

SUPPORTING INFORMATION

Formation of Infinite 2D Water Layer in Lanthanide Coordination Polymers with 6-Methyl-2,3,5-Pyridinetricarboxylate as a Novel Bridging Ligand

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S1. Selected bond lengths (Å) and angles (°) for {[Pr(mptc)(H₂O)₄].3H₂O}_n (1)

Pr(1)-O(4)#1	2.389(2)	Pr(1)-O(10)	2.450(2)	Pr(1)-O(9)	2.513(3)
Pr(1)-O(1)	2.389(3)	Pr(1)-O(8)	2.489(2)	Pr(1)-O(6)#2	2.516(3)
Pr(1)-O(5)#1	2.410(2)	Pr(1)-O(7)	2.506(2)		
O(4)#1-Pr(1)-O(1)	82.07(8)	O(4)#1-Pr(1)-O(7)	135.90(8)	O(7)-Pr(1)-O(9)	141.76(8)
O(4)#1-Pr(1)-O(5)#1	72.65(8)	O(1)-Pr(1)-O(7)	72.08(8)	O(4)#1-Pr(1)-O(6)#2	114.02(8)
O(1)-Pr(1)-O(5)#1	82.75(8)	O(5)#1-Pr(1)-O(7)	69.18(8)	O(1)-Pr(1)-O(6)#2	144.06(8)
O(4)#1-Pr(1)-O(10)	79.64(8)	O(10)-Pr(1)-O(7)	125.98(8)	O(5)#1-Pr(1)-O(6)#2	72.91(8)
O(1)-Pr(1)-O(10)	77.06(8)	O(8)-Pr(1)-O(7)	75.12(7)	O(10)-Pr(1)-O(6)#2	135.47(8)
O(5)#1-Pr(1)-O(10)	147.62(8)	O(4)#1-Pr(1)-O(9)	71.68(8)	O(8)-Pr(1)-O(6)#2	76.23(7)
O(4)#1-Pr(1)-O(8)	148.19(8)	O(1)-Pr(1)-O(9)	146.11(8)	O(7)-Pr(1)-O(6)#2	74.70(8)
O(1)-Pr(1)-O(8)	107.54(8)	O(5)#1-Pr(1)-O(9)	108.44(8)	O(9)-Pr(1)-O(6)#2	68.58(8)
O(5)#1-Pr(1)-O(8)	137.58(8)	O(10)-Pr(1)-O(9)	77.42(8)		
O(10)-Pr(1)-O(8)	73.45(8)	O(8)-Pr(1)-O(9)	85.97(8)		

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

S2. Selected bond lengths (Å) and angles (°) for {[Nd(mptc)(H₂O)₄].3H₂O}_n (2)

Nd(1)-O(4)#1	2.378(3)	Nd(1)-O(10)	2.442(3)	Nd(1)-O(9)	2.496(3)
Nd(1)-O(1)	2.384(4)	Nd(1)-O(8)	2.471(3)	Nd(1)-O(6)#2	2.504(3)
Nd(1)-O(5)#1	2.398(3)	Nd(1)-O(7)	2.486(3)		
O(4)#1-Nd(1)-O(1)	81.83(11)	O(4)#1-Nd(1)-O(7)	136.46(10)	O(7)-Nd(1)-O(9)	141.53(10)
O(4)#1-Nd(1)-O(5)#1	72.99(10)	O(1)-Nd(1)-O(7)	72.56(11)	O(4)#1-Nd(1)-O(6)#2	114.17(10)
O(1)-Nd(1)-O(5)#1	82.87(11)	O(5)#1-Nd(1)-O(7)	69.43(10)	O(1)-Nd(1)-O(6)#2	144.33(11)
O(4)#1-Nd(1)-O(10)	79.21(10)	O(10)-Nd(1)-O(7)	125.96(10)	O(5)#1-Nd(1)-O(6)#2	72.85(10)
O(1)-Nd(1)-O(10)	76.82(11)	O(8)-Nd(1)-O(7)	75.06(9)	O(10)-Nd(1)-O(6)#2	135.56(10)
O(5)#1-Nd(1)-O(10)	147.54(10)	O(4)#1-Nd(1)-O(9)	71.72(11)	O(8)-Nd(1)-O(6)#2	76.27(9)
O(4)#1-Nd(1)-O(8)	147.67(10)	O(1)-Nd(1)-O(9)	145.81(11)	O(7)-Nd(1)-O(6)#2	74.59(10)
O(1)-Nd(1)-O(8)	107.79(10)	O(5)#1-Nd(1)-O(9)	108.64(11)	O(9)-Nd(1)-O(6)#2	68.62(11)
O(5)#1-Nd(1)-O(8)	137.73(9)	O(10)-Nd(1)-O(9)	77.25(11)		
O(10)-Nd(1)-O(8)	73.44(10)	O(8)-Nd(1)-O(9)	85.54(10)		

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

S3. Selected bond lengths (Å) and angles (°) for {[Sm(mptc)(H₂O)₄].3H₂O}_n (3)

Sm(1)-O(4)#1	2.350(2)	Sm(1)-O(10)	2.411(2)	Sm(1)-O(9)	2.459(2)
Sm(1)-O(1)	2.353(2)	Sm(1)-O(8)	2.435(2)	Sm(1)-O(6)#2	2.475(2)
Sm(1)-O(5)#1	2.362(2)	Sm(1)-O(7)	2.457(2)		
O(4)#1-Sm(1)-O(1)	81.23(8)	O(4)#1-Sm(1)-O(7)	137.08(7)	O(7)-Sm(1)-O(9)	141.58(7)
O(4)#1-Sm(1)-O(5)#1	73.65(8)	O(1)-Sm(1)-O(7)	73.02(8)	O(4)#1-Sm(1)-O(6)#2	114.82(7)
O(1)-Sm(1)-O(5)#1	83.00(8)	O(5)#1-Sm(1)-O(7)	69.67(7)	O(1)-Sm(1)-O(6)#2	144.74(8)
O(4)#1-Sm(1)-O(10)	78.40(7)	O(10)-Sm(1)-O(7)	125.99(7)	O(5)#1-Sm(1)-O(6)#2	72.94(7)
O(1)-Sm(1)-O(10)	76.76(8)	O(8)-Sm(1)-O(7)	75.21(7)	O(10)-Sm(1)-O(6)#2	135.30(7)
O(5)#1-Sm(1)-O(10)	147.58(7)	O(4)#1-Sm(1)-O(9)	71.67(8)	O(8)-Sm(1)-O(6)#2	76.21(7)
O(4)#1-Sm(1)-O(8)	146.75(7)	O(1)-Sm(1)-O(9)	145.29(8)	O(7)-Sm(1)-O(6)#2	74.61(7)
O(1)-Sm(1)-O(8)	108.17(7)	O(5)#1-Sm(1)-O(9)	108.75(8)	O(9)-Sm(1)-O(6)#2	68.72(7)
O(5)#1-Sm(1)-O(8)	138.02(7)	O(10)-Sm(1)-O(9)	76.87(8)		
O(10)-Sm(1)-O(8)	73.22(7)	O(8)-Sm(1)-O(9)	85.16(8)		

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

S4. Selected bond lengths (Å) and angles (°) for {[Tb(mptc)(H₂O)₄].3H₂O}_n (4)

Tb(1)-O(1)	2.327(7)	Tb(1)-O(10)	2.361(7)	Tb(1)-O(7)	2.419(7)
Tb(1)-O(5)#1	2.328(7)	Tb(1)-O(8)	2.385(7)	Tb(1)-O(6)#2	2.469(7)
Tb(1)-O(4)#1	2.330(7)	Tb(1)-O(9)	2.415(8)		
O(1)-Tb(1)-O(5)#1	84.1(3)	O(1)-Tb(1)-O(9)	144.5(3)	O(9)-Tb(1)-O(7)	141.3(3)
O(1)-Tb(1)-O(4)#1	80.5(3)	O(5)#1-Tb(1)-O(9)	108.2(3)	O(1)-Tb(1)-O(6)#2	145.8(2)
O(5)#1-Tb(1)-O(4)#1	74.3(3)	O(4)#1-Tb(1)-O(9)	71.6(3)	O(5)#1-Tb(1)-O(6)#2	72.7(3)
O(1)-Tb(1)-O(10)	76.1(3)	O(10)-Tb(1)-O(9)	77.0(3)	O(4)#1-Tb(1)-O(6)#2	115.3(3)
O(5)#1-Tb(1)-O(10)	148.2(3)	O(8)-Tb(1)-O(9)	85.3(3)	O(10)-Tb(1)-O(6)#2	134.8(3)
O(4)#1-Tb(1)-O(10)	78.1(3)	O(1)-Tb(1)-O(7)	74.0(3)	O(8)-Tb(1)-O(6)#2	76.0(2)
O(1)-Tb(1)-O(8)	108.2(3)	O(5)#1-Tb(1)-O(7)	69.9(2)	O(9)-Tb(1)-O(6)#2	68.4(3)
O(5)#1-Tb(1)-O(8)	137.7(3)	O(4)#1-Tb(1)-O(7)	137.6(3)	O(7)-Tb(1)-O(6)#2	74.6(3)
O(4)#1-Tb(1)-O(8)	146.4(3)	O(10)-Tb(1)-O(7)	125.9(2)		
O(10)-Tb(1)-O(8)	73.0(2)	O(8)-Tb(1)-O(7)	75.0(2)		

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

S5: Hydrogen bonds (Å, °) in **1**.

D-H...A ^a	<i>d</i> (D-H)	<i>d</i> (H...A)	<i>d</i> (D...A)	∠(DHA)
O8-H8A...O13#1	0.851	2.011	2.743(16)	144
O9-H9A...O11#2	0.851	1.966	2.791(31)	163
O10-H10A...O10#1	0.851	2.528	3.192(13)	136
O10-H10A...O13#3	0.851	2.566	2.836(22)	100
O11-H11B...O12#4	0.853	2.010	2.836(1)	163
O12-H12A...O11#5	0.856	2.179	2.857(9)	136
O13-H13A...O9#2	0.855	2.266	3.063(1)	155
O13-H13B...O12	0.857	2.007	2.859(32)	172

^a D = donor; A = acceptor.

Symmetry code: #1 -x+1, -y+2, -z+1; #2 -x+1, -y+1, -z+1; #3 x, y, z; #4 x, y-1, z; #5 -x+3/2, y+1/2, -z+1/2.

S6: Hydrogen bonds (Å, °) in **2**.

D-H...A ^a	<i>d</i> (D-H)	<i>d</i> (H...A)	<i>d</i> (D...A)	∠(DHA)
O8-H8A...O13#1	0.850	2.008	2.736(16)	143
O9-H9A...O11#2	0.850	1.956	2.779(31)	163
O10-H10A...O10#1	0.850	2.525	3.194(14)	136
O10-H10A...O13#3	0.850	2.556	2.831(22)	100
O11-H11B...O12#4	0.850	2.002	2.827(1)	163
O12-H12A...O11#5	0.855	2.187	2.862(9)	136
O13-H13A...O9#2	0.853	2.290	3.082(1)	154
O13-H13B...O12	0.856	2.027	2.879(32)	173

^a D = donor; A = acceptor.

Symmetry code: #1 -x+1, -y+2, -z+1; #2 -x+1, -y+1, -z+1; #3 x, y, z; #4 x, y-1, z; #5 -x+3/2, y+1/2, -z+1/2.

S7: Hydrogen bonds (Å, °) in **3**.

D-H...A ^a	<i>d</i> (D-H)	<i>d</i> (H...A)	<i>d</i> (D...A)	∠(DHA)
O8-H8A...O13#1	0.847	2.016	2.736(1)	142
O9-H9A...O11#2	0.846	1.952	2.772(2)	163
O10-H10A...O10#1	0.848	2.527	3.204(1)	138
O10-H10A...O13#3	0.848	2.544	2.828(2)	101
O11-H11B...O12#4	0.847	2.003	2.824(1)	163
O12-H12A...O11#5	0.852	2.196	2.866(1)	135
O13-H13A...O9#2	0.849	2.327	3.112(1)	154
O13-H13B...O12	0.852	2.028	2.877(2)	174

^a D = donor; A = acceptor.

Symmetry code: #1 -x+1, -y+2, -z+1; #2 -x+1, -y+1, -z+1; #3 x, y, z; #4 x, y-1, z; #5 -x+3/2, y+1/2, -z+1/2.

S8: Hydrogen bonds (Å, °) in **4**.

D-H...A ^a	<i>d</i> (D-H)	<i>d</i> (H...A)	<i>d</i> (D...A)	∠(DHA)
O8-H8A...O13#1	0.843	2.019	2.730(18)	142
O9-H9A...O11#2	0.845	1.950	2.767(32)	162
O10-H10A...O10#1	0.843	2.545	3.228(18)	139
O10-H10A...O13#3	0.843	2.570	2.865(24)	102
O11-H11B...O12#4	0.843	2.004	2.821(1)	163
O12-H12A...O11#5	0.848	2.214	2.870(11)	134
O13-H13A...O9#2	0.846	2.353	3.132(2)	153
O13-H13B...O12	0.851	2.016	2.865(32)	175

^a D = donor; A = acceptor.

Symmetry code: #1 -x+1, -y+2, -z+1; #2 -x+1, -y+1, -z+1; #3 x, y, z;; #4 x, y-1, z; #5 -x+3/2, y+1/2, -z+1/2.