Construction of Three Metal−Organic Frameworks Based on Multifunctional T-shaped Tripodal Ligands, H_3PyImDC

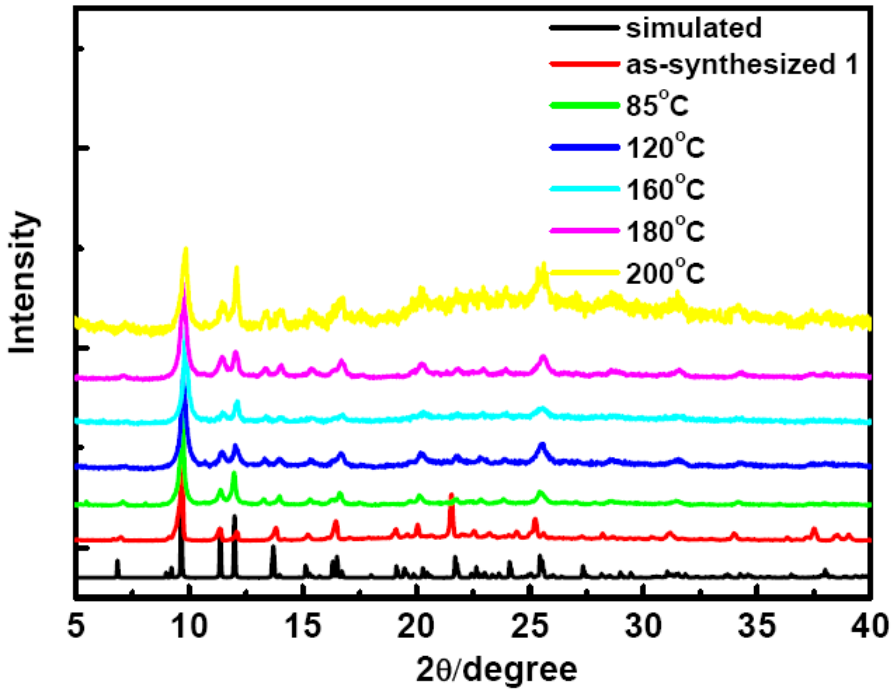
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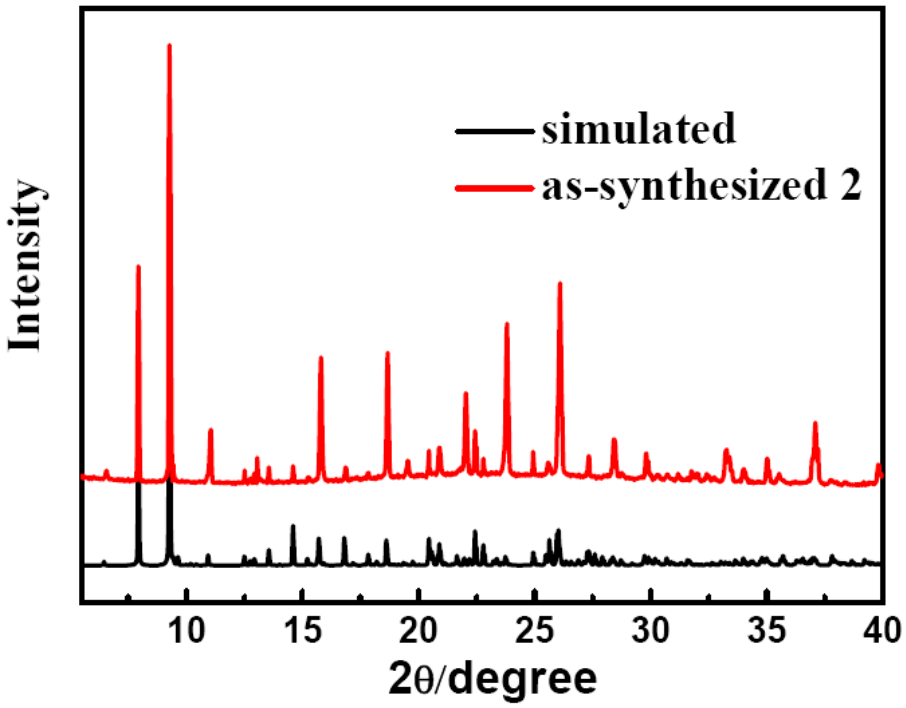
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Figure S1. Powder X-ray diffraction patterns of the simulated and as-synthesized samples **1-3**, indicating the phase purity of the as-synthesized samples. Compounds **1** and **3** are recorded at various temperatures.





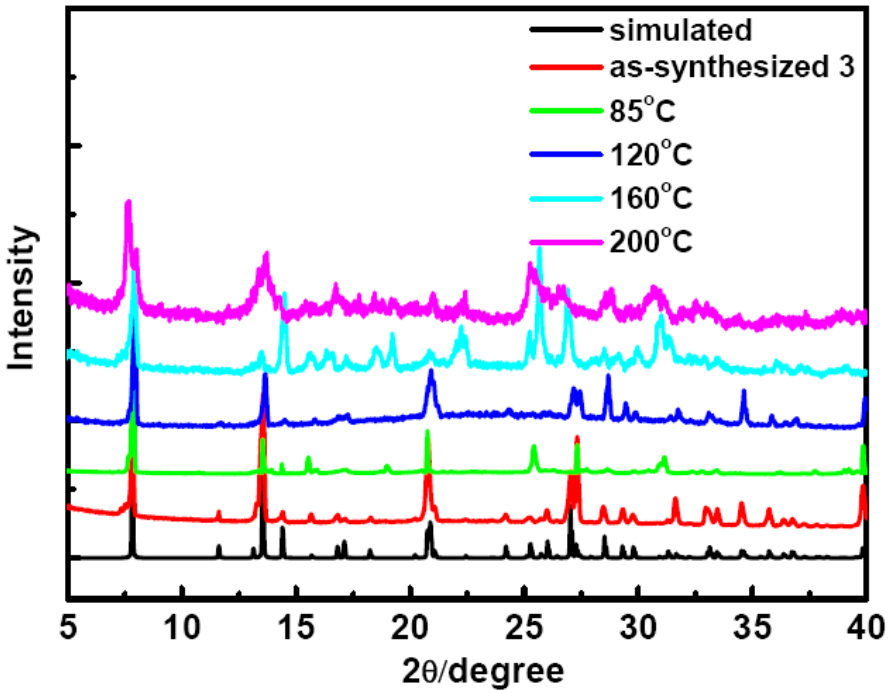


Figure S2. FT-IR spectra for compound **1-3**.

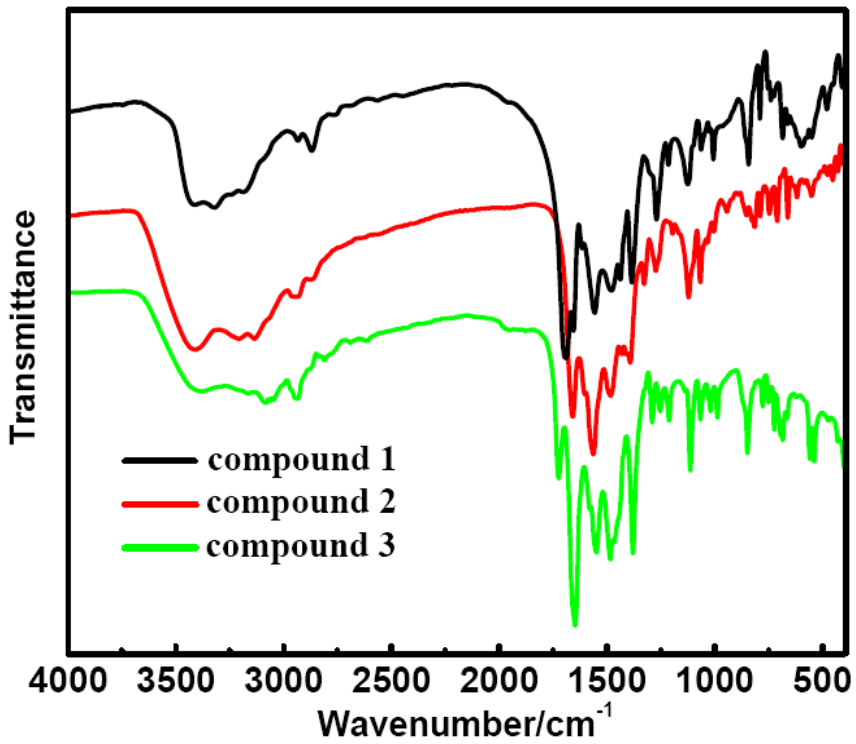


Figure S3. Tiles and face symbols for the three-periodic nets for (a) **1** and (b) **3**.

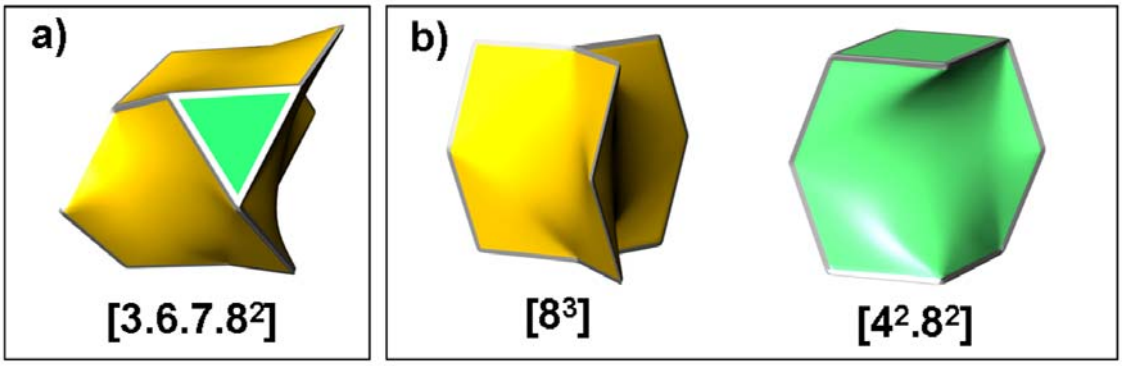


Figure S4. (a) Space-filling model of the open channels along [100] direction in compound **1**. (b) Hydrogen-bonding model between the water cluster and organic ligand in compound **2**. Color scheme: carbon = gray, nitrogen = blue, oxygen = red, zinc = green, all the guest molecules and H atoms in compound **1** were omitted.

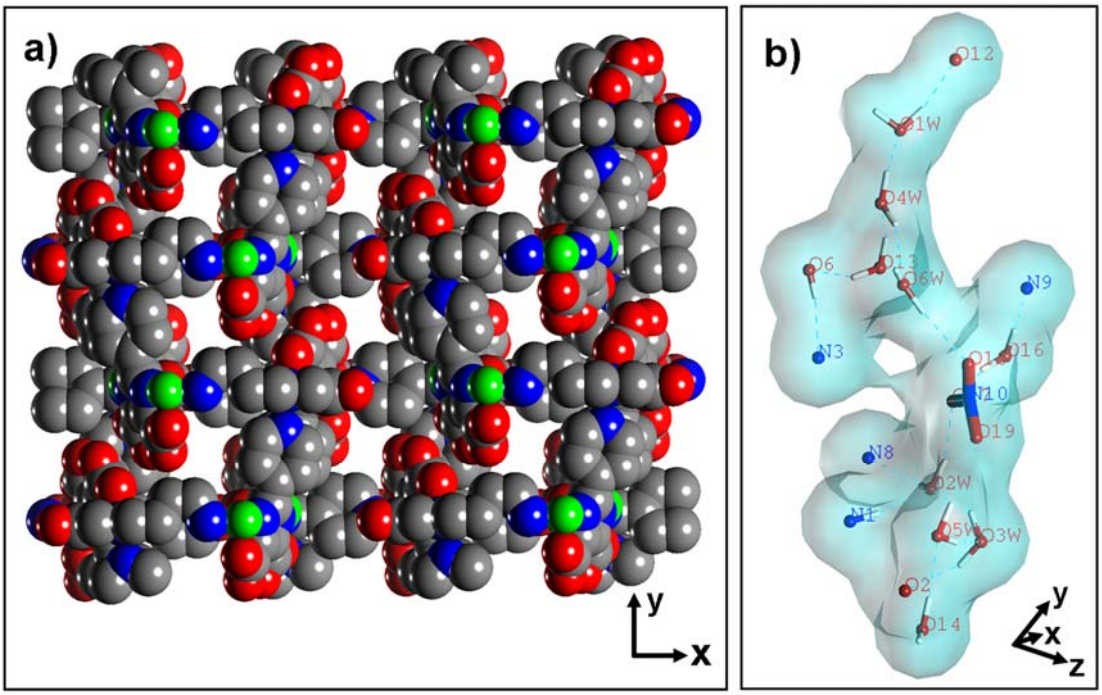


Figure S5. TGA curves for **1-3** (35-800^{o}C).

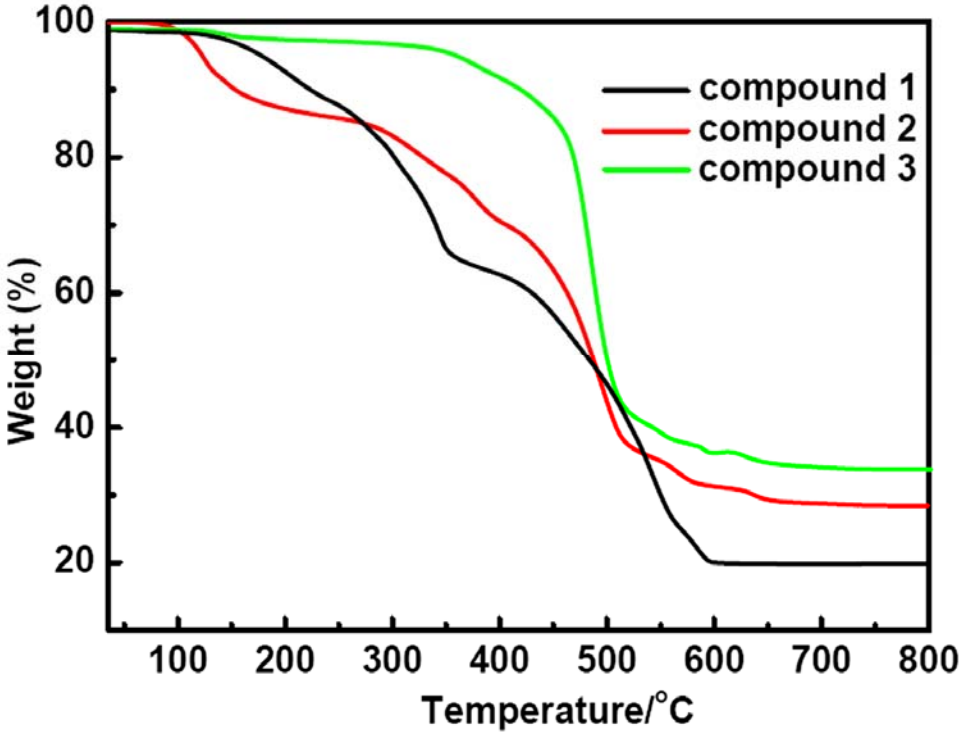


Table S1. Topological information for compounds **1** and **3**.

Name	Compound **1**	Compound **3**
Net	**bbm**	**ant**
T_1 $CS_{1\text{-}10}$	4.10.24.42.64.92.124.162.204.252	3.13.16.54.42.119.81210.133.327
T_2 $CS_{1\text{-}10}$	4.10.24.40.66.90.124.160.206.250	6.8.32.28.84.60.162.106.266.164
Cum_{10}	979 & 975	999 & 917
Vertex symbols	T_1 [3.6.6.7.7.8_2] T_2 [3.7.6.6.7.7]	T_1 [4.4.8_{10}] T_2 [4.4.4.4.8_4.8_4.8_4.8_4.8_5.8_5.8_5.8_5.*.*.*]
Tilling	[3.6.7.8^2]	[8^3] +[4^2.8^2]

Table S2. Selected bond lengths [Å] and angles [º] for **1**

Zn(1)-O(7)	2.072(5)	Zn(2)-N(2)#2	2.025(6)
Zn(1)-N(4)	2.074(6)	Zn(2)-N(2)	2.025(6)
Zn(1)-N(1)	2.100(6)	Zn(2)-N(5)#3	2.061(8)
Zn(1)-N(3)#1	2.130(6)	Zn(2)-O(3)	2.139(5)
Zn(1)-O(5)	2.214(5)	Zn(2)-O(3)#2	2.139(5)
Zn(1)-O(1)	2.246(5)	N(3)-Zn(1)#1	2.130(6)
O(7)-Zn(1)-N(4)	100.1(2)	N(5)#3-Zn(2)-O(3)#2	86.63(13)
O(7)-Zn(1)-N(1)	94.2(2)	O(3)-Zn(2)-O(3)#2	173.3(3)
N(4)-Zn(1)-N(1)	158.3(2)	C(4)-O(1)-Zn(1)	111.3(5)
O(7)-Zn(1)-N(3)#1	89.4(2)	C(4)-O(2)-H(2)	122(8)
N(4)-Zn(1)-N(3)#1	92.8(2)	C(5)-O(3)-Zn(2)	112.5(5)
N(1)-Zn(1)-N(3)#1	103.6(2)	C(13)-O(5)-Zn(1)	111.3(5)
O(7)-Zn(1)-O(5)	176.0(2)	C(13)-O(6)-H(6)	109(7)
N(4)-Zn(1)-O(5)	78.9(2)	C(17)-O(7)-Zn(1)	127.3(5)
N(1)-Zn(1)-O(5)	85.8(2)	C(1)-N(1)-C(2)	103.9(6)
N(3)#1-Zn(1)-O(5)	94.6(2)	C(1)-N(1)-Zn(1)	142.5(5)
O(7)-Zn(1)-O(1)	91.6(2)	C(2)-N(1)-Zn(1)	111.7(4)
N(4)-Zn(1)-O(1)	85.6(2)	C(1)-N(2)-C(3)	104.1(6)
N(1)-Zn(1)-O(1)	77.8(2)	C(1)-N(2)-Zn(2)	145.7(5)
N(3)#1-Zn(1)-O(1)	178.3(2)	C(3)-N(2)-Zn(2)	110.1(5)
O(5)-Zn(1)-O(1)	84.49(19)	C(10)-N(3)-C(6)	118.0(7)
N(2)#2-Zn(2)-N(2)	129.8(3)	C(10)-N(3)-Zn(1)#1	123.2(5)
N(2)#2-Zn(2)-N(5)#3	115.11(16)	C(6)-N(3)-Zn(1)#1	118.8(5)
N(2)-Zn(2)-N(5)#3	115.11(16)	C(11)-N(4)-C(12)	106.2(6)
N(2)#2-Zn(2)-O(3)	101.8(2)	C(11)-N(4)-Zn(1)	142.8(5)
N(2)-Zn(2)-O(3)	81.1(2)	C(12)-N(4)-Zn(1)	110.9(4)
N(5)#3-Zn(2)-O(3)	86.63(13)	C(14)#4-N(5)-C(14)	116.2(9)
N(2)#2-Zn(2)-O(3)#2	81.1(2)	C(14)#4-N(5)-Zn(2)#5	121.9(4)
N(2)-Zn(2)-O(3)#2	101.8(2)	C(14)-N(5)-Zn(2)#5	121.9(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2 #2 -x+1/2,-y+1/2,-z+2 #3 -x+1,y,-z+3/2 #4 x+1/2,y-1/2,z #5 x-1/2,y+1/2, z

Table S3. Selected bond lengths (Å) and angles (°) for **2**.

Nd(1)-O(9)#1	2.360(3)	Nd(2)-O(3)	2.349(2)
Nd(1)-O(5)	2.392(3)	Nd(2)-O(16)	2.410(3)
Nd(1)-O(10)	2.447(2)	Nd(2)-O(4)#2	2.411(2)
Nd(1)-O(7)	2.492(3)	Nd(2)-O(15)	2.453(3)
Nd(1)-O(13)	2.502(3)	Nd(2)-O(1)	2.486(2)
Nd(1)-O(14)	2.526(3)	Nd(2)-O(8)	2.532(3)
Nd(1)-O(11)#1	2.536(2)	Nd(2)-O(11)#1	2.605(3)
Nd(1)-O(1)	2.540(2)	Nd(2)-O(12)#1	2.644(3)
Nd(1)-O(2)	2.689(2)	Nd(2)-O(7)	2.779(3)
O(9)#1-Nd(1)-O(5)	77.79(11)	O(3)-Nd(2)-O(16)	74.65(10)
O(9)#1-Nd(1)-O(10)	85.23(9)	O(3)-Nd(2)-O(4)#2	98.84(8)
O(5)-Nd(1)-O(10)	78.18(9)	O(16)-Nd(2)-O(4)#2	85.68(10)
O(9)#1-Nd(1)-O(7)	105.61(9)	O(3)-Nd(2)-O(15)	73.62(10)
O(5)-Nd(1)-O(7)	70.03(9)	O(16)-Nd(2)-O(15)	144.51(10)
O(10)-Nd(1)-O(7)	142.90(9)	O(4)#2-Nd(2)-O(15)	83.86(9)
O(9)#1-Nd(1)-O(13)	74.22(11)	O(3)-Nd(2)-O(1)	69.86(8)
O(5)-Nd(1)-O(13)	145.06(10)	O(16)-Nd(2)-O(1)	87.81(9)
O(10)-Nd(1)-O(13)	79.04(10)	O(4)#2-Nd(2)-O(1)	168.16(8)
O(7)-Nd(1)-O(13)	137.89(10)	O(15)-Nd(2)-O(1)	95.85(9)
O(9)#1-Nd(1)-O(14)	148.41(11)	O(3)-Nd(2)-O(8)	147.08(10)
O(5)-Nd(1)-O(14)	72.24(10)	O(16)-Nd(2)-O(8)	136.63(9)
O(10)-Nd(1)-O(14)	79.17(11)	O(4)#2-Nd(2)-O(8)	77.93(8)
O(7)-Nd(1)-O(14)	73.40(10)	O(15)-Nd(2)-O(8)	73.47(9)
O(13)-Nd(1)-O(14)	128.26(10)	O(1)-Nd(2)-O(8)	113.39(8)
O(9)#1-Nd(1)-O(11)#1	68.73(9)	O(3)-Nd(2)-O(11)#1	129.79(9)
O(5)-Nd(1)-O(11)#1	111.76(8)	O(16)-Nd(2)-O(11)#1	79.70(10)
O(10)-Nd(1)-O(11)#1	148.36(9)	O(4)#2-Nd(2)-O(11)#1	121.56(8)
O(7)-Nd(1)-O(11)#1	64.91(9)	O(15)-Nd(2)-O(11)#1	133.94(9)
O(13)-Nd(1)-O(11)#1	76.83(10)	O(1)-Nd(2)-O(11)#1	66.70(8)
O(14)-Nd(1)-O(11)#1	132.22(10)	O(8)-Nd(2)-O(11)#1	75.56(9)
O(9)#1-Nd(1)-O(1)	132.90(9)	O(3)-Nd(2)-O(12)#1	142.19(10)
O(5)-Nd(1)-O(1)	133.98(10)	O(16)-Nd(2)-O(12)#1	68.08(9)
O(10)-Nd(1)-O(1)	128.51(8)	O(4)#2-Nd(2)-O(12)#1	72.70(8)
O(7)-Nd(1)-O(1)	68.75(8)	O(15)-Nd(2)-O(12)#1	138.72(8)
O(13)-Nd(1)-O(1)	80.92(10)	O(1)-Nd(2)-O(12)#1	113.81(8)
O(14)-Nd(1)-O(1)	77.18(10)	O(8)-Nd(2)-O(12)#1	68.75(9)
O(11)#1-Nd(1)-O(1)	66.97(7)	O(11)#1-Nd(2)-O(12)#1	49.28(7)
O(9)#1-Nd(1)-O(2)	137.84(11)	O(3)-Nd(2)-O(7)	120.04(9)
O(5)-Nd(1)-O(2)	134.92(9)	O(16)-Nd(2)-O(7)	137.45(9)
O(10)-Nd(1)-O(2)	79.08(8)	O(4)#2-Nd(2)-O(7)	125.76(8)
O(7)-Nd(1)-O(2)	110.47(8)	O(15)-Nd(2)-O(7)	73.90(9)
O(13)-Nd(1)-O(2)	64.52(10)	O(1)-Nd(2)-O(7)	65.04(7)
O(14)-Nd(1)-O(2)	65.56(10)	O(8)-Nd(2)-O(7)	48.62(8)

O(11)#1-Nd(1)-O(2)	108.02(8)	O(11)#1-Nd(2)-O(7)	60.05(8)
O(1)-Nd(1)-O(2)	49.51(7)	O(12)#1-Nd(2)-O(7)	92.63(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x,-y+1,-z

Table S4. Hydrogen bonds for **2** [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(6)-H(6)...N(3)#3	0.82	1.90	2.707(4)	166.2
N(1)-H(1)...O(2W)	0.86	2.15	2.928(5)	150.1
N(5)-H(5)...O(5W)#4	0.86	2.33	3.164(6)	164.7
N(7)-H(7)...O(3W)	0.86	2.02	2.880(4)	175.5
O(13)-H(13A)...O(4W)	0.988(19)	1.97(4)	2.872(5)	150(5)
O(13)-H(13B)...O(6)#1	0.97(2)	1.90(3)	2.800(4)	153(5)
O(14)-H(14A)...O(5W)	0.972(19)	2.08(3)	3.033(7)	167(5)
O(14)-H(14B)...O(6W)	0.997(19)	1.75(2)	2.735(6)	169(5)
O(15)-H(15A)...N(6)#5	0.985(19)	1.86(3)	2.795(4)	157(6)
O(15)-H(15B)...O(18)#6	0.983(19)	1.97(3)	2.894(7)	155(6)
O(15)-H(15B)...N(10)#6	0.983(19)	2.57(2)	3.542(8)	170(4)
O(16)-H(16A)...N(9)#7	0.986(19)	1.70(2)	2.682(4)	178(6)
O(16)-H(16B)...O(17)	0.96(2)	1.84(3)	2.777(7)	164(6)
O(16)-H(16B)...N(10)	0.96(2)	2.64(4)	3.440(8)	141(5)
O(1W)-H(1A)...N(2)#8	0.98(2)	2.10(3)	3.005(4)	153(5)
O(1W)-H(1A)...O(4)#8	0.98(2)	2.26(5)	2.990(4)	130(4)
O(1W)-H(1B)...O(12)	0.979(19)	1.88(3)	2.838(4)	165(5)
O(2W)-H(2A)...O(17)#9	0.969(19)	1.95(3)	2.882(8)	161(6)
O(2W)-H(2A)...O(19)#9	0.969(19)	2.50(4)	3.190(8)	128(4)
O(2W)-H(2A)...N(10)#9	0.969(19)	2.68(3)	3.558(10)	151(5)
O(2W)-H(2B)...N(8)#7	0.964(19)	2.22(5)	3.027(5)	141(6)
O(3W)-H(3A)...O(2W)	0.992(19)	2.09(4)	2.922(6)	140(4)
O(3W)-H(3A)...O(19)#9	0.992(19)	2.52(4)	3.261(7)	132(4)
O(3W)-H(3B)...O(2)	0.985(19)	1.94(3)	2.873(4)	158(5)
O(3W)-H(3B)...O(10)	0.985(19)	2.61(5)	3.095(5)	111(4)
O(4W)-H(4A)...O(1W)#7	0.986(19)	1.94(3)	2.869(5)	155(5)
O(4W)-H(4B)...O(6W)#10	0.997(19)	2.07(3)	2.997(8)	153(5)
O(5W)-H(5B)...O(8)#5	1.052(19)	2.54(3)	3.517(6)	155(5)
O(5W)-H(5C)...O(3W)	1.03(2)	1.89(3)	2.902(7)	166(6)
O(6W)-H(6A)...O(18)#6	1.010(19)	2.18(2)	3.185(9)	174(6)
O(6W)-H(6B)...O(4W)#6	0.97(2)	2.28(5)	2.997(8)	130(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x,-y+1,-z #3 x,-y+1/2,z+1/2 #4 -x,y+1/2,-z+1/2 #5 -x,y-1/2,-z+1/2

#6 x-1, y, z #7 x,-y+1/2,z-1/2 #8 x+1,y,z+1 #9 -x+1,y-1/2,-z+1/2 #10 x+1, y, z

Table S5. Selected bond lengths (Å) and angles (°) for **3**.

Nd(1)-O(1)	2.359(4)	Nd(2)-O(2)#4	2.361(4)
Nd(1)-O(1)#1	2.359(4)	Nd(2)-O(2)#5	2.361(4)
Nd(1)-O(4)#2	2.486(4)	Nd(2)-O(2)#6	2.361(4)
Nd(1)-O(4)#3	2.486(4)	Nd(2)-O(2)	2.361(4)
Nd(1)-O(3)#2	2.547(3)	Nd(2)-O(3)#5	2.490(4)
Nd(1)-O(3)#3	2.547(3)	Nd(2)-O(3)	2.490(4)
Nd(1)-N(1)#1	2.601(4)	Nd(2)-O(3)#4	2.490(4)
Nd(1)-N(1)	2.601(4)	Nd(2)-O(3)#6	2.490(4)
O(1)-Nd(1)-O(1)#1	179.24(19)	O(2)#4-Nd(2)-O(2)#5	85.5(2)
O(1)-Nd(1)-O(4)#2	96.82(15)	O(2)#4-Nd(2)-O(2)#6	150.3(2)
O(1)#1-Nd(1)-O(4)#2	83.10(15)	O(2)#5-Nd(2)-O(2)#6	102.1(2)
O(1)-Nd(1)-O(4)#3	83.10(15)	O(2)#4-Nd(2)-O(2)	102.1(2)
O(1)#1-Nd(1)-O(4)#3	96.82(15)	O(2)#5-Nd(2)-O(2)	150.3(2)
O(4)#2-Nd(1)-O(4)#3	168.76(17)	O(2)#6-Nd(2)-O(2)	85.5(2)
O(1)-Nd(1)-O(3)#2	92.91(14)	O(2)#4-Nd(2)-O(3)#5	79.59(14)
O(1)#1-Nd(1)-O(3)#2	86.45(13)	O(2)#5-Nd(2)-O(3)#5	71.73(13)
O(4)#2-Nd(1)-O(3)#2	51.38(12)	O(2)#6-Nd(2)-O(3)#5	75.82(14)
O(4)#3-Nd(1)-O(3)#2	117.39(12)	O(2)-Nd(2)-O(3)#5	137.65(13)
O(1)-Nd(1)-O(3)#3	86.45(13)	O(2)#4-Nd(2)-O(3)	75.82(14)
O(1)#1-Nd(1)-O(3)#3	92.91(14)	O(2)#5-Nd(2)-O(3)	137.65(13)
O(4)#2-Nd(1)-O(3)#3	117.39(12)	O(2)#6-Nd(2)-O(3)	79.59(14)
O(4)#3-Nd(1)-O(3)#3	51.38(12)	O(2)-Nd(2)-O(3)	71.73(13)
O(3)#2-Nd(1)-O(3)#3	66.02(16)	O(3)#5-Nd(2)-O(3)	67.72(16)
O(1)-Nd(1)-N(1)#1	115.72(14)	O(2)#4-Nd(2)-O(3)#4	71.73(13)
O(1)#1-Nd(1)-N(1)#1	64.95(13)	O(2)#5-Nd(2)-O(3)#4	79.59(14)
O(4)#2-Nd(1)-N(1)#1	116.19(13)	O(2)#6-Nd(2)-O(3)#4	137.65(13)
O(4)#3-Nd(1)-N(1)#1	73.46(13)	O(2)-Nd(2)-O(3)#4	75.82(14)
O(3)#2-Nd(1)-N(1)#1	150.94(13)	O(3)#5-Nd(2)-O(3)#4	140.68(18)
O(3)#3-Nd(1)-N(1)#1	117.91(13)	O(3)-Nd(2)-O(3)#4	127.27(17)
O(1)-Nd(1)-N(1)	64.95(13)	O(2)#4-Nd(2)-O(3)#6	137.65(13)
O(1)#1-Nd(1)-N(1)	115.72(14)	O(2)#5-Nd(2)-O(3)#6	75.82(14)
O(4)#2-Nd(1)-N(1)	73.46(13)	O(2)#6-Nd(2)-O(3)#6	71.73(13)
O(4)#3-Nd(1)-N(1)	116.19(13)	O(2)-Nd(2)-O(3)#6	79.59(14)
O(3)#2-Nd(1)-N(1)	117.91(13)	O(3)#5-Nd(2)-O(3)#6	127.27(17)
O(3)#3-Nd(1)-N(1)	150.94(13)	O(3)-Nd(2)-O(3)#6	140.68(18)
N(1)#1-Nd(1)-N(1)	73.68(18)	O(3)#4-Nd(2)-O(3)#6	67.72(16)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/4,-y-1/4,z #2 x+1/4,-y,z+1/4 #3 -x+1/2,y-1/4,z+1/4 #4 x,-y+1/4,-z+1/4

#5 -x+1/4,-y+1/4,z #6 -x+1/4,y,-z+1/4 #7 x-1/4,-y,z-1/4 #8 -x+1/4,y,-z+5/4