Supporting Information

From 1D to 3D Lanthanide Coordination Polymers Constructed with Pyridine-3,5-dicarboxylic Acid: Synthesis, Crystal Structures, and Catalytic Properties

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Contents

Table S1 Selected bond lengths (Å) and bond angles (º) for **1-7**.

Compound **1**

La(1)-O(6)#1	2.426(4)	La(2')-O(2W)	3.025(11)
La(1)-O(4)#2	2.426(4)	O(6)#1-La(1)-O(9)#1	80.86(15)
La(1)-O(9)#1	2.468(4)	O(4)#2-La(1)-O(9)#1	83.64(15)
La(1)-O(13)	2.524(5)	O(6)#1-La(1)-O(13)	140.60(18)
La(1)-O(12)#3	2.543(4)	O(4)#2-La(1)-O(13)	74.93(17)
La(1)-O(1)	2.605(5)	O(9)#1-La(1)-O(13)	125.67(19)
La(1)-O(7)#4	2.653(5)	O(6)#1-La(1)-O(12)#3	76.20(15)
La(1)-O(2)	2.719(4)	O(4)#2-La(1)-O(12)#3	154.19(15)
La(1)-O(8)#4	2.821(4)	O(9)#1-La(1)-O(12)#3	81.27(14)
La(1)-La(2)	4.1536(11)	O(13)-La(1)-O(12)#3	130.80(16)
La(2)-O(10)	2.423(4)	O(6)#1-La(1)-O(1)	75.73(16)
La(2)-O(3)#5	2.471(4)	O(4)#2-La(1)-O(1)	78.64(16)
La(2)-O(5)	2.484(4)	O(9)#1-La(1)-O(1)	152.51(15)
La(2)-O(8)#4	2.558(4)	O(13)-La(1)-O(1)	69.42(19)
La(2)-O(2W)	2.559(5)	O(6)#1-La(1)-O(7)#4	148.96(16)
La(2)-O(2)	2.560(4)	O(4)#2-La(1)-O(7)#4	100.92(18)
La(2)-O(1W)	2.583(5)	O(9)#1-La(1)-O(7)#4	68.68(15)
La(2)-O(11)#3	2.705(4)	O(13)-La(1)-O(7)#4	67.43(19)
La(2)-O(12)#3	2.791(4)	O(12)#3-La(1)-O(7)#4	92.93(16)
La(1')-O(13)	2.231(10)	O(1)-La(1)-O(7)#4	135.23(17)
La(1')-O(7)#4	2.241(10)	O(6)#1-La(1)-O(2)	92.68(15)
La(1')-O(4)#2	2.297(9)	O(4)#2-La(1)-O(2)	126.68(14)
La(1')-O(9)#1	2.393(9)	O(9)#1-La(1)-O(2)	147.83(14)
La(1')-O(8)#4	2.718(9)	O(13)-La(1)-O(2)	78.10(18)
La(1')-O(6)#1	2.854(10)	O(12)#3-La(1)-O(2)	66.60(13)
La(1')-O(1)	2.870(9)	O(1)-La(1)-O(2)	48.84(13)
La(1')-O(12)#3	2.873(9)	O(7)#4-La(1)-O(2)	109.79(14)
La(1')-O(2)	3.020(9)	O(6)#1-La(1)-O(8)#4	138.84(15)
La(1')-La(2')	4.176(11)	O(4)#2-La(1)-O(8)#4	140.33(16)
La(2')-O(8)#4	2.145(11)	O(9)#1-La(1)-O(8)#4	100.21(14)
La(2')-O(10)	2.194(10)	O(13)-La(1)-O(8)#4	70.93(16)
La(2')-O(3)#5	2.227(10)	O(12)#3-La(1)-O(8)#4	63.52(14)
La(2')-O(2)	2.639(10)	O(1)-La(1)-O(8)#4	106.86(14)
La(2')-O(11)#3	2.695(10)	O(7)#4-La(1)-O(8)#4	47.17(13)

Symmetry transformations used to generate equivalent atoms: #1 x-1,y,z ,#2 -x-1,-y+1,-z+2 ,#3 -x,-y+1,-z+1 ,#4 x,y-1,z #5 -x,-y+1,-z+2 , #6 x,y+1,z ,#7 x+1,y,z

Compound **2**

Pr(1)-O(7)#1	2.367(3)	O(4)#2-Pr(1)-O(2)	78.76(13)
Pr(1)-O(4)#2	2.411(4)	O(4)#2-Pr(1)-O(2)	78.76(13)
Pr(1)-O(10)	2.495(3)	O(10)-Pr(1)-O(2)	70.65(12)
Pr(1)-O(2)	2.514(3)	O(7)#1-Pr(1)-O(1W)	138.55(14)
Pr(1)-O(1W)	2.514(4)	O(4)#2-Pr(1)-O(1W)	132.21(14)
Pr(1)-O(2W)	2.558(4)	O(11)#3-Pr(1)-O(1W)	71.27(14)
Pr(1)-O(6)	2.659(4)	O(10)-Pr(1)-O(1W)	127.37(13)
Pr(1)-O(5)	2.769(4)	O(2)-Pr(1)-O(1W)	71.38(13)
Pr(2)-O(3)#4	2.376(4)	O(4)#2-Pr(1)-O(2W)	128.24(14)
Pr(2)-O(12)#5	2.403(4)	O(11)#3-Pr(1)-O(2W)	71.05(14)
Pr(2)-O(8)#6	2.422(3)	O(10)-Pr(1)-O(2W)	140.91(13)
Pr(2)-O(13)	2.470(4)	O(2)-Pr(1)-O(2W)	138.83(13)
Pr(2)-O(5)	2.492(3)	O(1W)-Pr(1)-O(2W)	67.61(14)
O(7)#1-Pr(1)-O(4)#2	77.97(13)	O(2)-Pr(1)-O(6)	112.29(12)
O(7)#1-Pr(1)-O(11)#3	98.58(13)	O(1W)-Pr(1)-O(6)	86.71(14)
O(4)#2-Pr(1)-O(11)#3	73.92(13)	O(2W)-Pr(1)-O(6)	69.18(14)
O(7)#1-Pr(1)-O(10)	84.44(13)	O(7)#1-Pr(1)-O(5)	119.15(11)
O(4)#2-Pr(1)-O(10)	72.28(13)	O(4)#2-Pr(1)-O(5)	129.96(11)
O(11)#3-Pr(1)-O(10)	144.60(13)	O(11)#3-Pr(1)-O(5)	137.32(11)
O(7)#1-Pr(1)-O(2)	150.06(13)	O(10)-Pr(1)-O(5)	64.17(12)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z , #2 -x+1,-y+1,-z+1, #3 x,y+1,z ,#4 -x,-y+1,-z+1 ,#5 x-1,y+1,z , #6 -x,-y+1,-z , #7 x,y-1,z, #8 x+1,y-1,z

Compound **3**

Sm(1)-O(3)#1	2.334(6)	O(3)#1-Sm(1)-O(10)	98.7(2)
Sm(1)-O(5)	2.404(6)	O(5)-Sm(1)-O(10)	142.33(18)
Sm(1)-O(10)	2.445(6)	O(3)#1-Sm(1)-O(12)#2	84.3(2)
Sm(1)-O(12)#2	2.485(6)	O(5)-Sm(1)-O(12)#2	72.2(2)
Sm(1)-O(8)#3	2.507(6)	O(10)-Sm(1)-O(12)#2	144.6(2)
Sm(1)-O(2W)	2.509(6)	O(3)#1-Sm(1)-O(8)#3	150.0(2)
Sm(1)-O(1W)	2.543(7)	O(5)-Sm(1)-O(8)#3	78.1(2)
Sm(1)-O(1)	2.638(6)	O(10)-Sm(1)-O(8)#3	92.8(2)
Sm(1)-O(2)	2.752(6)	O(12)#2-Sm(1)-O(8)#3	70.7(2)
Sm(1)-Sm(2)	4.0932(9)	O(3)#1-Sm(1)-O(2W)	138.9(3)
Sm(2)-O(12)#2	2.815(6)	O(5)-Sm(1)-O(2W)	131.6(2)
Sm(2)-O(11)#2	2.586(6)	O(10)-Sm(1)-O(2W)	71.4(2)
O(3)#1-Sm(1)-O(5)	78.6(2)	O(8)#3-Sm(1)-O(1W)	138.9(2)
Sm(2)-O(8)#3	2.680(6)	O(4)#5-Sm(2)-Sm(1)	115.05(16)
Sm(2)-O(12)#2	2.815(6)	O(13)-Sm(2)-Sm(1)	90.78(18)
O(6)#4-Sm(2)-Sm(1)	161.55(16)	O(2)-Sm(2)-Sm(1)	40.96(13)
O(9)#4-Sm(2)-Sm(1)	104.74(15)	O(7)#3-Sm(2)-Sm(1)	86.20(14)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+3/2,-z; #2 x,y-1,z; #3 -x,y,-z+1/2; #4 x,y+1,z; #5 -x+1,-y+1,-z.

Compound **4**

Tb(1)-O(11)	2.339(3)	O(8)-Tb(1)-O(3)#1	83.83(12)
Tb(1)-O(1W)	2.360(3)	O(11)-Tb(1)-O(2W)	78.22(12
Tb(1)-O(2)	2.378(3)	O(1W)-Tb(1)-O(2W)	71.31(13)
Tb(1)-O(8)	2.380(3)	O(2)-Tb(1)-O(2W)	133.49(12)
Tb(1)-O(3)#1	2.403(3)	O(8)-Tb(1)-O(2W)	146.77(13)
Tb(1)-O(2W)	2.409(3)	O(3)#1-Tb(1)-O(2W)	74.87(12)
Tb(1)-O(6)	2.444(3)	O(11)-Tb(1)-O(6)	91.97(11)
Tb(1)-O(5)	2.508(3)	O(1W)-Tb(1)-O(6)	96.14(13)
Tb(1)-O(7)	2.881(3)	O(2)-Tb(1)-O(6)	73.97(12)
Tb(2)-O(7)	2.317(3)	O(8)-Tb(1)-O(6)	127.49(11)
Tb(2)-O(1)	2.353(3)	O(3)#1-Tb(1)-O(6)	145.37(12)
Tb(2)-O(9)#2	2.501(3)	O(2W)-Tb(1)-O(6)	70.54(12)
Tb(2)-O(11)	2.770(3)	O(11)-Tb(1)-O(5)	137.16(11)
O(11)-Tb(1)-O(1W)	143.59(12)	O(1W)-Tb(1)-O(5)	71.86(12)
O(11)-Tb(1)-O(2)	73.93(12)	O(2)-Tb(1)-O(5)	73.63(11)
O(1W)-Tb(1)-O(2)	142.34(12)	O(8)-Tb(1)-O(5)	77.07(11)
O(11)-Tb(1)-O(8)	122.89(11)	O(3)#1-Tb(1)-O(5)	143.45(11)
O(1W)-Tb(1)-O(8)	78.52(12)	O(2W)-Tb(1)-O(5)	105.55(12)
O(2)-Tb(1)-O(8)	79.52(12)	O(6)-Tb(1)-O(5)	52.40(10)

Symmetry transformations used to generate equivalent atoms: #1 -x,y+1/2,-z-1/2, #2 x-1,y,z ,#3 -x,y-1/2,-z-1/2 #4 x+1,y,z

Compound **5**

Ho(1)-O(7)	2.301(3)	O(7)-Ho(1)-O(13)	147.25(11)
Ho(1)-O(4)#1	2.344(3)	O(4)#1-Ho(1)-O(13)	72.67(11)
Ho(1)-O(1)	2.360(3)	O(1)-Ho(1)-O(13)	138.14(11)
Ho(1)-O(13)	2.374(3)	O(1W)-Ho(1)-O(13)	74.21(13)
Ho(1)-O(1W)	2.368(4)	O(7)-Ho(1)-O(12)	134.16(12)
Ho(1)-O(12)	2.412(3)	O(4)#1-Ho(1)-O(12)	145.50(12)
Ho(1)-O(10)	2.438(3)	O(1)-Ho(1)-O(12)	75.61(11)
Ho(1)-O(11)	2.484(3)	O(1W)-Ho(1)-O(12)	99.23(13)
Ho(1)-O(9)	2.766(3)	O(13)-Ho(1)-O(12)	72.91(12)
Ho(2)-O(9)	2.327(3)	O(7)-Ho(1)-O(10)	125.17(11)
Ho(2)-O(3W)	2.347(3)	O(4)#1-Ho(1)-O(10)	89.88(12)
Ho(2)-O(8)	2.366(3)	O(1)-Ho(1)-O(10)	74.78(12)
O(7)-Ho(1)-O(4)#1	79.22(12)	O(1W)-Ho(1)-O(10)	145.44(12)
O(7)-Ho(1)-O(1)	74.04(11)	O(13)-Ho(1)-O(10)	71.92(12)
O(4)#1-Ho(1)-O(1)	132.02(11)	O(12)-Ho(1)-O(10)	77.27(11)
O(7)-Ho(1)-O(1W)	82.09(13)	O(7)-Ho(1)-O(11)	84.89(11)
O(4)#1-Ho(1)-O(1W)	73.57(13)	O(13)-Ho(1)-O(10)	71.92(12)
O(1)-Ho(1)-O(1W)	138.38(13)	O(12)-Ho(1)-O(10)	77.27(11)

Symmetry transformations used to generate equivalent atoms: #1 -x,y+1/2,-z-1/2 ,#2 x-1,y,z ,#3 -x,y-1/2,-z-1/2, #4 x+1,y,z

Compound **6**

Er(1)-O(12)	2.240(11)	O(11)#2-Er(1)-O(2)	74.2(5)
Er(1)-O(5)	2.246(11)	O(12)-Er(1)-O(1W)	86.5(4)
Er(1)-O(6)#1	2.281(11)	O(5)-Er(1)-O(1W)	73.2(4)
Er(1)-O(11)#2	2.384(13)	O(6)#1-Er(1)-O(1W)	138.4(5)
Er(1)-O(2)	2.392(10)	O(11)#2-Er(1)-O(1W)	73.7(5)
Er(1)-O(1W)	2.401(10)	O(2)-Er(1)-O(1W)	127.5(3)
Er(1)-O(2W)	2.452(11)	O(12)-Er(1)-O(2W)	72.3(4)
Er(1)-O(1)	2.524(10)	O(5)-Er(1)-O(2W)	83.7(4)
Er(1)-O(1)	2.524(10)	O(6)#1-Er(1)-O(2W)	71.8(5)
O(12)-Er(1)-O(5)	152.3(2)	O(11)#2-Er(1)-O(2W)	139.0(5)
O(12)-Er(1)-O(6)#1	104.1(4)	O(2)-Er(1)-O(2W)	146.6(3)
O(5)-Er(1)-O(6)#1	80.7(5)	O(1W)-Er(1)-O(2W)	73.6(2)
O(12)-Er(1)-O(11)#2	81.6(4)	O(12)-Er(1)-O(1)	76.0(4)
O(5)-Er(1)-O(11)#2	109.6(4)	O(5)-Er(1)-O(1)	131.3(4)
O(6)#1-Er(1)-O(11)#2	146.9(3)	O(6)#1-Er(1)-O(1)	78.2(5)
O(12)-Er(1)-O(2)	127.9(4)	O(11)#2-Er(1)-O(1)	71.5(5)
O(5)-Er(1)-O(2)	79.9(4)	O(2)-Er(1)-O(1)	52.82(18)
O(6)#1-Er(1)-O(2)	77.0(4)	O(1W)-Er(1)-O(1)	142.9(3)

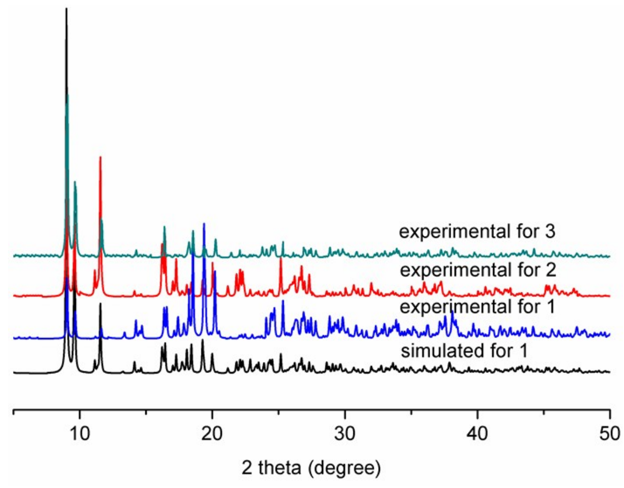
Symmetry transformations used to generate equivalent atoms: #1 x,-y+1,z-1/2 , #2 x,-y+1,z+1/2 #5 -x+2,-y+1,-z.

Compound **7**

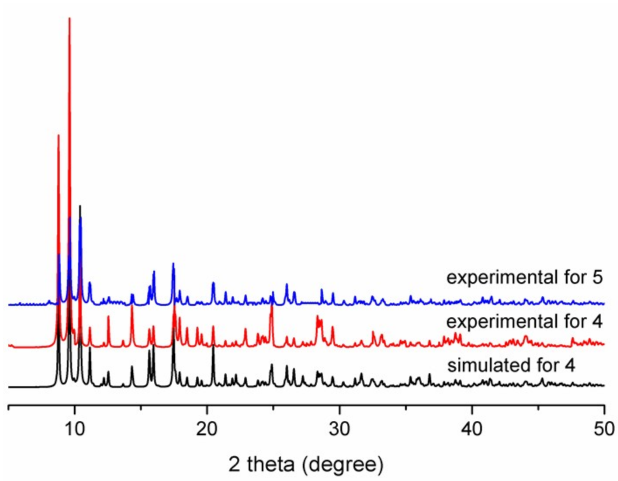
Lu(1)-O(5)#1	2.205(13)	O(6)-Lu(1)-O(1)	76.0(5)
Lu(1)-O(9)	2.235(12)	O(10)#1-Lu(1)-O(1)	75.0(5)
Lu(1)-O(6)	2.267(13)	O(5)#1-Lu(1)-O(1W)	73.4(5)
Lu(1)-O(10)#1	2.346(14)	O(9)-Lu(1)-O(1W)	86.9(5)
Lu(1)-O(1)	2.384(13)	O(6)-Lu(1)-O(1W)	136.2(6)
Lu(1)-O(1W)	2.393(13)	O(10)#1-Lu(1)-O(1W)	75.0(6)
Lu(1)-O(2W)	2.432(12)	O(1)-Lu(1)-O(1W)	128.9(4)
Lu(1)-O(2)	2.483(13)	O(5)#1-Lu(1)-O(2W)	83.4(5)
Ag(1)-N(1)	2.149(6)	O(9)-Lu(1)-O(2W)	72.2(5)
Ag(1)-N(1)#3	2.149(5)	O(6)-Lu(1)-O(2W)	70.1(6)
O(5)#1-Lu(1)-O(9)	152.3(3)	O(10)#1-Lu(1)-O(2W)	140.8(6)
O(5)#1-Lu(1)-O(6)	79.2(5)	O(1)-Lu(1)-O(2W)	144.0(4)
O(9)-Lu(1)-O(6)	103.8(5)	O(1W)-Lu(1)-O(2W)	73.4(3)
O(5)#1-Lu(1)-O(10)#1	109.0(5)	O(5)#1-Lu(1)-O(2)	130.4(5)
O(9)-Lu(1)-O(10)#1	83.6(5)	O(9)-Lu(1)-O(2)	76.4(5)
O(6)-Lu(1)-O(10)#1	147.4(3)	O(6)-Lu(1)-O(2)	77.7(6)
O(5)#1-Lu(1)-O(1)	78.6(5)	O(1)-Lu(1)-O(2)	53.4(2)
O(9)-Lu(1)-O(1)	129.1(5)	O(1W)-Lu(1)-O(2)	145.5(4)

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

(a)



(b)



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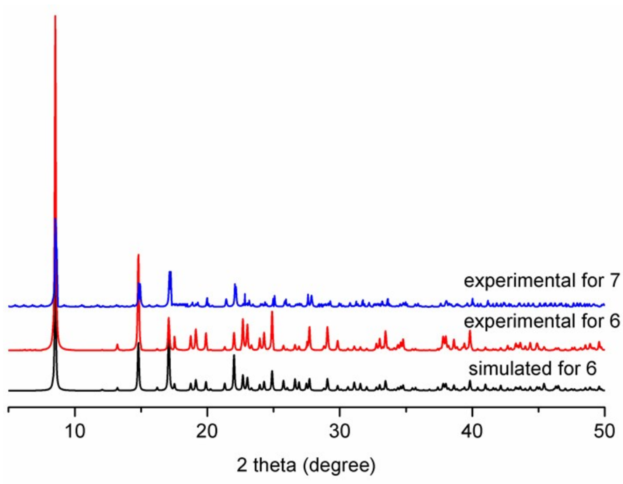

Fig. S1 Experimental and simulated PXRD patterns for **1** to **7**.

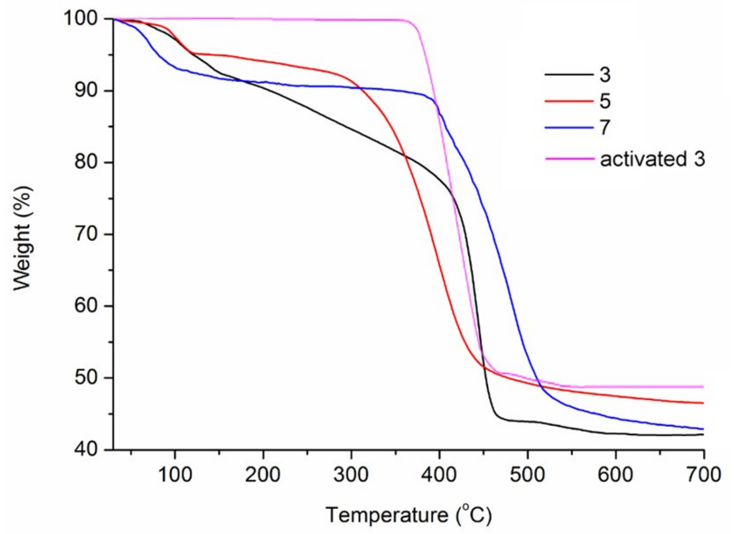

Fig. S2 TGA curves of compounds **3**, **5**, **7** and activated **3**.

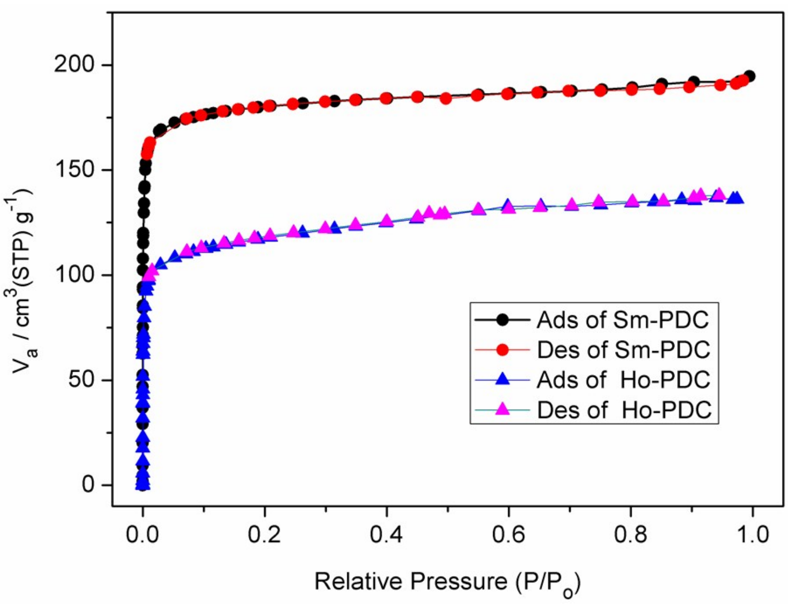

Fig. S3 N_2 adsorption/desorption isotherms of **3** (Sm-PDC) and **5** (Ho-PDC).

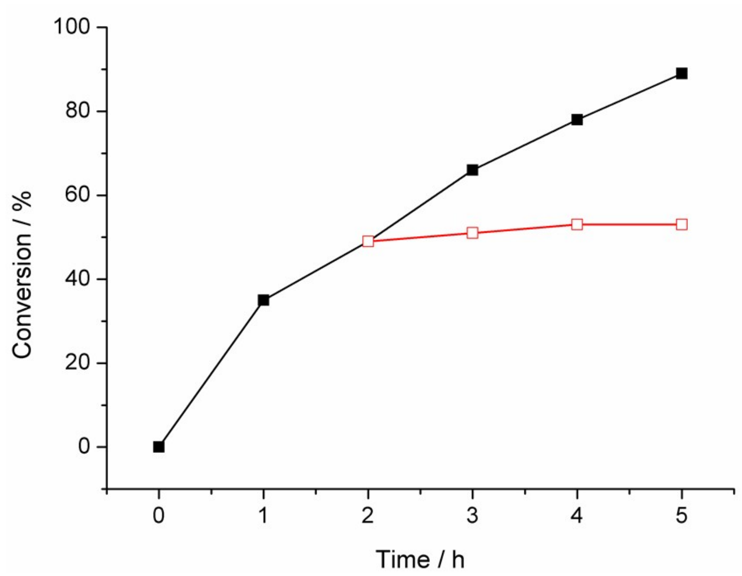

Fig. S4 Filtration experiment for **3** (Sm-PDC). The full square (■) represents the reaction with Sm-PDC as a catalyst. The open square (□) represents the reaction course after filtration of the catalyst at 2 hours.

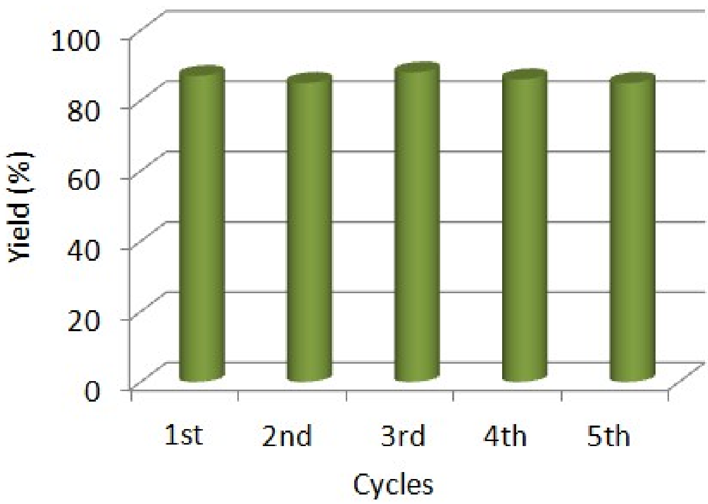

Fig. S5 Recycling experiments.

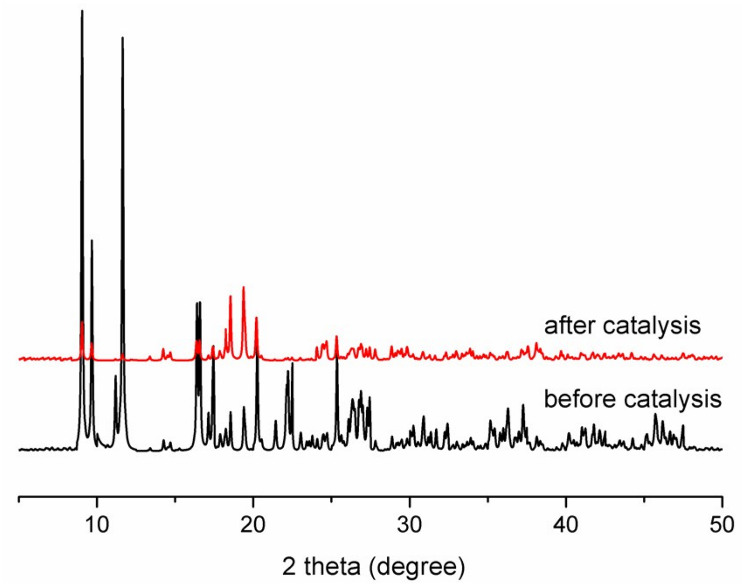

Fig. S6 Powder X-ray patterns for **3** (Sm-PDC) before and after catalytic studies.