Supporting Information

A Series of Lanthanide Compounds Based on Pyridine-3,5-dicarboxylate and Succinate Ligands: Syntheses, Structures and Properties

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Contents

Table S1. Crystal data and structure refinement of compounds **1-6.**

	1	**2**	**3**	**4**	**5**	**6**
Chemical formula	$C_9H_{15}NO_{11}Pr$	$C_9H_{15}NO_{11}Eu$	$C_9H_{15}NO_{11}Tb$	$C_9H_{15}NO_{11}Er$	$C_9H_{13}NO_{11}Yb$	$C_9H_{13}NO_{11}Lu$
Formula weight	454.13	465.18	472.14	480.48	468.24	470.17
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	triclinic
Space group	$P\,2_1/c$	$P\,2_1/c$	$P\,2_1/c$	$P\,2_1/c$	P -1	P -1
a /Å	15.930(6)	15.9131(14)	15.8734(12)	15.8585(14)	5.3448(6)	5.3400(8)
b /Å	13.588(5)	13.5396(11)	13.4525(10)	13.4190(11)	8.9517(10)	8.9530(14)
c /Å	6.663(2)	6.6475(6)	6.6309(5)	6.6158(6)	15.6623(18)	15.655(2)
α/°	90	90	90	90	104.912(1)	104.760(2)
β/°	97.392(5)	97.662(1)	97.8615(8)	97.925(1)	93.036(1)	93.015(2)
γ/°	90	90	90	90	97.157(1)	97.273(2)
V/Å^3	1430.2(9)	1419.5(2)	1402.63(18)	1394.4(2)	715.65(14)	715.11(18)
Z	4	4	4	4	2	2
T/K	296(2)	296(2)	296(2)	296(2)	293(2)	293(2)
F(000)	892	908	916	928	448	450
Dcalcd/g·cm^{-3}	2.109	2.177	2.236	2.289	2.173	2.184
μ/mm^{-1}	3.465	4.478	5.102	6.078	6.583	6.952
λ/Å	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Reflections collected	6748	7176	7014	7079	3715	3672
GOF	1.055	1.061	1.052	1.001	1.068	1.044
$R_1[I=2\sigma(I)]$[a]	0.0525	0.0325	0.0227	0.0304	0.0245	0.0269
$wR_2[I=2\sigma(I)]$[b]	0.1503	0.0843	0.0626	0.0812	0.0616	0.0774

[a] $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$

Table S2. Selected bond lengths (Å) and bond angles (º) for compounds **1**-**6**.

Compound **1**

Pr(1)-O(2)#1	2.405(6)	O(5)-Pr(1)-O(3W)	77.9(3)
Pr(1)-O(1)	2.498(6)	O(2)#1-Pr(1)-O(4)#2	92.4(2)
Pr(1)-O(2W)	2.522(7)	O(1)-Pr(1)-O(4)#2	74.2(2)
Pr(1)-O(1W)	2.528(7)	O(2W)-Pr(1)-O(4)#2	87.4(2)
Pr(1)-O(5)	2.530(6)	O(1W)-Pr(1)-O(4)#2	72.8(2)
Pr(1)-O(3W)	2.537(7)	O(5)-Pr(1)-O(4)#2	127.0(2)
Pr(1)-O(4)#2	2.543(6)	O(3W)-Pr(1)-O(4)#2	147.8(3)
Pr(1)-O(3)#2	2.561(6)	O(2)#1-Pr(1)-O(3)#2	133.1(2)
Pr(1)-O(6)	2.562(8)	O(1)-Pr(1)-O(3)#2	113.18(19)
O(2)#1-Pr(1)-O(1)	74.4(2)	O(2W)-Pr(1)-O(3)#2	70.3(2)
O(2)#1-Pr(1)-O(2W)	145.6(2)	O(1W)-Pr(1)-O(3)#2	70.4(2)
O(1)-Pr(1)-O(2W)	72.4(2)	O(5)-Pr(1)-O(3)#2	76.1(2)
O(2)#1-Pr(1)-O(1W)	71.2(2)	O(3W)-Pr(1)-O(3)#2	143.1(3)
O(1)-Pr(1)-O(1W)	130.5(2)	O(4)#2-Pr(1)-O(3)#2	51.0(2)
O(2W)-Pr(1)-O(1W)	140.2(2)	O(2)#1-Pr(1)-O(6)	77.3(3)
O(2)#1-Pr(1)-O(5)	127.9(2)	O(1)-Pr(1)-O(6)	135.9(3)
O(1)-Pr(1)-O(5)	141.5(3)	O(2W)-Pr(1)-O(6)	122.3(3)
O(2W)-Pr(1)-O(5)	76.7(3)	O(1W)-Pr(1)-O(6)	67.6(3)
O(1W)-Pr(1)-O(5)	88.0(3)	O(5)-Pr(1)-O(6)	50.6(3)
O(2)#1-Pr(1)-O(3W)	83.8(3)	O(3W)-Pr(1)-O(6)	69.8(3)
O(1)-Pr(1)-O(3W)	74.0(3)	O(4)#2-Pr(1)-O(6)	140.4(3)
O(2W)-Pr(1)-O(3W)	78.5(3)	O(3)#2-Pr(1)-O(6)	110.9(3)
O(1W)-Pr(1)-O(3W)	134.2(3)		

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

Compound **2**

Eu(1)-O(4)#1	2.373(4)	O(5)-Eu(1)-O(1W)	77.23(16)
Eu(1)-O(3)#2	2.485(4)	O(4)#1-Eu(1)-O(1)	92.45(14)
Eu(1)-O(3W)	2.508(5)	O(3)#2-Eu(1)-O(1)	74.10(13)
Eu(1)-O(2W)	2.511(4)	O(3W)-Eu(1)-O(1)	146.64(17)
Eu(1)-O(5)	2.507(4)	O(2W)-Eu(1)-O(1)	73.41(14)
Eu(1)-O(1W)	2.511(4)	O(5)-Eu(1)-O(1)	126.94(15)
Eu(1)-O(1)	2.522(4)	O(1W)-Eu(1)-O(1)	86.58(16)
Eu(1)-O(2)	2.552(4)	O(4)#1-Eu(1)-O(2)	133.19(14)
Eu(1)-O(6)	2.558(5)	O(3)#2-Eu(1)-O(2)	113.03(12)
O(4)#1-Eu(1)-O(3)#2	74.48(14)	O(3W)-Eu(1)-O(2)	142.75(17)
O(4)#1-Eu(1)-O(3W)	84.05(18)	O(2W)-Eu(1)-O(2)	70.46(14)
O(3)#2-Eu(1)-O(3W)	73.00(16)	O(5)-Eu(1)-O(2)	76.09(14)
O(4)#1-Eu(1)-O(2W)	71.52(16)	O(1W)-Eu(1)-O(2)	69.74(15)
O(3)#2-Eu(1)-O(2W)	131.14(15)	O(1)-Eu(1)-O(2)	50.97(12)
O(3W)-Eu(1)-O(2W)	135.00(19)	O(4)#1-Eu(1)-O(6)	77.24(16)
O(4)#1-Eu(1)-O(5)	127.88(15)	O(3)#2-Eu(1)-O(6)	135.83(17)
O(3)#2-Eu(1)-O(5)	141.62(16)	O(3W)-Eu(1)-O(6)	70.9(2)
O(3W)-Eu(1)-O(5)	78.62(17)	O(2W)-Eu(1)-O(6)	67.21(19)
O(2W)-Eu(1)-O(5)	87.24(18)	O(5)-Eu(1)-O(6)	50.65(17)
O(4)#1-Eu(1)-O(1W)	145.59(15)	O(1W)-Eu(1)-O(6)	122.91(18)
O(3)#2-Eu(1)-O(1W)	72.20(14)	O(1)-Eu(1)-O(6)	140.58(18)
O(3W)-Eu(1)-O(1W)	78.3(2)	O(2)-Eu(1)-O(6)	111.09(17)

O(2W)-Eu(1)-O(1W)	139.67(14)		

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

Compound **3**

Tb(1)-O(1)	2.342(3)	O(3W)-Tb(1)-O(2W)	140.13(11)
Tb(1)-O(2)#1	2.462(3)	O(1)-Tb(1)-O(4)#2	92.07(10)
Tb(1)-O(6)	2.474(3)	O(2)#1-Tb(1)-O(4)#2	73.88(9)
Tb(1)-O(1W)	2.472(3)	O(6)-Tb(1)-O(4)#2	127.26(10)
Tb(1)-O(3W)	2.475(3)	O(1W)-Tb(1)-O(4)#2	146.08(13)
Tb(1)-O(2W)	2.480(3)	O(3W)-Tb(1)-O(4)#2	86.82(11)
Tb(1)-O(4)#2	2.505(3)	O(2W)-Tb(1)-O(4)#2	73.75(11)
Tb(1)-O(3)#2	2.531(3)	O(1)-Tb(1)-O(3)#2	133.63(10)
Tb(1)-O(5)	2.544(4)、	O(2)#1-Tb(1)-O(3)#2	113.12(9)
O(1)-Tb(1)-O(2)#1	74.66(10)	O(6)-Tb(1)-O(3)#2	75.61(10)
O(1)-Tb(1)-O(6)	128.01(11)	O(1W)-Tb(1)-O(3)#2	141.42(12)
O(2)#1-Tb(1)-O(6)	141.39(11)	O(3W)-Tb(1)-O(3)#2	69.82(11)
O(1)-Tb(1)-O(1W)	84.94(13)	O(2W)-Tb(1)-O(3)#2	70.82(10)
O(2)#1-Tb(1)-O(1W)	72.75(12)	O(4)#2-Tb(1)-O(3)#2	51.79(9)
O(6)-Tb(1)-O(1W)	78.39(12)	O(1)-Tb(1)-O(5)	76.68(11)
O(1)-Tb(1)-O(3W)	145.11(11)	O(2)#1-Tb(1)-O(5)	135.41(12)
O(2)#1-Tb(1)-O(3W)	71.55(10)	O(6)-Tb(1)-O(5)	51.33(11)
O(6)-Tb(1)-O(3W)	77.47(11)	O(1W)-Tb(1)-O(5)	71.35(16)
O(1W)-Tb(1)-O(3W)	77.09(15)	O(3W)-Tb(1)-O(5)	123.52(12)
O(1)-Tb(1)-O(2W)	71.59(12)	O(2W)-Tb(1)-O(5)	66.90(13)
O(2)#1-Tb(1)-O(2W)	131.59(11)	O(4)#2-Tb(1)-O(5)	140.63(13)
O(6)-Tb(1)-O(2W)	87.02(12)	O(3)#2-Tb(1)-O(5)	111.41(12)
O(1W)-Tb(1)-O(2W)	135.59(14)	O(3W)-Tb(1)-O(2W)	140.13(11)
Tb(1)-O(1)	2.342(3)	O(1)-Tb(1)-O(4)#2	92.07(10)
Tb(1)-O(2)#1	2.462(3)	O(2)#1-Tb(1)-O(4)#2	73.88(9)
Tb(1)-O(6)	2.474(3)	O(6)-Tb(1)-O(4)#2	127.26(10)
Tb(1)-O(1W)	2.472(3)	O(1W)-Tb(1)-O(4)#2	146.08(13)
Tb(1)-O(3W)	2.475(3)	O(3W)-Tb(1)-O(4)#2	86.82(11)
Tb(1)-O(2W)	2.480(3)	O(2W)-Tb(1)-O(4)#2	73.75(11)
Tb(1)-O(4)#2	2.505(3)	O(1)-Tb(1)-O(3)#2	133.63(10)
Tb(1)-O(3)#2	2.531(3)	O(2)#1-Tb(1)-O(3)#2	113.12(9)
Tb(1)-O(5)	2.544(4)	O(6)-Tb(1)-O(3)#2	75.61(10)
O(1)-Tb(1)-O(2)#1	74.66(10)		

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

Compound **4**

Er(1)-O(4)#1	2.328(2)	O(1W)-Er(1)-O(5)	76.70(6)
Er(1)-O(3)#2	2.452(3)	O(4)#1-Er(1)-O(1)	91.93(7)
Er(1)-O(3W)	2.454(5)	O(3)#2-Er(1)-O(1)	73.64(10)
Er(1)-O(2W)	2.459(5)	O(3W)-Er(1)-O(1)	145.89(16)
Er(1)-O(1W)	2.459(3)	O(2W)-Er(1)-O(1)	73.77(15)
Er(1)-O(5)	2.464(2)	O(1W)-Er(1)-O(1)	87.66(7)
Er(1)-O(1)	2.4873(18)	O(5)-Er(1)-O(1)	127.21(8)
Er(1)-O(2)	2.5121(18)	O(4)#1-Er(1)-O(2)	133.84(8)
Er(1)-O(6)	2.529(2)	O(3)#2-Er(1)-O(2)	113.0
O(4)#1-Er(1)-O(3)#2	74.68(9)	O(3W)-Er(1)-O(2)	140.97(15)

O(4)#1-Er(1)-O(3W)	85.19(17)	O(2W)-Er(1)-O(2)	70.53(13)
O(3)#2-Er(1)-O(3W)	72.83(16)	O(1W)-Er(1)-O(2)	70.02(5)
O(4)#1-Er(1)-O(2W)	72.12(17)	O(5)-Er(1)-O(2)	75.25(6)
O(3)#2-Er(1)-O(2W)	131.93(18)	O(1)-Er(1)-O(2)	52.1
O(3W)-Er(1)-O(2W)	136.0(2)	O(4)#1-Er(1)-O(6)	76.46(13)
O(4)#1-Er(1)-O(1W)	145.27(14)	O(3)#2-Er(1)-O(6)	135.42(10)
O(3)#2-Er(1)-O(1W)	71.91(9)	O(3W)-Er(1)-O(6)	71.55(17)
O(3W)-Er(1)-O(1W)	76.23(17)	O(2W)-Er(1)-O(6)	66.80(16)
O(2W)-Er(1)-O(1W)	139.89(14)	O(1W)-Er(1)-O(6)	122.97(8)
O(4)#1-Er(1)-O(5)	128.23(10)	O(5)-Er(1)-O(6)	51.8
O(3)#2-Er(1)-O(5)	141.44(9)	O(1)-Er(1)-O(6)	140.57(11)
O(3W)-Er(1)-O(5)	78.46(14)	O(2)-Er(1)-O(6)	111.51(9)
O(2W)-Er(1)-O(5)	86.63(17)		

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

Compound **5**

Yb(1)-O(4)#1	2.217(4)	O(4)#1-Yb(1)-O(2)	72.51(13)
Yb(1)-O(3)#2	2.239(3)	O(3)#2-Yb(1)-O(2)	79.69(13)
Yb(1)-O(2W)	2.267(4)	O(2W)-Yb(1)-O(2)	82.74(13)
Yb(1)-O(1W)	2.288(3)	O(1W)-Yb(1)-O(2)	128.40(12)
Yb(1)-O(6)	2.389(4)	O(6)-Yb(1)-O(2)	137.12(13)
Yb(1)-O(2)	2.412(3)	O(4)#1-Yb(1)-O(5)	81.96(12)
Yb(1)-O(5)	2.422(3)	O(3)#2-Yb(1)-O(5)	126.85(12)
Yb(1)-O(1)	2.449(3)	O(2W)-Yb(1)-O(5)	74.14(12)
O(4)#1-Yb(1)-O(3)#2	94.77(14)	O(1W)-Yb(1)-O(5)	79.14(12)
O(4)#1-Yb(1)-O(2W)	91.17(14)	O(6)-Yb(1)-O(5)	53.94(11)
O(3)#2-Yb(1)-O(2W)	158.79(13)	O(2)-Yb(1)-O(5)	145.03(13)
O(4)#1-Yb(1)-O(1W)	159.08(14)	O(4)#1-Yb(1)-O(1)	126.12(12)
O(3)#2-Yb(1)-O(1W)	89.48(12)	O(3)#2-Yb(1)-O(1)	80.71(12)
O(2W)-Yb(1)-O(1W)	92.20(13)	O(2W)-Yb(1)-O(1)	79.34(12)
O(4)#1-Yb(1)-O(6)	77.00(15)	O(1W)-Yb(1)-O(1)	74.77(12)
O(3)#2-Yb(1)-O(6)	73.52(12)	O(6)-Yb(1)-O(1)	147.04(13)
O(2W)-Yb(1)-O(6)	127.69(12)	O(2)-Yb(1)-O(1)	53.77(11)
O(1W)-Yb(1)-O(6)	84.64(14)	O(5)-Yb(1)-O(1)	141.71(11)

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

Compound **6**

Lu(1)-O(4)#1	2.206(5)	O(4)#1-Lu(1)-O(2)	72.43(17)
Lu(1)-O(3)#2	2.234(5)	O(3)#2-Lu(1)-O(2)	79.88(18)
Lu(1)-O(2W)	2.269(5)	O(2W)-Lu(1)-O(2)	82.51(19)
Lu(1)-O(1W)	2.273(5)	O(1W)-Lu(1)-O(2)	128.42(17)
Lu(1)-O(6)	2.381(5)	O(6)-Lu(1)-O(2)	137.27(19)
Lu(1)-O(2)	2.407(5)	O(4)#1-Lu(1)-O(5)	81.94(17)
Lu(1)-O(5)	2.408(4)	O(3)#2-Lu(1)-O(5)	126.72(16)
Lu(1)-O(1)	2.447(5)	O(2W)-Lu(1)-O(5)	74.17(17)
O(4)#1-Lu(1)-O(3)#2	94.88(19)	O(1W)-Lu(1)-O(5)	79.10(17)
O(4)#1-Lu(1)-O(2W)	90.7(2)	O(6)-Lu(1)-O(5)	53.98(16)
O(3)#2-Lu(1)-O(2W)	158.93(18)	O(2)-Lu(1)-O(5)	144.96(17)
O(4)#1-Lu(1)-O(1W)	159.14(19)	O(4)#1-Lu(1)-O(1)	125.78(17)
O(3)#2-Lu(1)-O(1W)	89.55(17)	O(3)#2-Lu(1)-O(1)	80.97(17)

O(2W)-Lu(1)-O(1W)	92.40(18)	O(2W)-Lu(1)-O(1)	79.29(16)
O(4)#1-Lu(1)-O(6)	77.3(2)	O(1W)-Lu(1)-O(1)	75.04(17)
O(3)#2-Lu(1)-O(6)	73.32(17)	O(6)-Lu(1)-O(1)	147.14(17)
O(2W)-Lu(1)-O(6)	127.75(17)	O(2)-Lu(1)-O(1)	53.52(15)
O(1W)-Lu(1)-O(6)	84.5(2)	O(5)-Lu(1)-O(1)	141.79(16)

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

Table S3. Bond lengths (Å) of Ln-O in lanthanide complexes **1-6**

Ln	Pr	Eu	Tb	Er	Yb	Lu
Ln(1)-O(1)	2.498(6)	2.485(4)	2.462(3)	2.452(3)	2.239(3)	2.234(5)
Ln (1)-O(2)	2.405(6)	2.373(4)	2.342(3)	2.328(2)	2.217(4)	2.206(5)
Ln (1)-O(3)	2.561(6)	2.552(4)	2.531(3)	2.5121(18)	2.422(3)	2.408(4)
Ln (1)-O(4)	2.543(6)	2.522(4)	2.505(3)	2.4873(18)	2.412(3)	2.407(5)
Ln (1)-O(5)	2.530(6)	2.507(4)	2.475(3)	2.459(3)	2.389(4)	2.381(5)
Ln (1)-O(6)	2.562(8)	2.558(5)	2.544(4)	2.529(2)	2.449(3)	2.447(5)
Ln (1)-O(1W)	2.528(7)	2.511(4)	2.472(3)	2.459(5)	2.288(3)	2.273(5)
Ln (1)-O(2W)	2.522(7)	2.508(5)	2.474(3)	2.454(5)	2.267(4)	2.269(5)
Ln (1)-O(3W)	2.537(7)	2.511(4)	2.480(3)	2.464(2)		

Scheme S1

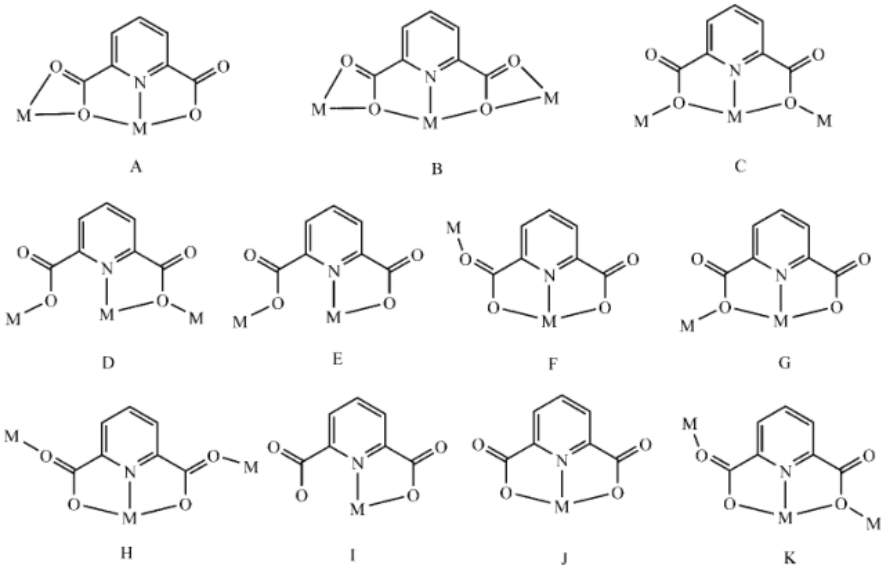


Figure S1.

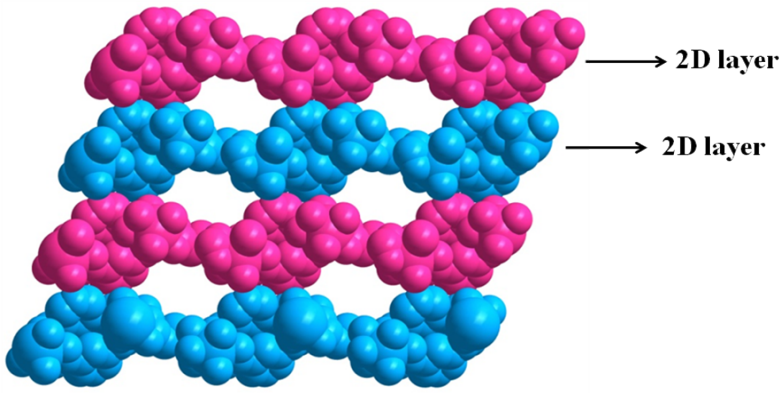


Figure S2.

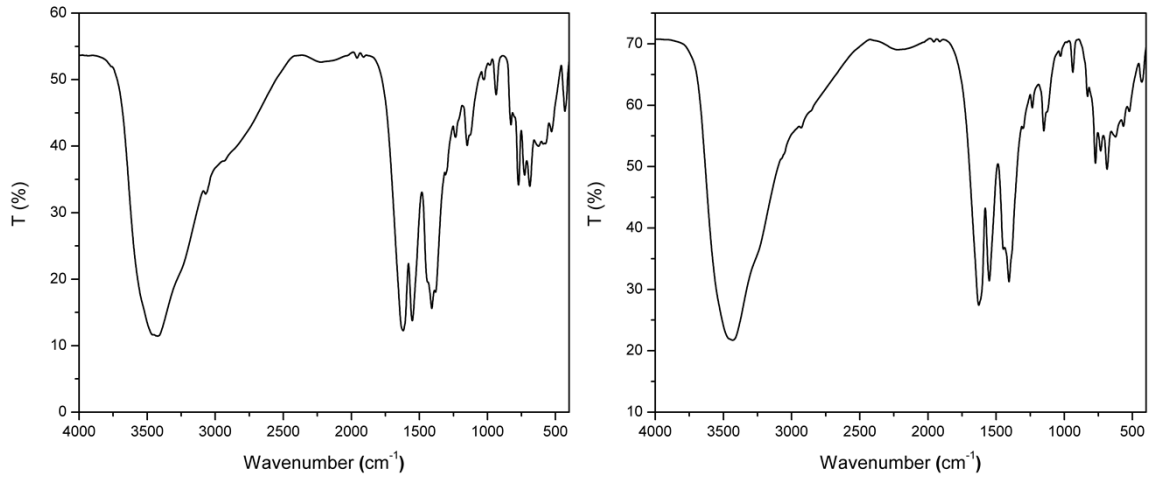


Fig. S2a. The IR spectra of **1** (left)and **2** (right).

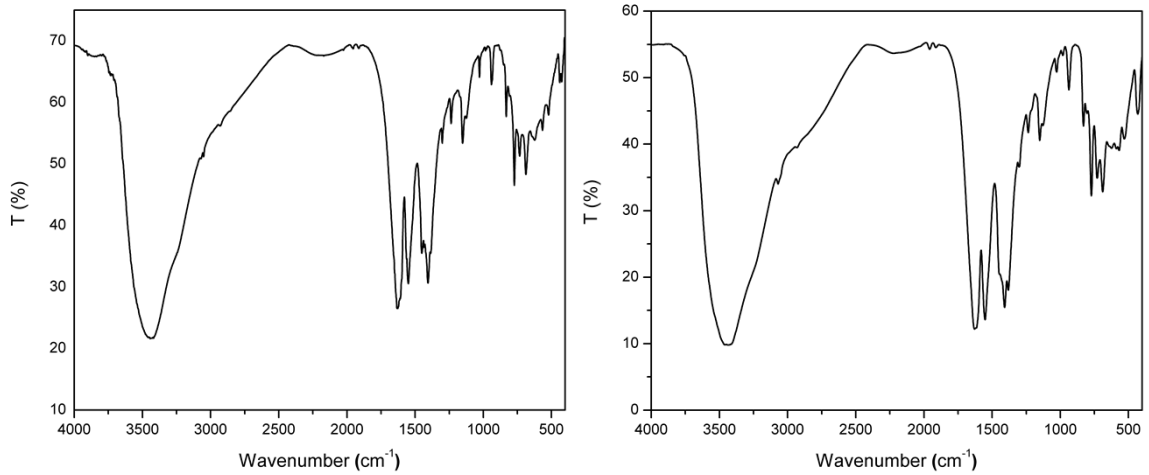


Fig. S2b. The IR spectra of **3** (left) and **4** (right).

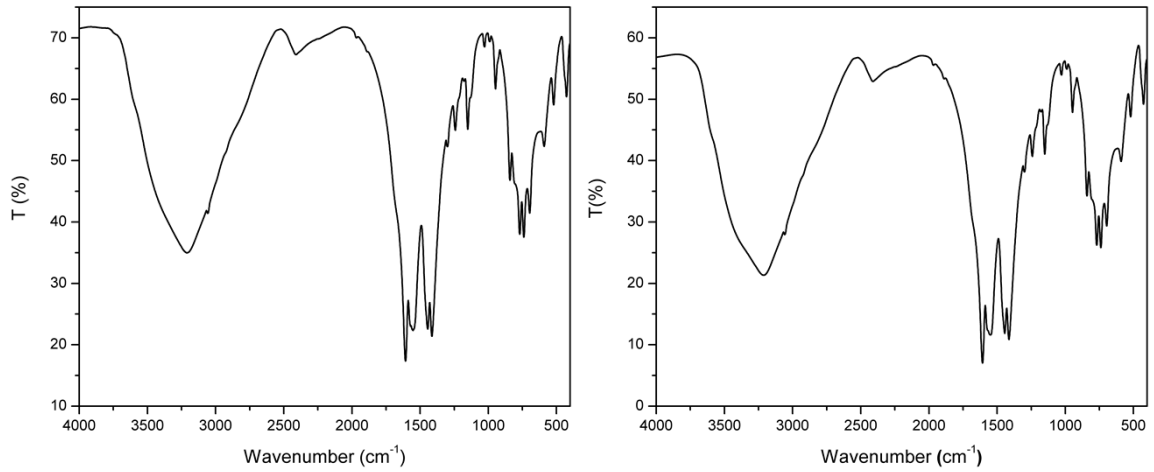
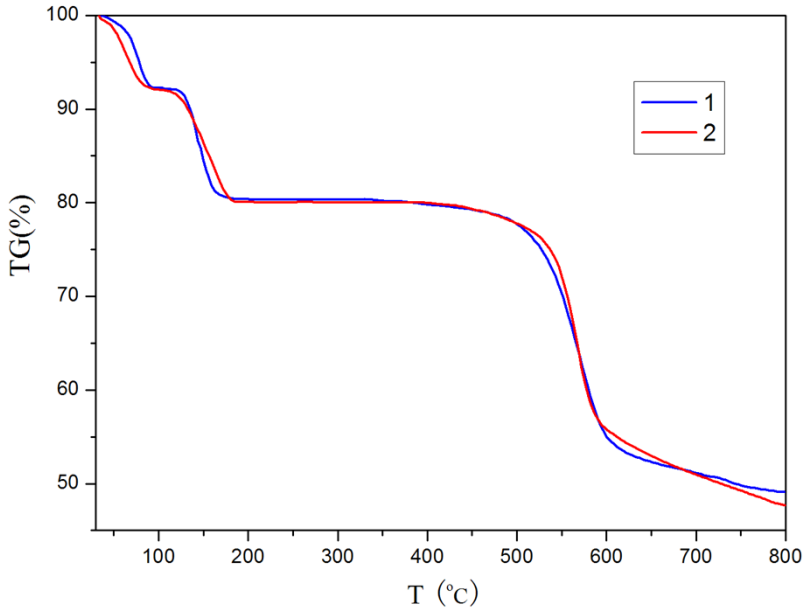


Fig. S2c. The IR spectra of **5** (left) and **6** (right).

Figure S3.

(a)


100
90
80
70
60
50
TG(%)
100
200
300
400
500
600
700
800
T (°C)
1
2

(b)

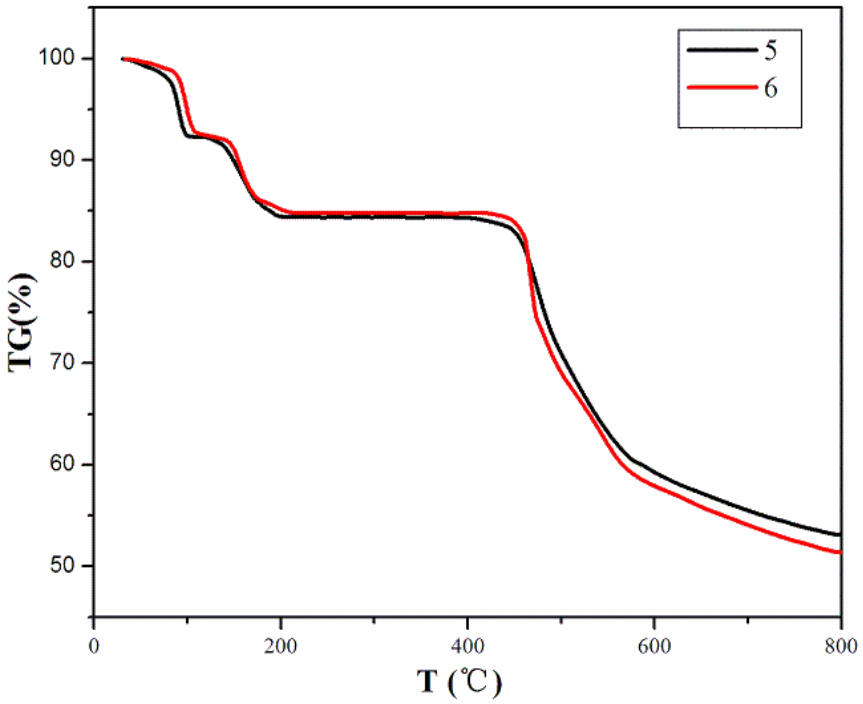
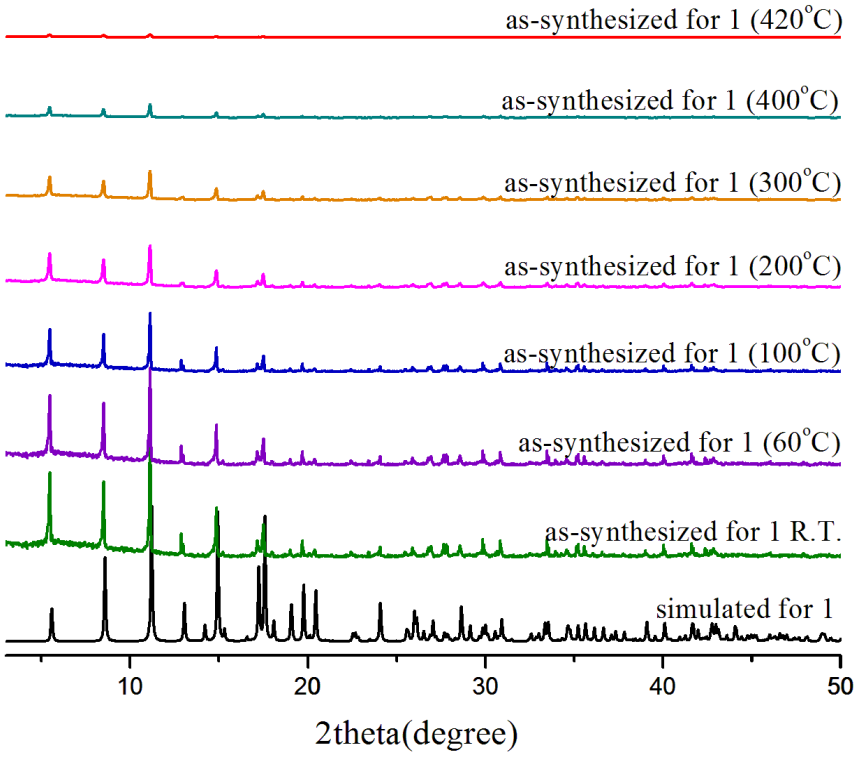
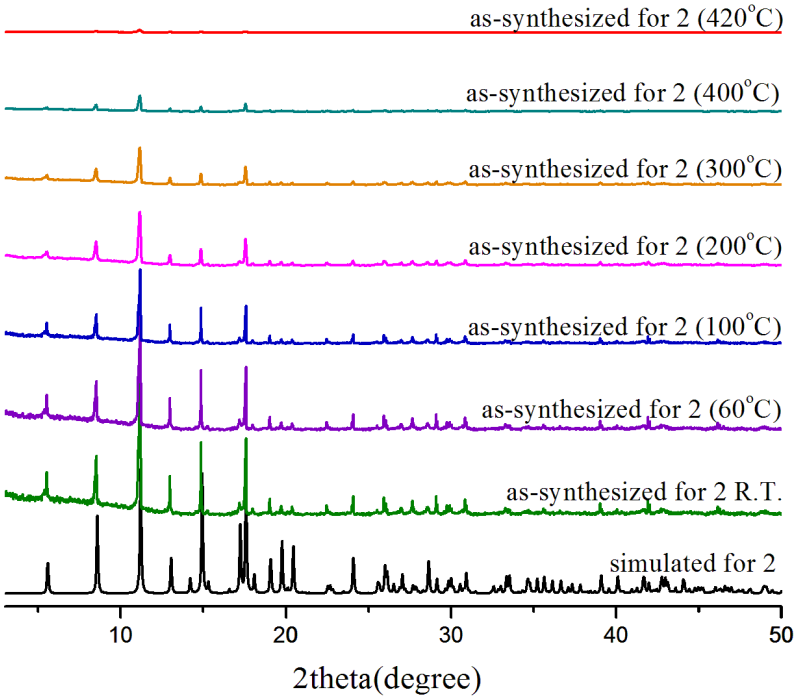

100
90
80
70
60
50
TG(%)
0
200
400
600
800
T (℃)
5
6

Figure S4.

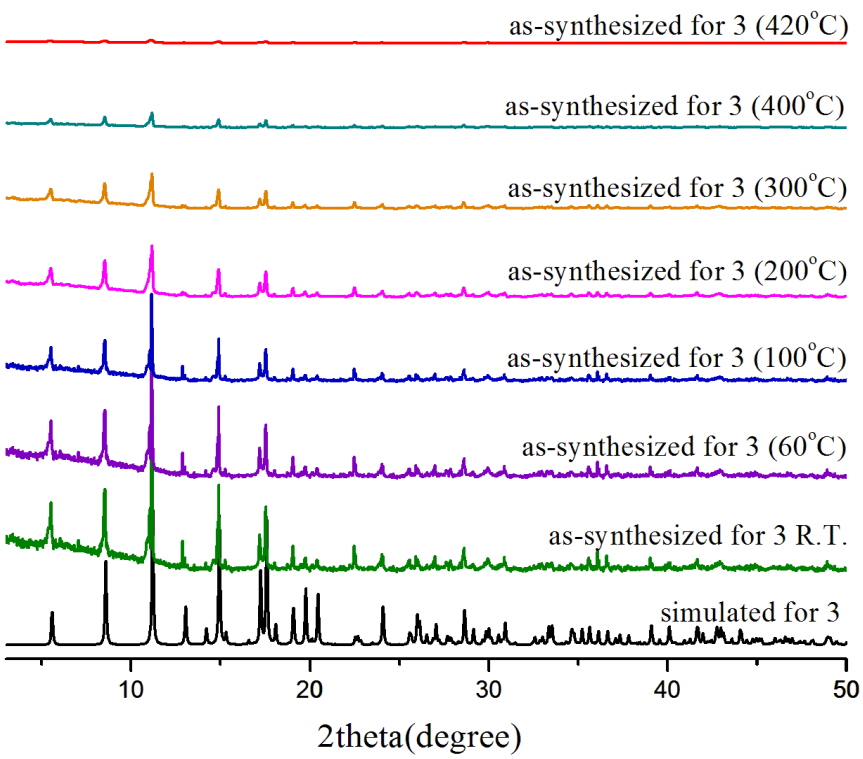
(a) For compound **1**



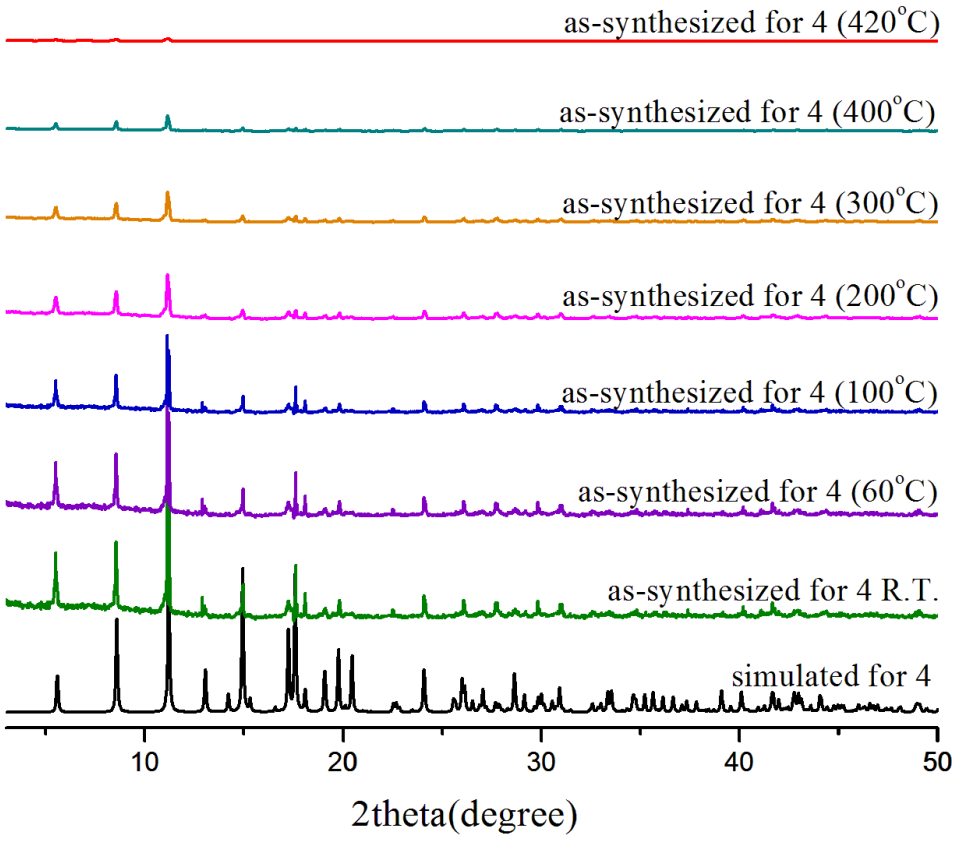
(b) for compound **2**



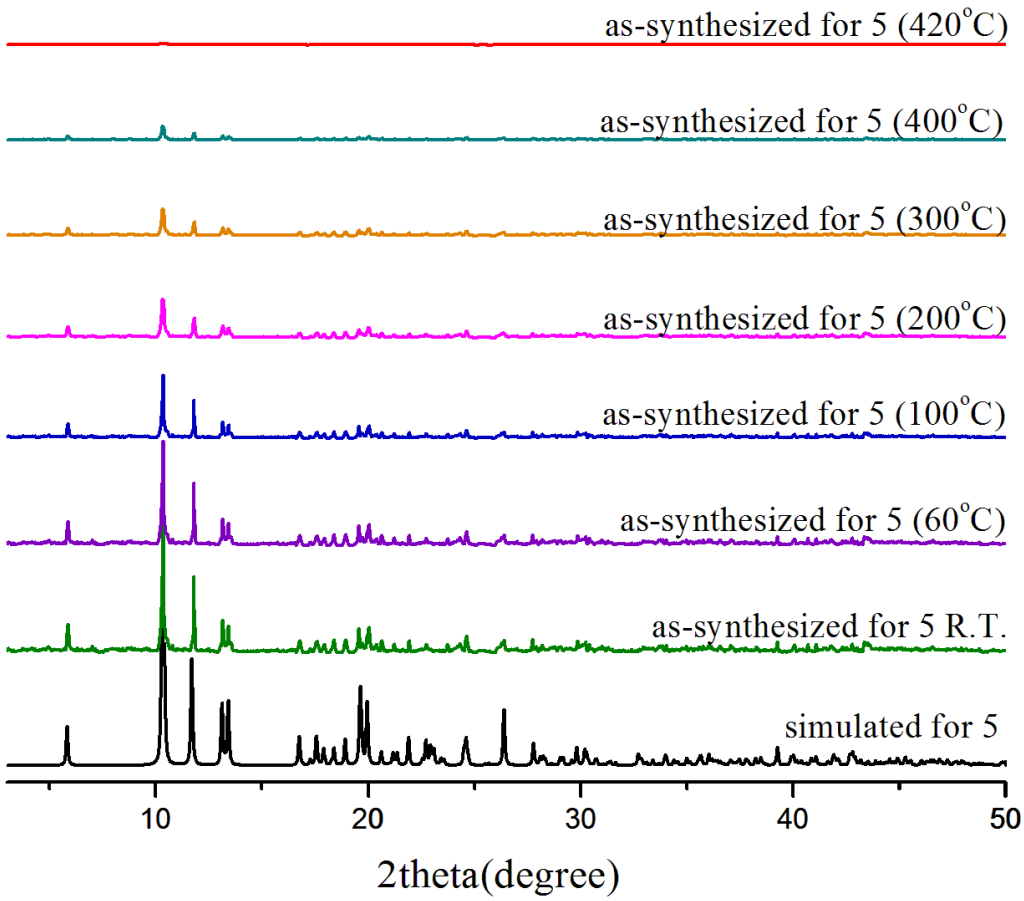
(c) for compound **3**



(d) for compound **4**



(e) for compound **5**



(f) for compound **6**

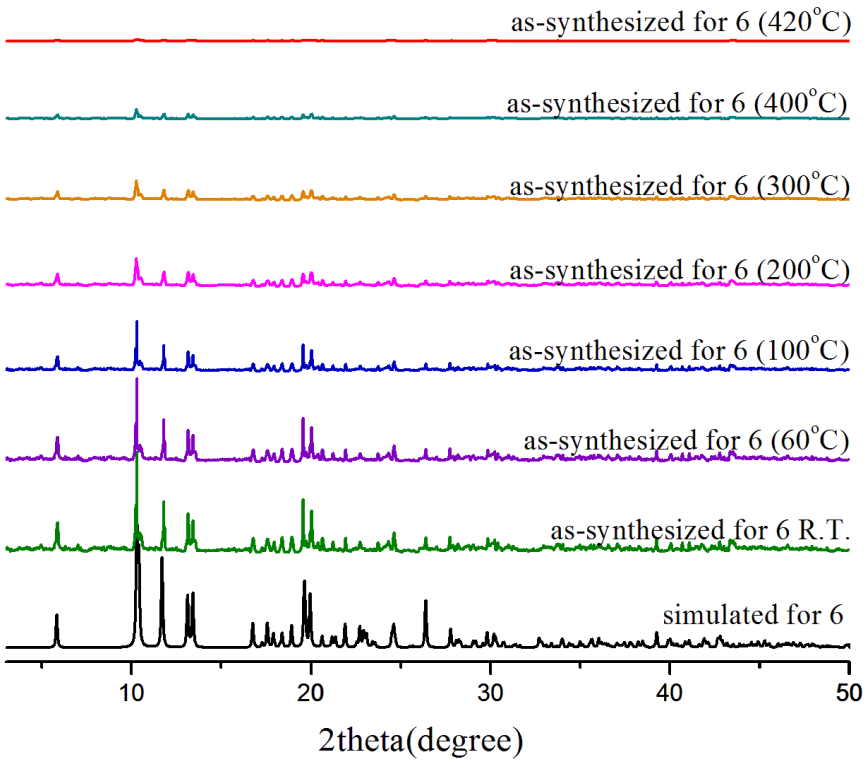


Figure S5.

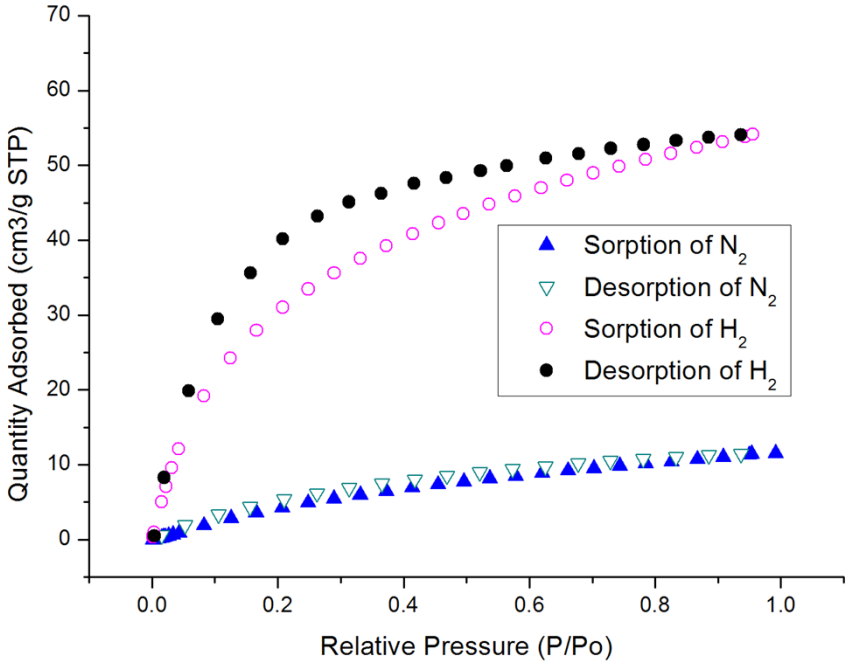


Figure S6.