Supplemental Material for:

Synthesis and structural characterization of 3d-4f heterometallic coordination polymers: from cluster to chain

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Table S1. Selected bond lengths [Å] and bond angles [°] for compound **1**

Ce(1)-O(13)#1	2.299(10)	Ce(1)-O(13)	2.299(10)
Ce(1)-O(2)	2.326(9)	Ce(1)-O(2)#1	2.326(9)
Ce(1)-O(1W)#1	2.445(14)	Ce(1)-O(1W)	2.445(14)
Ce(1)-O(5)	2.435(15)	Ce(1)-O(1)	2.471(15)
Ce(2)-O(13)	2.301(9)	Ce(2)-O(10)	2.318(7)
Ce(2)-O(4)	2.331(8)	Ce(2)-O(2)	2.333(10)
Ce(2)-O(2W)	2.390(10)	Ce(2)-O(9)	2.447(10)
Ce(2)-O(11)	2.438(10)	Ce(2)-O(7)	2.454(10)
Ce(2)-O(15)	2.542(10)		
Mn(1)-O(4)	1.818(12)	Mn(1)-O(13)#1	1.835(9)
Mn(1)-O(13)	1.835(9)	Mn(1)-O(12)	1.968(13)
Mn(1)-O(3)#2	1.985(9)	Mn(1)-O(3)#3	1.985(9)
Mn(2)-O(2)#1	1.812(9)	Mn(2)-O(2)	1.812(9)
Mn(2)-O(10)	1.830(13)	Mn(2)-O(8)	1.971(9)
Mn(2)-O(8)#1	1.971(9)	Mn(2)-O(14)	2.023(14)
O(13)#1-Ce(1)-O(13)	66.7(4)	O(13)#1-Ce(1)-O(2)	103.1(3)
O(13)-Ce(1)-O(2)	67.9(3)	O(13)#1-Ce(1)-O(2)#1	67.9(3)
O(13)-Ce(1)-O(2)#1	103.1(3)	O(2)-Ce(1)-O(2)#1	66.5(5)
O(13)#1-Ce(1)-O(1W)#1	81.4(4)	O(13)-Ce(1)-O(1W)#1	142.0(4)
O(2)-Ce(1)-O(1W)#1	142.9(4)	O(2)#1-Ce(1)-O(1W)#1	82.1(5)
O(13)#1-Ce(1)-O(1W)	142.0(4)	O(13)-Ce(1)-O(1W)	81.4(4)
O(2)-Ce(1)-O(1W)	82.1(5)	O(2)#1-Ce(1)-O(1W)	142.9(4)
O(1W)#1-Ce(1)-O(1W)	117.0(9)	O(13)#1-Ce(1)-O(5)	76.2(3)
O(13)-Ce(1)-O(5)	76.2(3)	O(2)-Ce(1)-O(5)	140.4(3)
O(2)#1-Ce(1)-O(5)	140.4(3)	O(1W)#1-Ce(1)-O(5)	76.6(4)
O(1W)-Ce(1)-O(5)	76.6(4)	O(13)#1-Ce(1)-O(1)	140.0(3)
O(13)-Ce(1)-O(1)	140.0(3)	O(2)-Ce(1)-O(1)	75.6(4)
O(2)#1-Ce(1)-O(1)	75.6(4)	O(1W)#1-Ce(1)-O(1)	78.0(4)
O(1W)-Ce(1)-O(1)	78.0(4)	O(5)-Ce(1)-O(1)	130.1(5)
O(13)-Ce(2)-O(10)	103.3(3)	O(13)-Ce(2)-O(4)	66.8(4)
O(10)-Ce(2)-O(4)	69.4(4)	O(13)-Ce(2)-O(2)	67.7(3)
O(10)-Ce(2)-O(2)	66.7(4)	O(4)-Ce(2)-O(2)	104.5(4)
O(13)-Ce(2)-O(2W)	81.0(3)	O(10)-Ce(2)-O(2W)	140.4(4)
O(4)-Ce(2)-O(2W)	142.3(4)	O(2)-Ce(2)-O(2W)	79.4(4)
O(13)-Ce(2)-O(9)	75.7(3)	O(10)-Ce(2)-O(9)	140.8(4)
O(4)-Ce(2)-O(9)	74.7(4)	O(2)-Ce(2)-O(9)	139.7(3)
O(2W)-Ce(2)-O(9)	78.8(4)	O(13)-Ce(2)-O(11)	139.9(3)
O(10)-Ce(2)-O(11)	75.0(3)	O(4)-Ce(2)-O(11)	140.6(4)
O(2)-Ce(2)-O(11)	75.5(3)	O(9)-Ce(2)-O(11)	130.8(3)

O(2W)-Ce(2)-O(11)	77.1(4)	O(13)-Ce(2)-O(7)	141.3(3)
O(10)-Ce(2)-O(7)	75.0(4)	O(4)-Ce(2)-O(7)	77.0(4)
O(2)-Ce(2)-O(7)	137.7(3)	O(2W)-Ce(2)-O(7)	125.3(3)
O(9)-Ce(2)-O(7)	82.2(4)	O(11)-Ce(2)-O(7)	78.0(4)
O(13)-Ce(2)-O(15)	135.8(3)	O(10)-Ce(2)-O(15)	119.2(4)
O(4)-Ce(2)-O(15)	115.8(4)	O(2)-Ce(2)-O(15)	138.8(3)
O(2W)-Ce(2)-O(15)	74.1(4)	O(9)-Ce(2)-O(15)	64.1(3)
O(11)-Ce(2)-O(15)	68.3(3)	O(7)-Ce(2)-O(15)	51.5(3)
O(4)-Mn(1)-O(13)#1	88.6(4)	O(4)-Mn(1)-O(13)	88.6(4)
O(13)#1-Mn(1)-O(13)	87.1(6)	O(4)-Mn(1)-O(12)	174.1(6)
O(13)#1-Mn(1)-O(12)	95.7(4)	O(13)-Mn(1)-O(12)	95.7(4)
O(4)-Mn(1)-O(3)#2	94.0(4)	O(13)#1-Mn(1)-O(3)#2	94.8(4)
O(13)-Mn(1)-O(3)#2	176.9(4)	O(12)-Mn(1)-O(3)#2	81.6(4)
O(4)-Mn(1)-O(3)#3	94.0(4)	O(13)#1-Mn(1)-O(3)#3	176.9(4)
O(13)-Mn(1)-O(3)#3	94.8(4)	O(12)-Mn(1)-O(3)#3	81.6(4)
O(3)#2-Mn(1)-O(3)#3	83.3(6)	O(2)#1-Mn(2)-O(2)	89.5(6)
O(2)#1-Mn(2)-O(10)	89.2(4)	O(2)-Mn(2)-O(10)	89.2(4)
O(2)#1-Mn(2)-O(8)	174.9(4)	O(2)-Mn(2)-O(8)	94.4(4)
O(10)-Mn(2)-O(8)	94.0(4)	O(2)#1-Mn(2)-O(8)#1	94.4(4)
O(2)-Mn(2)-O(8)#1	174.9(4)	O(10)-Mn(2)-O(8)#1	94.0(4)
O(8)-Mn(2)-O(8)#1	81.6(6)	O(2)#1-Mn(2)-O(14)	93.9(4)
O(2)-Mn(2)-O(14)	93.9(4)	O(10)-Mn(2)-O(14)	175.5(6)
O(8)-Mn(2)-O(14)	82.6(4)	O(8)#1-Mn(2)-O(14)	82.6(4)

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

Table S2. Selected bond lengths [Å] and bond angles [°] for compound **2**

Nd(1)-O(8)	2.377(3)	Nd(1)-O(6)	2.411(3)
Nd(1)-O(5)	2.439(3)	Nd(1)-O(2W)	2.487(4)
Nd(1)-O(7)	2.490(3)	Nd(1)-O(3)	2.508(3)
Nd(1)-O(3W)	2.511(3)	Nd(1)-O(4)	2.590(3)
Nd(1)-O(6)#1	2.713(3)		
Mn(1)-O(1)#2	2.172(3)	Mn(1)-O(1)	2.172(3)
Mn(1)-O(7)	2.177(3)	Mn(1)-O(7)#2	2.177(3)
Mn(1)-O(2)	2.194(3)	Mn(1)-O(2)#2	2.194(3)
O(8)-Nd(1)-O(6)	83.93(12)	O(8)-Nd(1)-O(5)	76.33(12)
O(6)-Nd(1)-O(5)	82.99(11)	O(8)-Nd(1)-O(2W)	68.70(13)
O(6)-Nd(1)-O(2W)	87.67(14)	O(5)-Nd(1)-O(2W)	144.55(12)
O(8)-Nd(1)-O(7)	75.25(11)	O(6)-Nd(1)-O(7)	157.01(11)
O(5)-Nd(1)-O(7)	82.71(10)	O(2W)-Nd(1)-O(7)	93.65(14)
O(8)-Nd(1)-O(3)	142.63(11)	O(6)-Nd(1)-O(3)	114.35(11)
O(5)-Nd(1)-O(3)	74.20(12)	O(2W)-Nd(1)-O(3)	139.81(13)
O(7)-Nd(1)-O(3)	78.67(11)	O(8)-Nd(1)-O(3W)	137.30(11)
O(6)-Nd(1)-O(3W)	77.88(11)	O(5)-Nd(1)-O(3W)	137.60(11)
O(2W)-Nd(1)-O(3W)	72.23(13)	O(7)-Nd(1)-O(3W)	124.33(11)
O(3)-Nd(1)-O(3W)	79.85(12)	O(8)-Nd(1)-O(4)	111.70(12)
O(6)-Nd(1)-O(4)	150.20(11)	O(5)-Nd(1)-O(4)	124.47(11)
O(2W)-Nd(1)-O(4)	75.73(13)	O(7)-Nd(1)-O(4)	50.80(9)
O(3)-Nd(1)-O(4)	68.91(12)	O(3W)-Nd(1)-O(4)	73.58(10)
O(8)-Nd(1)-O(6)#1	136.24(12)	O(6)-Nd(1)-O(6)#1	65.37(11)
O(5)-Nd(1)-O(6)#1	69.89(11)	O(2W)-Nd(1)-O(6)#1	135.26(13)
O(7)-Nd(1)-O(6)#1	125.22(10)	O(3)-Nd(1)-O(6)#1	49.02(10)
O(3W)-Nd(1)-O(6)#1	67.76(11)	O(4)-Nd(1)-O(6)#1	110.14(10)
O(1)#2-Mn(1)-O(1)	180.0	O(1)#2-Mn(1)-O(7)	89.13(12)
O(1)-Mn(1)-O(7)	90.87(12)	O(1)#2-Mn(1)-O(7)#2	90.87(12)
O(1)-Mn(1)-O(7)#2	89.13(12)	O(7)-Mn(1)-O(7)#2	180.0
O(1)#2-Mn(1)-O(2)	83.05(13)	O(1)-Mn(1)-O(2)	96.95(13)
O(7)-Mn(1)-O(2)	91.90(12)	O(7)#2-Mn(1)-O(2)	88.10(12)
O(1)#2-Mn(1)-O(2)#2	96.95(13)	O(1)-Mn(1)-O(2)#2	83.05(13)
O(7)-Mn(1)-O(2)#2	88.10(12)	O(7)#2-Mn(1)-O(2)#2	91.90(12)
O(2)-Mn(1)-O(2)#2	180.0		

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

Table S3. Bond-valence Sums for the Mn and Ce Atoms of compound **1**

atom	Mn^{II}	Mn^{III}	Mn^{IV}	atom	Ce^{III}	Ce^{IV}
Mn1	4.50	4.15	4.04	Ce1	4.03	3.75
Mn2	4.54	4.19	4.08	Ce2	4.38	4.07

Table S4. Bond-valence Sums for the Mn and Nd Atoms of compound **2**

atom	Mn^{II}	Mn^{III}	Mn^{IV}	atom	Nd^{III}
Mn1	2.09	1.92	1.87	Nd1	3.27

Fig. S1 The distances between metals in the $[Ce_3Mn_2O_6]^{8+}$ core.

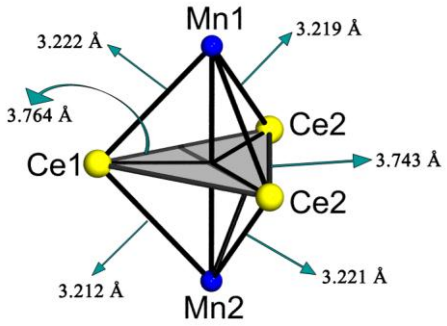

Fig. S2 The IR curves of compounds **1** and **2**.

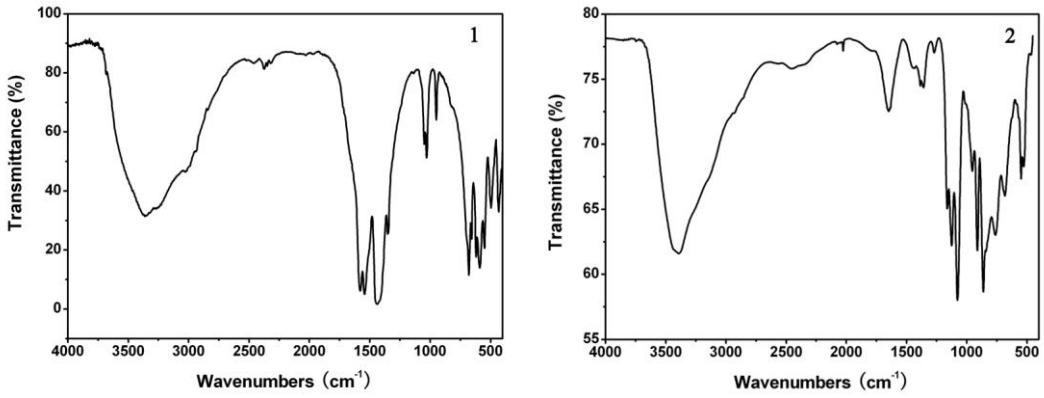

Fig. S3 The simulative (black) and experimental (red) PXRD patterns of compounds **1** and **2**.

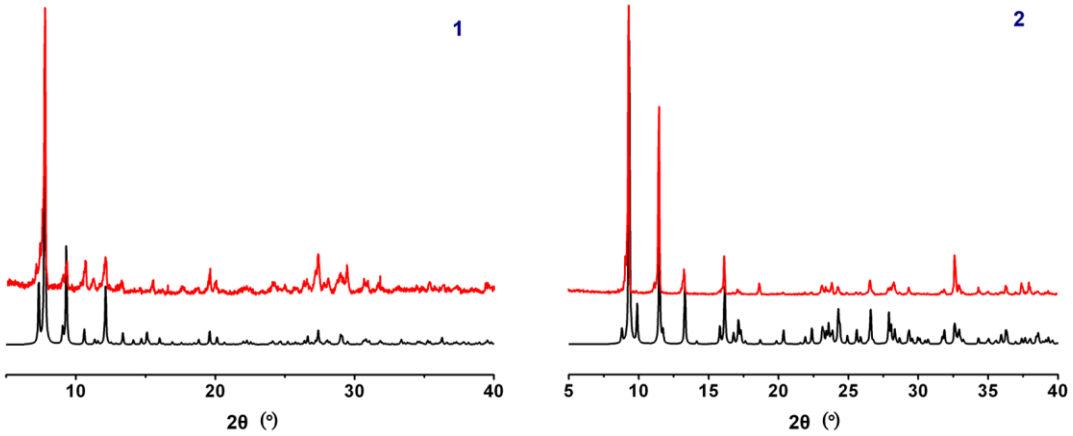

Fig. S4 TGA-DTA curves of compounds **1** and **2**.

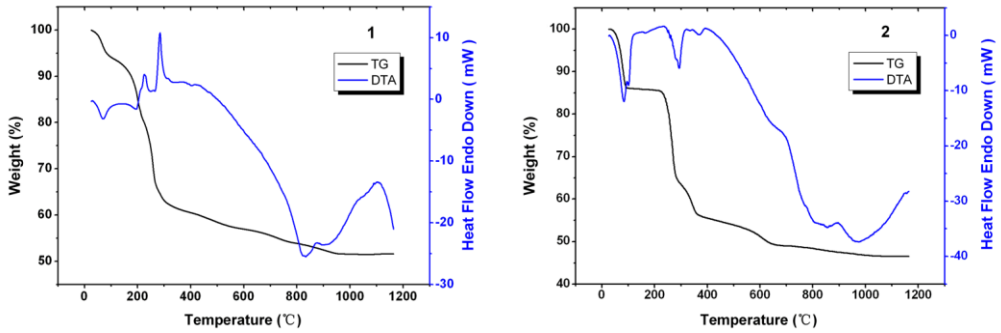

Fig. S5 The χ_m^{-1} versus T plots of compounds **1** and **2**.