

Assemblies of Three Nd(III) 2,6-Naphthalenedicarboxylates (ndc²⁻) 3D Coordination Polymers Based on Various Secondary Building Units (SBUs): Structural Diversity and Gas Sorption Property

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Supplementary Materials:

STable 1. Related bond lengths (Å) and angles (°) around the Nd(III) ion for **1**.

STable 2. Related bond lengths (Å) and angles (°) around the Nd(III) ion for **2**.

STable 3. Related bond lengths (Å) and angles (°) around the Nd(III) ion for **3**.

SFigure 1 The 3D porous framework of **1** views along the *a* axis showing 1D channels.

SFigure 2 The 3D porous framework of **2** views along the *b* axis showing the rod-shaped arrangement.

SFigure 3 The 3D porous framework of **3** views along the *b* axis showing the rod-shaped arrangement.

SFigure 4 (a) Thermogravimetric analysis (TGA) of **1**, (b) *in-situ* PXRD of **1**.

SFigure 5 (a) Thermogravimetric analysis (TGA) of **2**, (b) *in-situ* PXRD of **2**.

SFigure 6 (a) Thermogravimetric analysis (TGA) of **3**, (b) *in-situ* PXRD of **3**.

STable 1. Related bond lengths (Å) and angles (°) around the Nd(III) ion for **1**.

Nd(1)–O(6)#1	2.401(1)	Nd(1)–O(7)#3	2.470(1)
Nd(1)–O(2)#1	2.411(8)	Nd(1)–O(1)	2.481(9)
Nd(1)–O(8)#2	2.428(1)	Nd(1)–O(3)	2.501(7)
Nd(1)–O(9)	2.433(1)	Nd(1)–O(4)	2.511(8)
Nd(1)–O(5)	2.448(1)	Nd(1)–O(2)	2.659(8)
Nd(1)–O(10)	2.466(1)		
O(6)#1–Nd(1)–O(2)#1	68.4(5)	O(10)–Nd(1)–O(3)	73.8(3)
O(6)#1–Nd(1)–O(8)#2	12.4(4)	O(7)#3–Nd(1)–O(3)	149.1(4)
O(2)#1–Nd(1)–O(8)#2	77.8(4)	O(1)–Nd(1)–O(3)	80.5(3)
O(6)#1–Nd(1)–O(9)	129.1(5)	O(6)#1–Nd(1)–O(4)	67.1(4)
O(2)#1–Nd(1)–O(9)	80.8(3)	O(2)#1–Nd(1)–O(4)	86.1(3)
O(8)#2–Nd(1)–O(9)	141.0(5)	O(8)#2–Nd(1)–O(4)	74.9(4)
O(6)#1–Nd(1)–O(5)	133.8(5)	O(9)–Nd(1)–O(4)	71.4(4)
O(2)#1–Nd(1)–O(5)	84.3(4)	O(5)–Nd(1)–O(4)	149.6(4)
O(8)#2–Nd(1)–O(5)	130.4(5)	O(10)–Nd(1)–O(4)	105.8(3)
O(9)–Nd(1)–O(5)	78.6(5)	O(7)#3–Nd(1)–O(4)	134.7(4)
O(6)#1–Nd(1)–O(10)	145.4(5)	O(1)–Nd(1)–O(4)	128.3(3)
O(2)#1–Nd(1)–O(10)	146.1(4)	O(3)–Nd(1)–O(4)	51.7(3)
O(8)#2–Nd(1)–O(10)	135.6(5)	O(6)#1–Nd(1)–O(2)	73.3(4)
O(9)–Nd(1)–O(10)	73.7(4)	O(2)#1–Nd(1)–O(2)	74.7(3)
O(5)–Nd(1)–O(10)	69.4(4)	O(8)#2–Nd(1)–O(2)	67.1(4)
O(6)#1–Nd(1)–O(7)#3	134.4(5)	O(9)–Nd(1)–O(2)	136.3(4)
O(2)#1–Nd(1)–O(7)#3	73.6(4)	O(5)–Nd(1)–O(2)	63.7(4)
O(8)#2–Nd(1)–O(7)#3	135.6(5)	O(10)–Nd(1)–O(2)	109.6(3)
O(9)–Nd(1)–O(7)#3	65.6(5)	O(7)#3–Nd(1)–O(2)	73.0(4)
O(5)–Nd(1)–O(7)#3	16.0(3)	O(1)–Nd(1)–O(2)	50.3(3)
O(10)–Nd(1)–O(7)#3	75.8(4)	O(3)–Nd(1)–O(2)	123.1(3)
O(6)#1–Nd(1)–O(1)	85.2(5)	O(4)–Nd(1)–O(2)	140.1(3)
O(2)#1–Nd(1)–O(1)	124.1(3)	O(6)#1–Nd(1)–C(7)	68.3(4)
O(8)#2–Nd(1)–O(1)	72.9(5)	O(2)#1–Nd(1)–C(7)	109.3(3)
O(9)–Nd(1)–O(1)	145.2(4)	O(8)#2–Nd(1)–C(7)	70.9(4)
O(5)–Nd(1)–O(1)	80.3(4)	O(9)–Nd(1)–C(7)	86.3(4)
O(10)–Nd(1)–O(1)	73.1(4)	O(5)–Nd(1)–C(7)	157.8(4)
O(7)#3–Nd(1)–O(1)	96.1(4)	O(10)–Nd(1)–C(7)	91.0(3)
O(6)#1–Nd(1)–O(3)	76.3(4)	O(7)#3–Nd(1)–C(7)	151.2(4)
O(2)#1–Nd(1)–O(3)	133.4(3)	O(1)–Nd(1)–C(7)	104.4(3)

O(8)#2–Nd(1)–O(3)	73.0(4)	O(3)–Nd(1)–C(7)	26.2(3)
O(9)–Nd(1)–O(3)	100.0(4)	O(4)–Nd(1)–C(7)	25.6(3)
O(5)–Nd(1)–O(3)	142.0(4)	O(2)–Nd(1)–C(7)	135.8(3)

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

STable 2. Related bond lengths (Å) and angles (°) around the Nd(III) ion for 2.

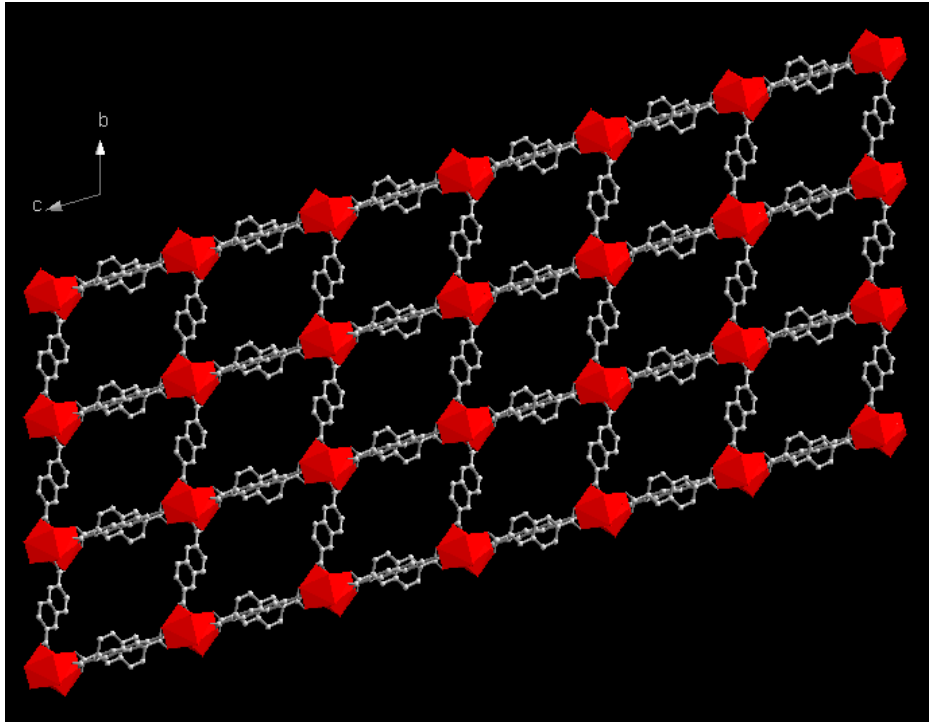
Nd(1)–O(5)#1	2.392(4)	Nd(2)–O(2)#3	2.353(4)
Nd(1)–O(5)#2	2.392(4)	Nd(2)–O(2)	2.353(3)
Nd(1)–O(1)	2.404(3)	Nd(2)–O(4)#6	2.391(4)
Nd(1)–O(1)#3	2.404(3)	Nd(2)–O(4)#7	2.391(4)
Nd(1)–O(3)#4	2.424(4)	Nd(2)–O(6)	2.429(4)
Nd(1)–O(3)#5	2.424(4)	Nd(2)–O(6)#3	2.429(4)
Nd(1)–O(7)	2.464(6)	Nd(2)–O(9)	2.559(5)
Nd(1)–O(8)	2.553(5)		
O(5)#1–Nd(1)–O(5)#2	73.0(2)	O(3)#4–Nd(1)–O(8)	74.71(1)
O(5)#1–Nd(1)–O(1)	145.43(1)	O(3)#5–Nd(1)–O(8)	74.71(1)
O(5)#2–Nd(1)–O(1)	85.12(1)	O(7)–Nd(1)–O(8)	127.64(2)
O(5)#1–Nd(1)–O(1)#3	85.12(1)	O(2)#3–Nd(2)–O(2)	84.68(2)
O(5)#2–Nd(1)–O(1)#3	145.43(1)	O(2)#3–Nd(2)–O(4)#6	74.76(1)
O(1)–Nd(1)–O(1)#3	99.63(2)	O(2)–Nd(2)–O(4)#6	124.91(1)
O(5)#1–Nd(1)–O(3)#4	70.18(1)	O(2)#3–Nd(2)–O(4)#7	124.91(1)
O(5)#2–Nd(1)–O(3)#4	112.12(1)	O(2)–Nd(2)–O(4)#7	74.76(1)
O(1)–Nd(1)–O(3)#4	144.18(1)	O(4)#6–Nd(2)–O(4)#7	76.6(2)
O(1)#3–Nd(1)–O(3)#4	83.78(1)	O(2)#3–Nd(2)–O(6)	145.67(1)
O(5)#1–Nd(1)–O(3)#5	112.12(1)	O(2)–Nd(2)–O(6)	83.47(1)
O(5)#2–Nd(1)–O(3)#5	70.18(1)	O(4)#6–Nd(2)–O(6)	137.13(1)
O(1)–Nd(1)–O(3)#5	83.78(1)	O(4)#7–Nd(2)–O(6)	82.42(1)
O(1)#3–Nd(1)–O(3)#5	144.18(1)	O(2)#3–Nd(2)–O(6)#3	83.47(1)
O(3)#4–Nd(1)–O(3)#5	74.0(2)	O(2)–Nd(2)–O(6)#3	145.67(1)
O(5)#1–Nd(1)–O(7)	74.01(1)	O(4)#6–Nd(2)–O(6)#3	82.42(1)
O(5)#2–Nd(1)–O(7)	74.01(1)	O(4)#7–Nd(2)–O(6)#3	137.13(1)
O(1)–Nd(1)–O(7)	74.42(1)	O(6)–Nd(2)–O(6)#3	88.44(2)
O(1)#3–Nd(1)–O(7)	74.42(1)	O(2)#3–Nd(2)–O(9)	71.16(1)
O(3)#4–Nd(1)–O(7)	139.30(1)	O(2)–Nd(2)–O(9)	71.16(1)
O(3)#5–Nd(1)–O(7)	139.30(1)	O(4)#6–Nd(2)–O(9)	140.49(1)
O(5)#1–Nd(1)–O(8)	140.03(1)	O(4)#7–Nd(2)–O(9)	140.49(1)
O(5)#2–Nd(1)–O(8)	140.03(1)	O(6)–Nd(2)–O(9)	74.52(1)
O(1)–Nd(1)–O(8)	72.51(1)	O(6)#3–Nd(2)–O(9)	74.52(1)
O(1)#3–Nd(1)–O(8)	72.51(1)		

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

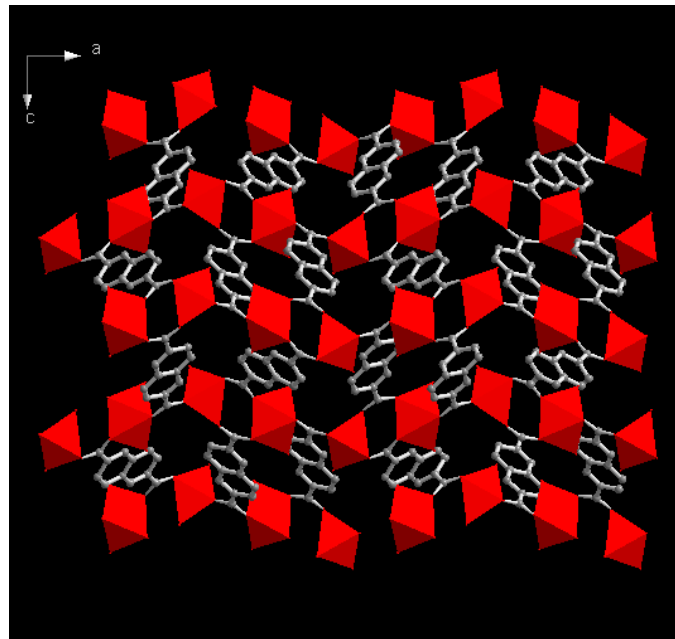
STable 3. Related bond lengths (Å) and angles (°) around the Nd(III) ion for **3**.

Nd–O(4)#1	2.363(4)	Nd–O(7)	2.516(4)
Nd–O(2)#2	2.391(4)	Nd–O(6)	2.519(4)
Nd–O(1)	2.395(4)	Nd–O(5)	2.548(4)
Nd–O(3)#3	2.451(4)	Nd–O(8)	2.472(3)
O(4)#1–Nd–O(2)#2	85.76(1)	O(3)#3–Nd–O(6)	72.66(1)
O(4)#1–Nd–O(1)	157.56(1)	O(8)–Nd–O(6)	126.98(1)
O(2)#2–Nd–O(1)	103.58(1)	O(7)–Nd–O(6)	147.80(1)
O(4)#1–Nd–O(3)#3	107.75(1)	O(4)#1–Nd–O(5)	123.31(1)
O(2)#2–Nd–O(3)#3	145.42(1)	O(2)#2–Nd–O(5)	71.37(1)
O(1)–Nd–O(3)#3	76.12(1)	O(1)–Nd–O(5)	79.14(1)
O(4)#1–Nd–O(8)	74.80(1)	O(3)#3–Nd–O(5)	74.72(1)
O(2)#2–Nd–O(8)	137.72(1)	O(8)–Nd–O(5)	149.98(1)
O(1)–Nd–O(8)	84.93(1)	O(7)–Nd–O(5)	126.64(1)
O(3)#3–Nd–O(8)	76.84(1)	O(6)–Nd–O(5)	51.37(1)
O(4)#1–Nd–O(7)	88.92(1)	O(4)#1–Nd–C(2)	99.21(1)
O(2)#2–Nd–O(7)	70.14(1)	O(2)#2–Nd–C(18)	74.89(1)
O(1)–Nd–O(7)	75.59(1)	O(1)–Nd–C(18)	102.91(1)
O(3)#3–Nd–O(7)	139.45(1)	O(3)#3–Nd–C(18)	71.63(1)
O(8)–Nd–O(7)	72.28(1)	O(8)–Nd–C(18)	144.34(1)
O(4)#1–Nd–O(6)	74.69(1)	O(7)–Nd–C(18)	143.36(1)
O(2)#2–Nd–O(6)	80.99(1)	O(6)–Nd–C(18)	25.73(1)
O(1)–Nd–O(6)	126.49(1)	O(5)–Nd–C(18)	25.65(1)

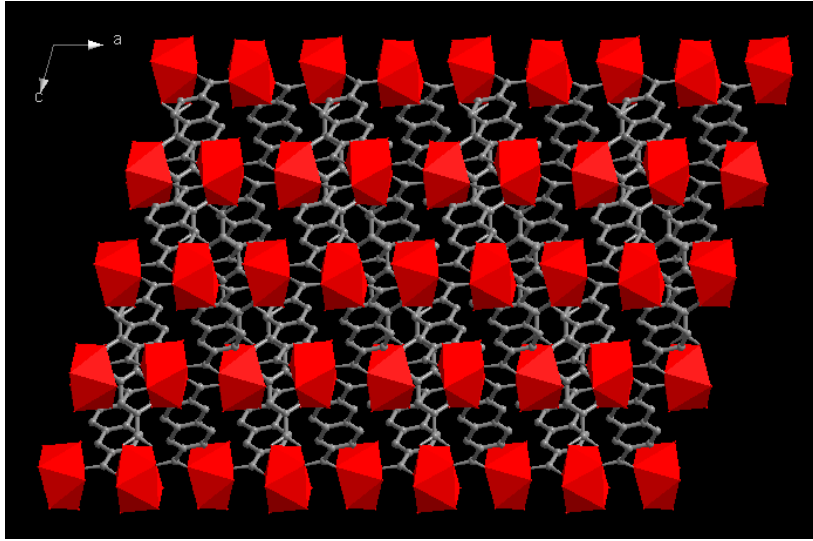
Symmetry transformations used to generate equivalent atoms: #1 $-x+1/2, y-1/2, -z+3/2$; #2 $-x, -y, -z+1$; #3 $x+1/2, -y+1/2, z-1/2$



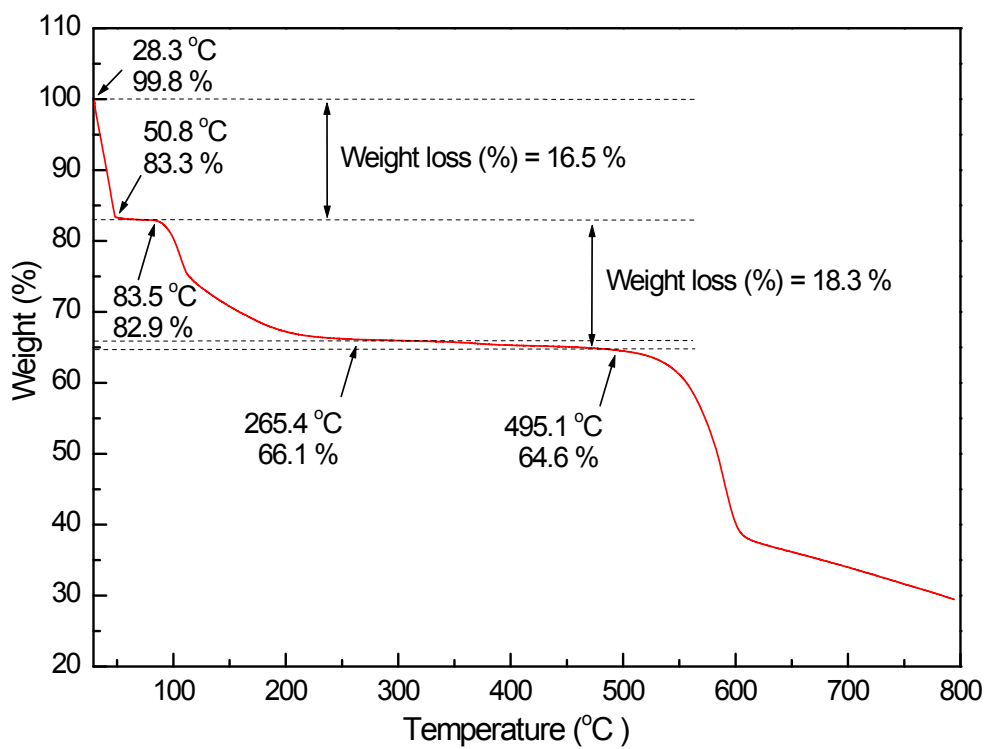
SFigure 1



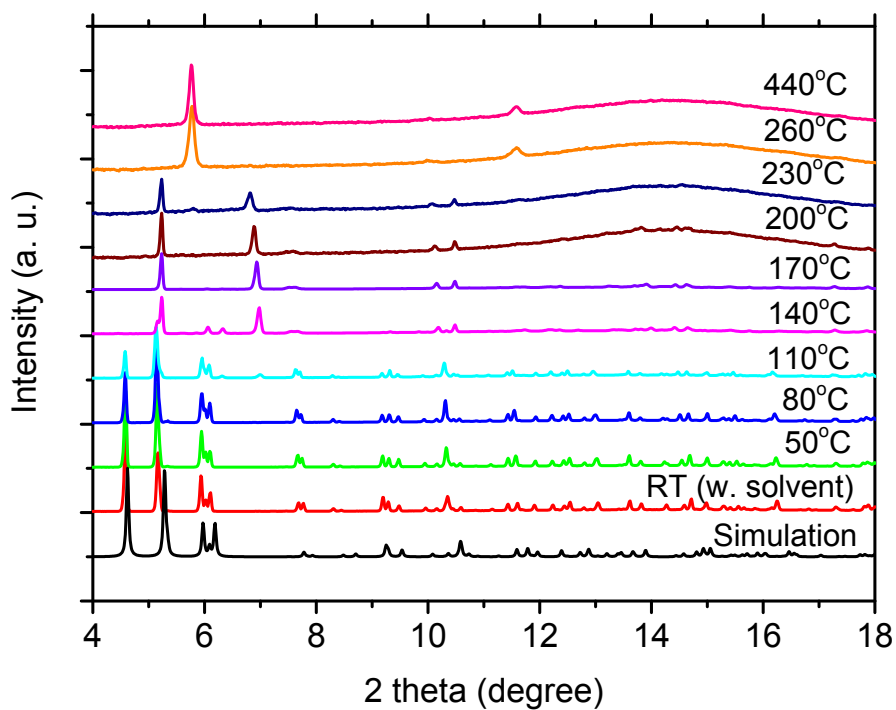
SFigure 2



SFigure 3

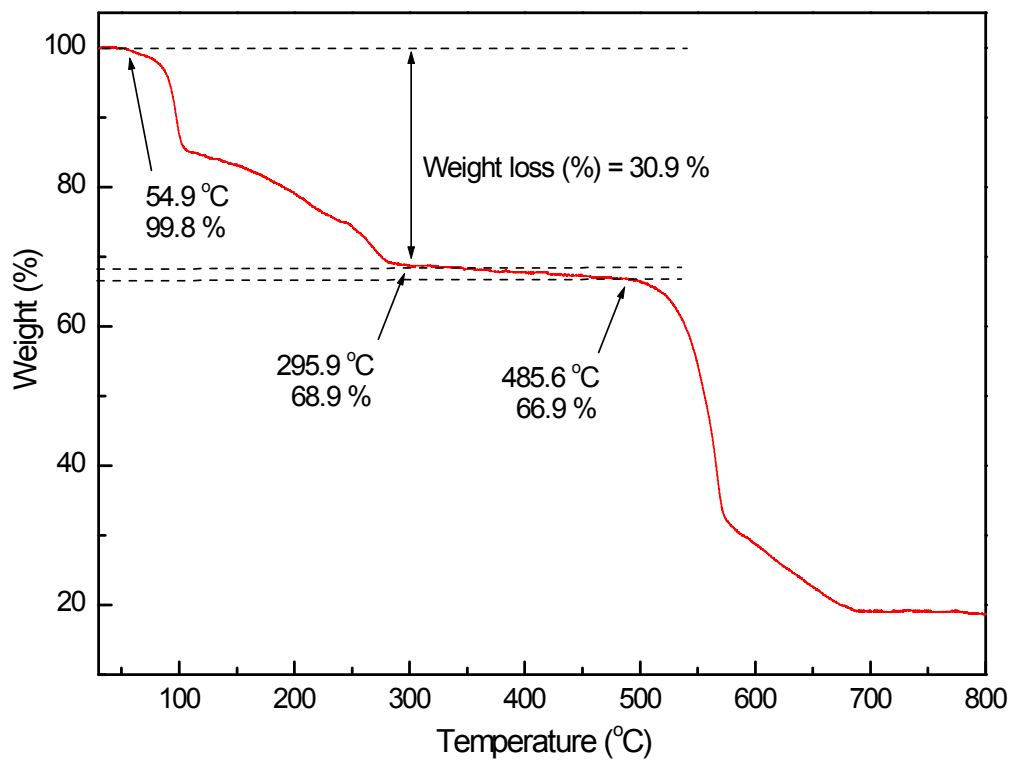


(a)

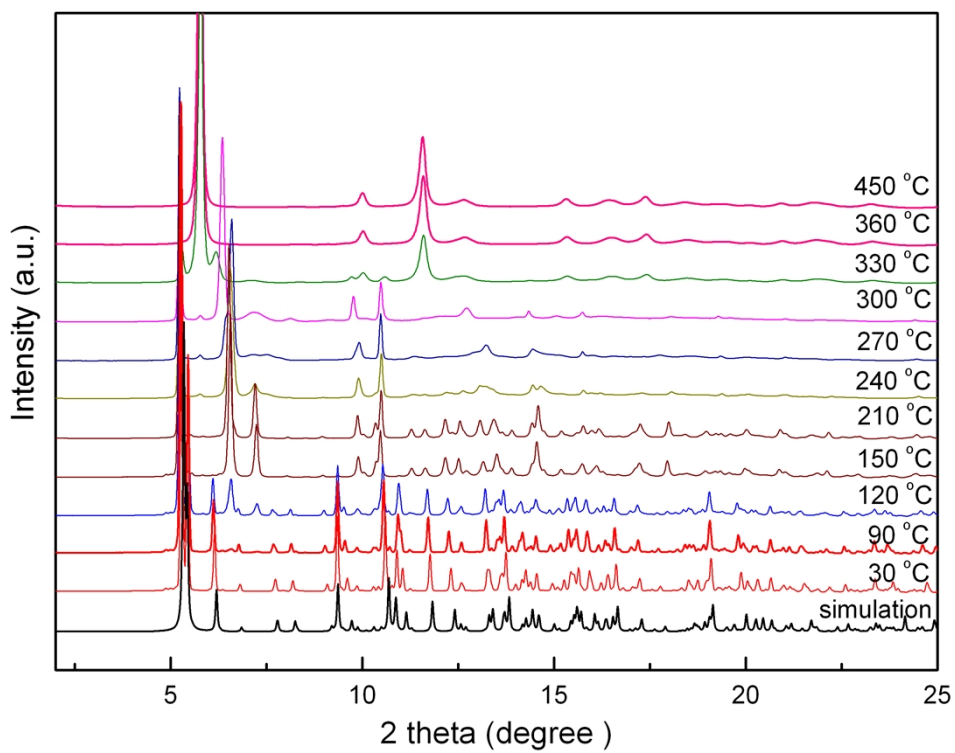


(b)

SFigure 4

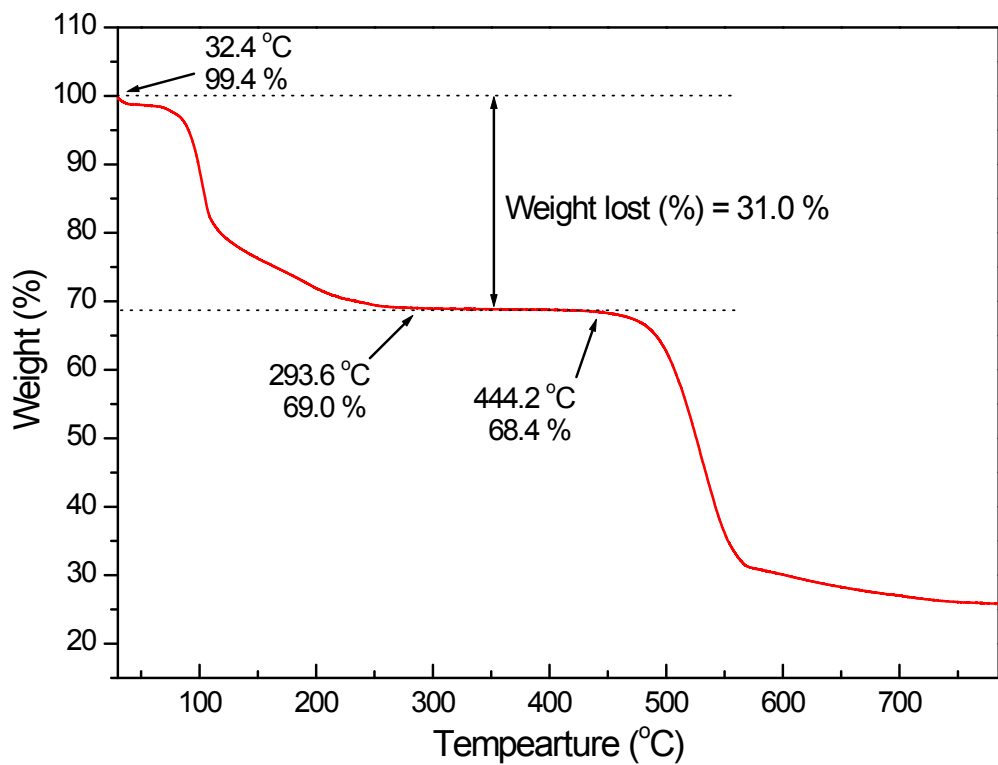


(a)

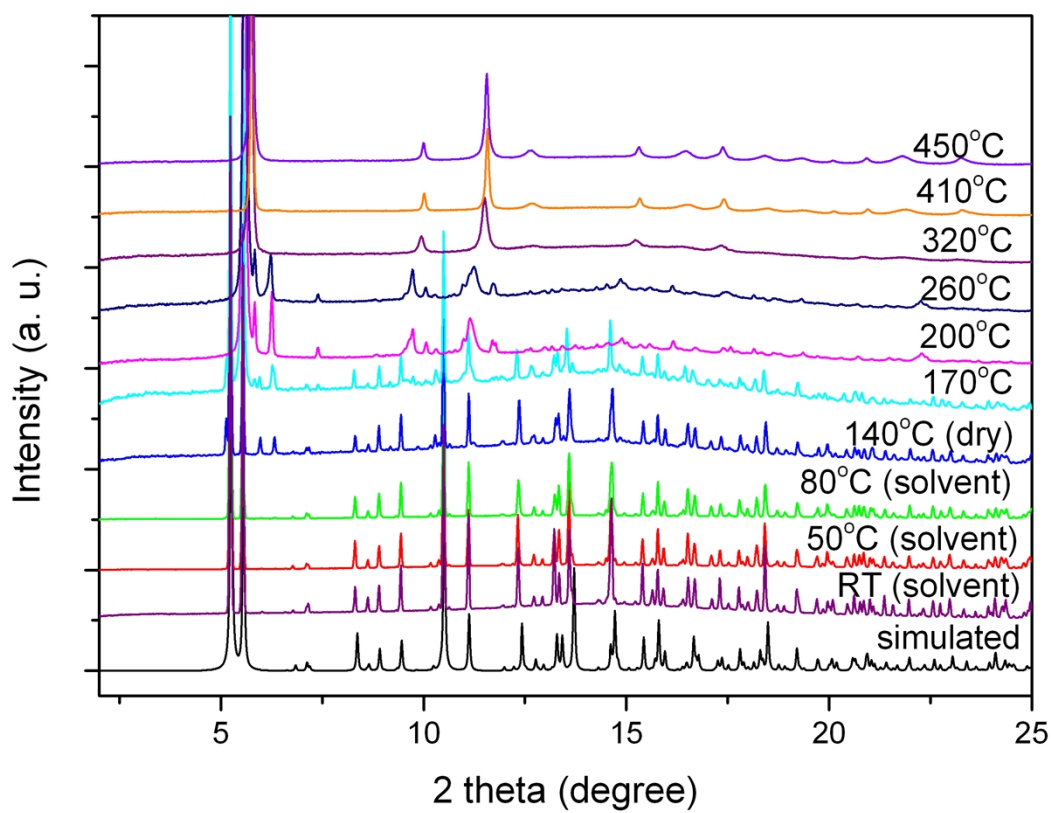


(b)

SFigure 5



(a)



(b)

SFigure 6