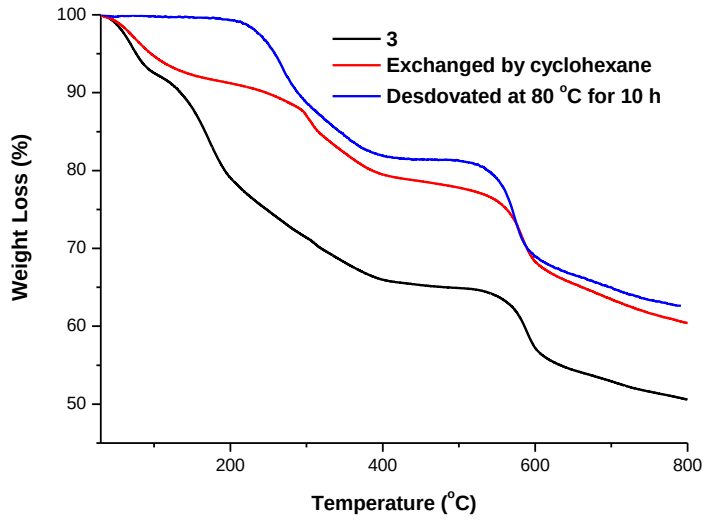
Fig. S5. A distance of 3.32 Å between two interpenetrating frameworks.


1
Exchanged by cyclohexane
Desolvated at 80 °C for 10 h
Exchanged by 1,4-dioxane
Weight Loss (%)
Temperature (°C)
100
90
80
70
60
50
40
100
200
300
400
500
600
700
800

(a)

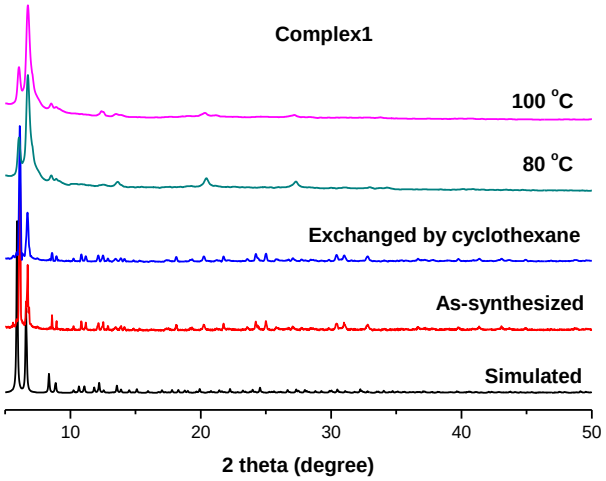

2
Exchanged by cyclohexane
Desolvated at 80 °C for 10 h
Weight Loss (%)
Temperature (°C)
100
90
80
70
60
50
100
200
300
400
500
600
700
800

(b)

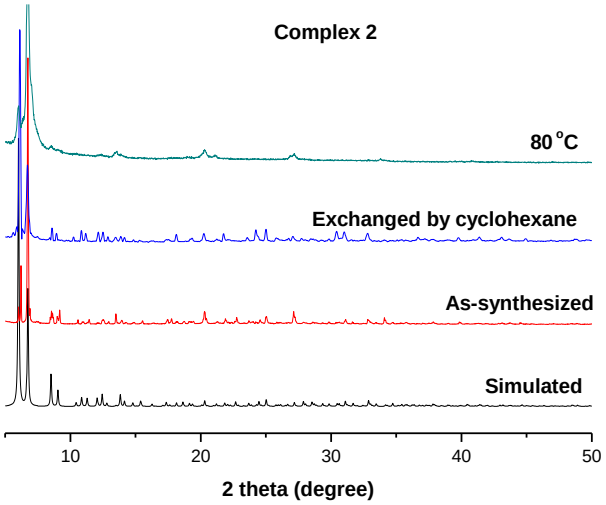


(c)

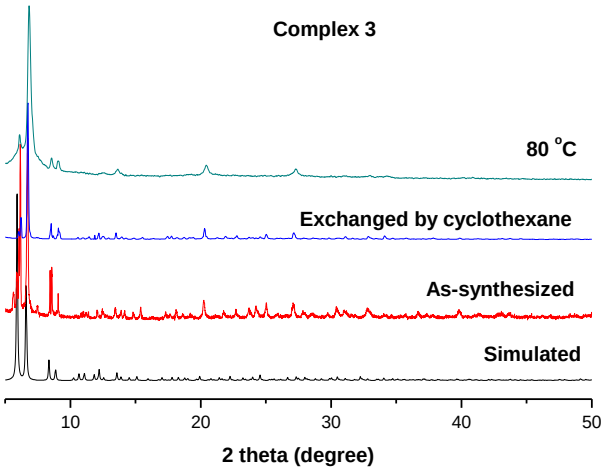
Fig. S6. The TGA curves of **1** - **3**.



(a)



(b)



(c)

Fig. S7. PXRD patterns of **1** - **3** under varied conditions.

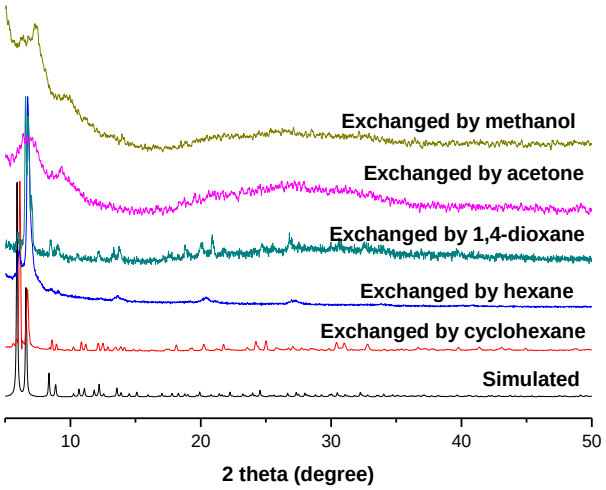
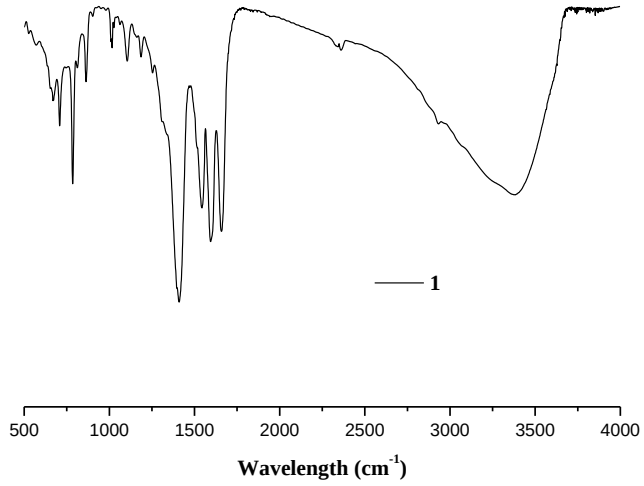
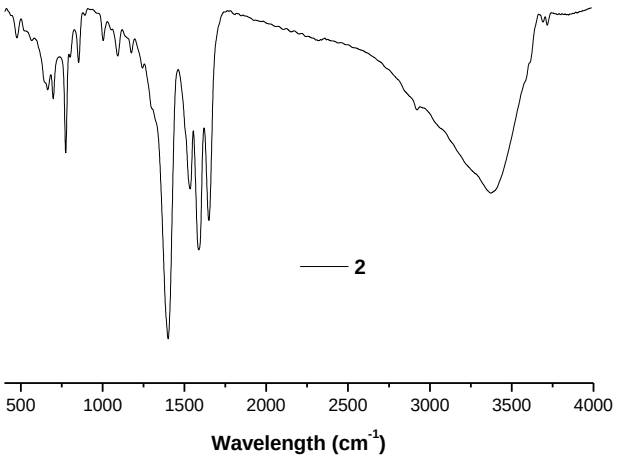


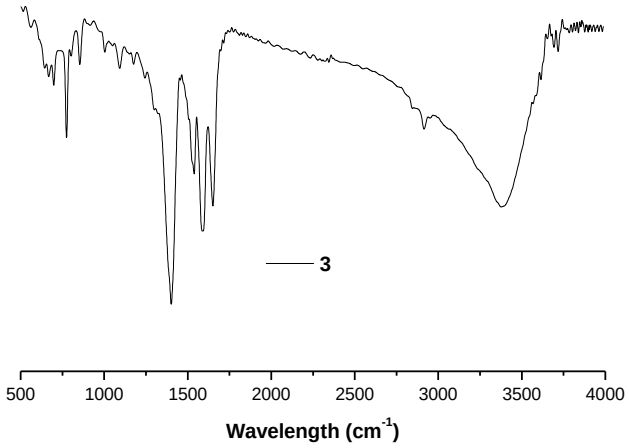
Fig. S8. PXRD patterns of **1** in different solvent.


1
500
1000
1500
2000
2500
3000
3500
4000
Wavelength (cm-1)

(a)


2
500
1000
1500
2000
2500
3000
3500
4000
Wavelength (cm-1)

(b)



(c)

Fig. S9. IR spectra of **1** - **3**.

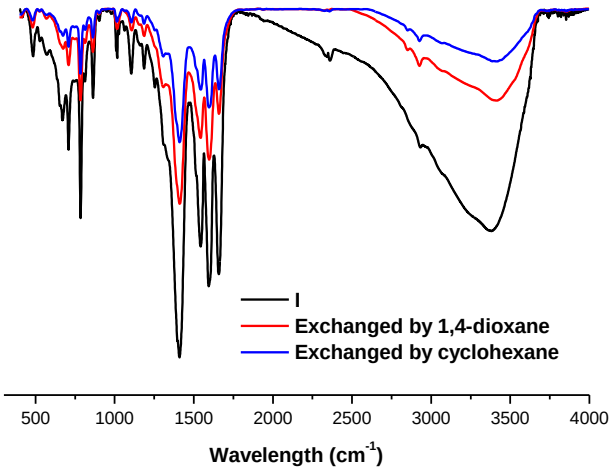


Fig. S10. IR spectra under varied conditions.