Supplementary Material (ESI) for CrystEngComm.

Syntheses of two coordination polymers with rutile-type topology and the single-crystal-to-single-crystal transformation of Mg(II) complex induced by methanol

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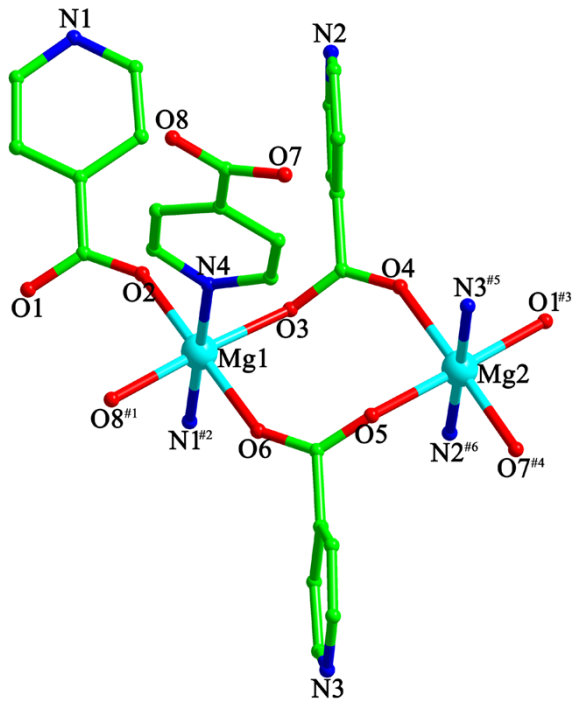


Fig. S1 ORTEP view of **1** showing the local coordination environments of Mg(II) ions.

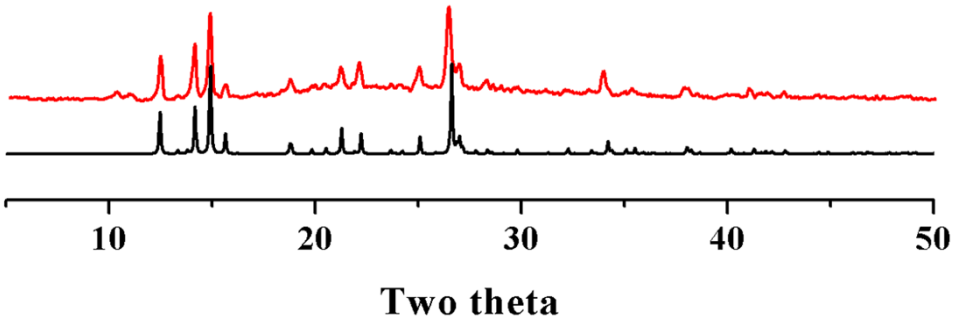
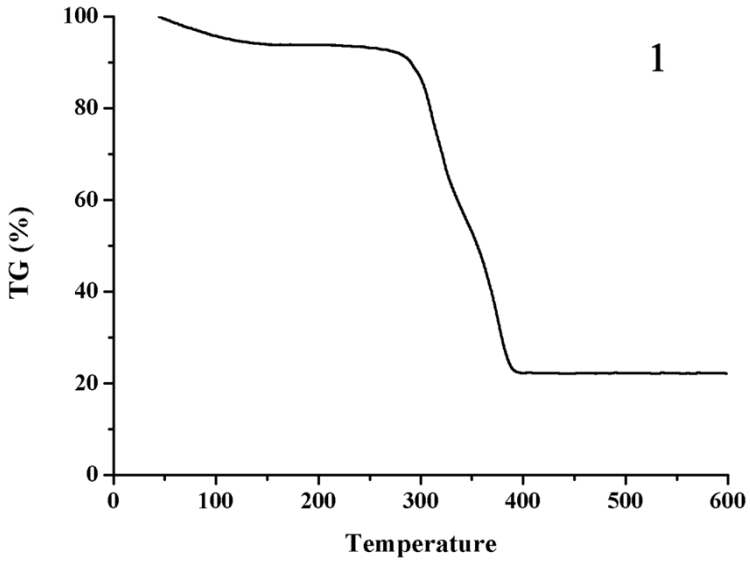
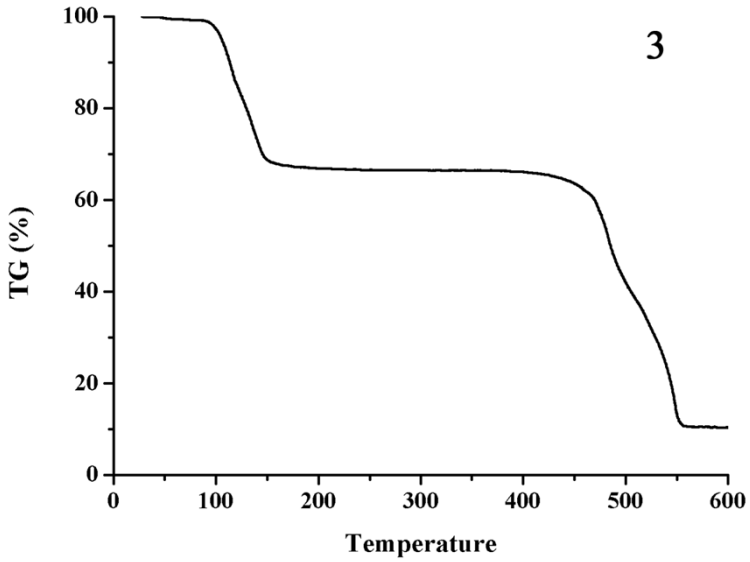


Fig. S2 PXRD patterns of **3** (black) and as-synthesized **3** (red).



(a)



(b)

Fig. S3 The TGA curves of compounds **1** and **3**.

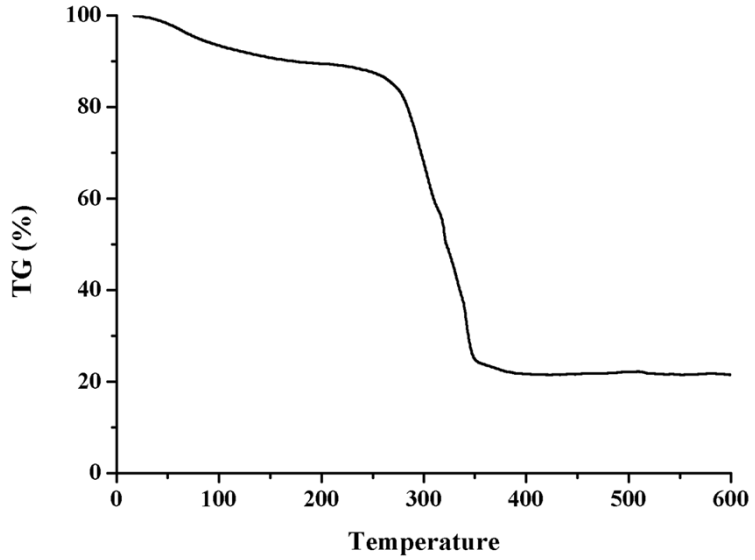


Fig. S4 The TGA curve of compound **1** after soaking in methanol.

Table S1. Selected bond distances (Å) and angles (°) for compound **1**.

Mn(1)-O(3)	2.115(5)	Mn(1)-O(8)#1	2.170(4)
Mn(1)-O(5)	2.170(5)	Mn(1)-O(2)	2.184(4)
Mn(1)-N(4)#2	2.249(6)	Mn(1)-N(2)#3	2.268(6)
Mn(2)-O(7)	2.139(5)	Mn(2)-O(1)	2.142(5)
Mn(2)-O(6)	2.156(4)	Mn(2)-N(3)#2	2.251(6)
Mn(2)-N(1)#5	2.296(6)	O(3)-Mn(1)-O(8)#1	94.38(18)
O(3)-Mn(1)-O(5)	176.9(3)	O(8)#1-Mn(1)-O(5)	86.96(19)
O(3)-Mn(1)-O(2)	88.41(18)	O(8)#1-Mn(1)-O(2)	176.7(3)
O(5)-Mn(1)-N(4)#2	94.5(2)	O(5)-Mn(1)-N(2)#3	85.1(2)
O(4)#4-Mn(2)-O(7)	95.07(17)	O(4)#4-Mn(2)-O(1)	86.82(18)
O(7)-Mn(2)-O(1)	178.1(2)	O(7)-Mn(2)-O(6)	86.19(19)
O(4)#4-Mn(2)-N(3)#2	93.01(19)	O(1)-Mn(2)-N(3)#2	87.4(2)
O(6)-Mn(2)-N(3)#2	86.3(2)	O(7)-Mn(2)-N(1)#5	87.1(2)

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

Table S2. Selected bond distances (Å) and angles (°) for compound **2**.

Mg(1)-O(2)	2.044(4)	Mg(1)-O(6)	2.052(5)
Mg(1)-O(8)#1	2.070(4)	Mg(1)-O(3)	2.078(5)
Mg(1)-N(4)	2.196(6)	Mg(1)-N(1)#2	2.217(6)
Mg(2)-O(1)#3	2.021(5)	Mg(2)-O(7)#4	2.031(4)
Mg(2)-O(5)	2.050(5)	Mg(2)-O(4)	2.075(5)
Mg(2)-N(3)#5	2.202(6)	Mg(2)-N(2)#6	2.239(6)
O(2)-Mg(1)-O(6)	178.3(3)	O(2)-Mg(1)-O(8)#1	94.14(17)
O(6)-Mg(1)-O(8)#1	86.64(18)	O(2)-Mg(1)-O(3)	88.55(18)
O(3)-Mg(1)-N(4)	93.0(2)	O(6)-Mg(1)-N(1)#2	87.4(2)

O(1)#3-Mg(2)-O(7)#4	94.79(18)	O(7)#4-Mg(2)-O(5)	86.68(18)
O(1)#3-Mg(2)-O(4)	86.93(18)	O(1)#3-Mg(2)-N(3)#5	93.2(2)
O(5)-Mg(2)-N(3)#5	87.6(2)		

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

Table S3a. Selected bond distances (Å) and angles (°) for compound **3**

Mg(1)-O(1)	2.0148(19)	Mg(1)-O(4)	2.058(2)
Mg(1)-O(3)	2.086(2)	O(1) -Mg(1)-O(4)	91.76(9)
O(1) -Mg(1)-O(3)	88.33(9)	O(4)-Mg(1)-O(3)	90.65(11)

Table S3b. Hydrogen bond for **3**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(3)-H(3A) ···N(1)#1	0.90	1.83	2.722(3)	170

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