Electronic Supplementary Information (ESI)

Dimensionality of luminescent coordination polymers of magnesium ions and 1, 1'–ethynebenzene–3, 3', 5, 5'–tetracarboxylic acid modulated by structural inducing agents

Zhu−Xi Yang,[a] Yin Qian,[a] Jing−Wei Yu,[a] Lu Zhai,*[a] Wen−Wei Zhang,[b] Xiao−Ming Ren*[a,b,c]

[a]*State Key Laboratory of Materials−Oriented Chemical Engineering and College of Chemistry & Molecular Engineering, Nanjing Tech University, Nanjing 210009, P. R. China*

[b]*State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023 P. R. China*

[c]*College of Materials Science& Engineering, Nanjing Tech University, Nanjing 210009, P. R. China*

Email: zhailu@njtech.edu.cn (LZ); xmren@njtech.edu.cn (XMR)

Contents

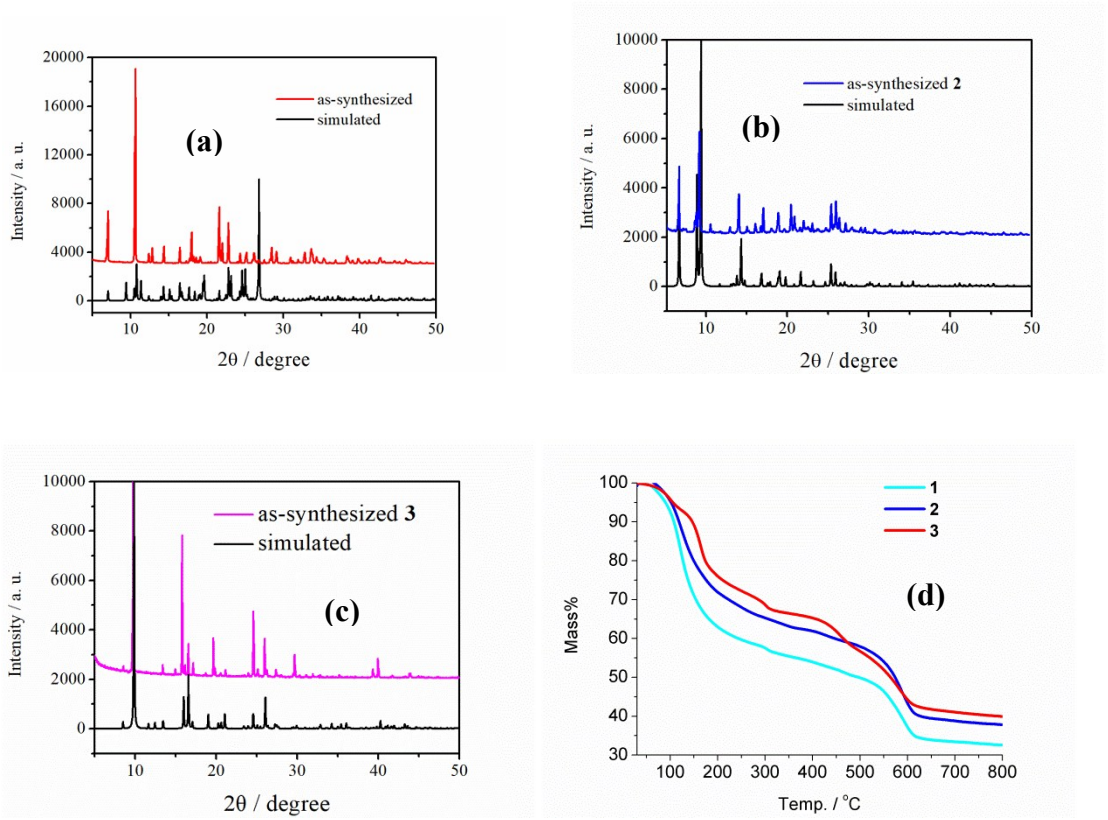
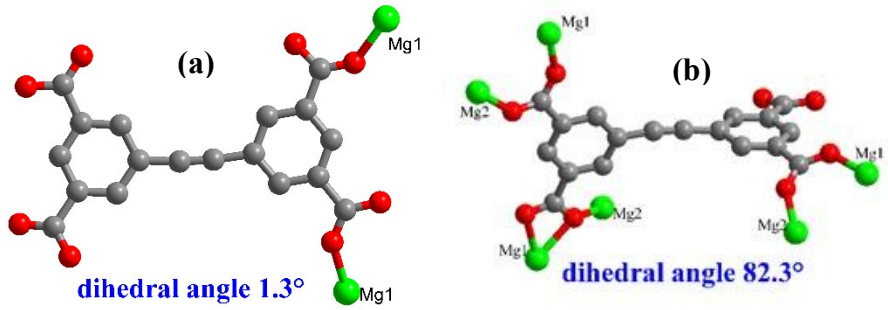


Fig. S1 PXRD patterns of (a) **1** (b) **2** (c) **3** as−synthesized samples and simulated one based on the single−crystal structures and (d) TG plots of **1**−**3**, indicating that three CPs start to release the coordination solvents or lattice solvents at room temperature.



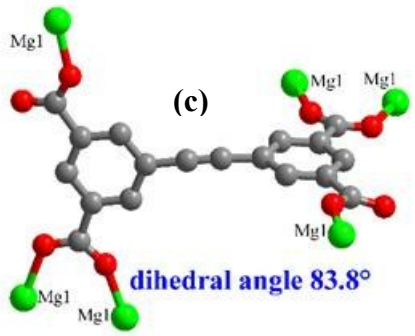


Fig. S2 Dihedral angle between two phenyl rings in (a) **1** (b) **2** (c) **3.**

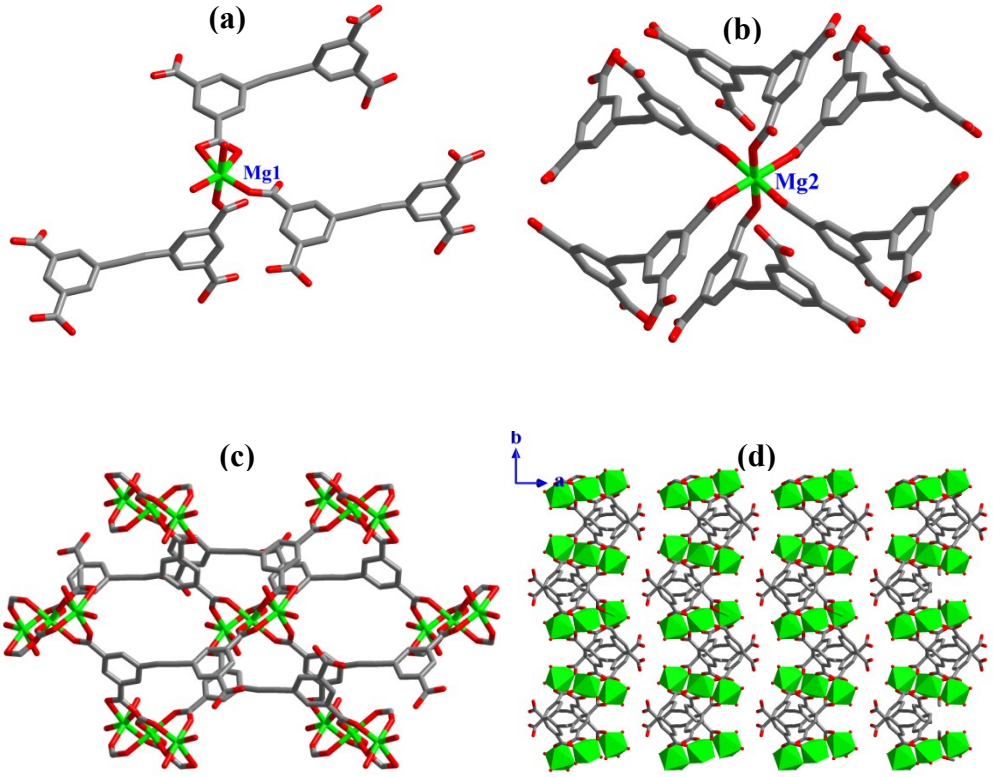


Fig. S3 The coordination environment of (a) Mg1 and (b) Mg2 (c) trinuclear cluster as node being connected to six $HEBTC^{3-}$ ligands (d) packing diagram viewed along c-axis, which shows the stack of two-dimensional coordination layers, in **2** (all H atoms were omitted for clarity).

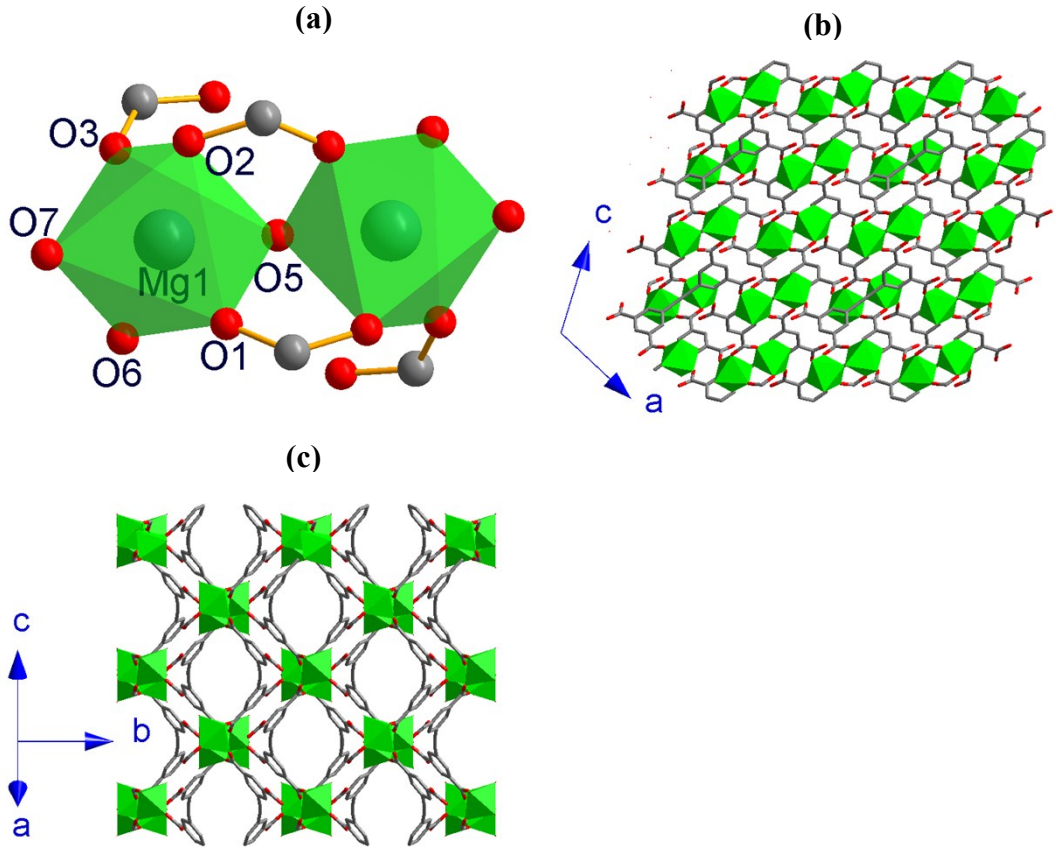


Fig. S4 (a) Mg^{2+}-binuclear unit and packing diagrams viewed along (b) b-axis (c) [101] direction in **3.**

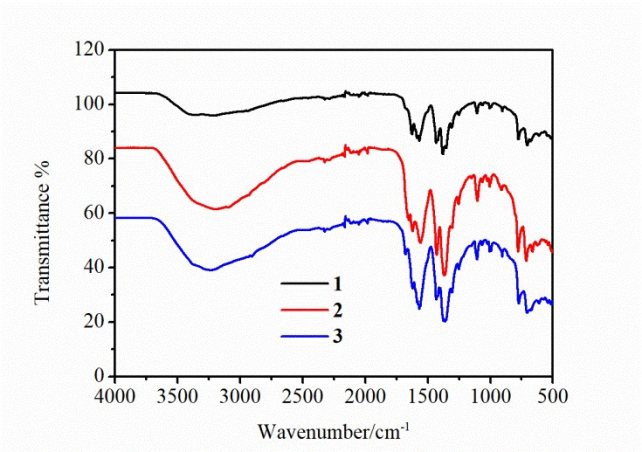


Fig. S5 IR spectra of **1**–**3** recorded using KBr pellet.

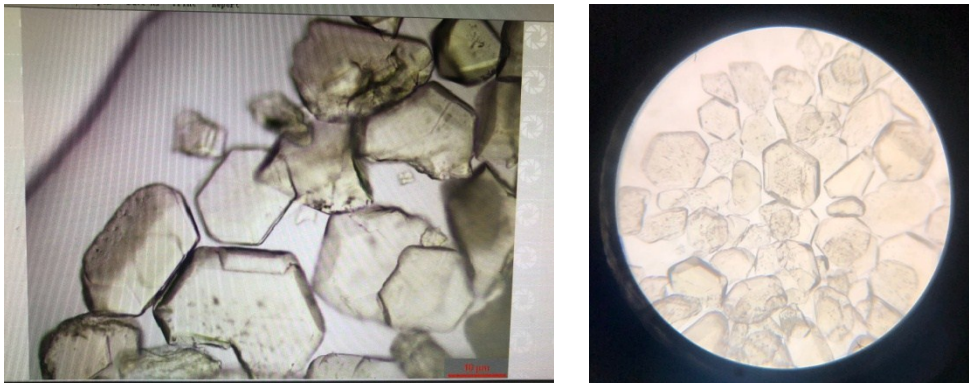


Fig. S6 Photographs of single crystals of **1**.

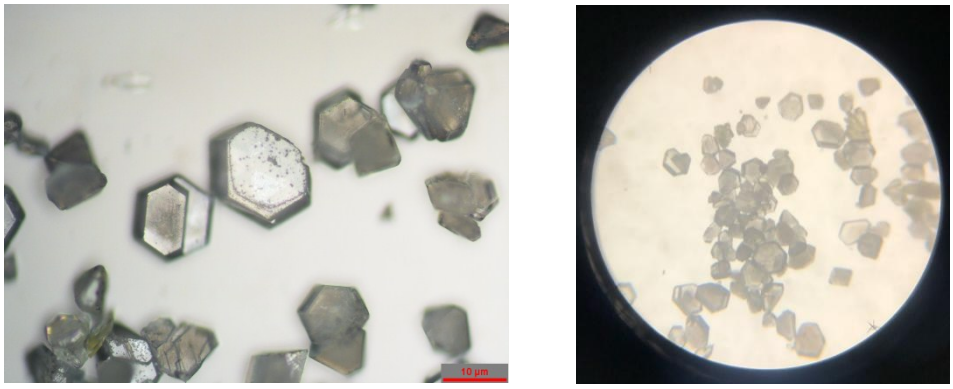


Fig. S7 Photographs of single crystals of **2**.

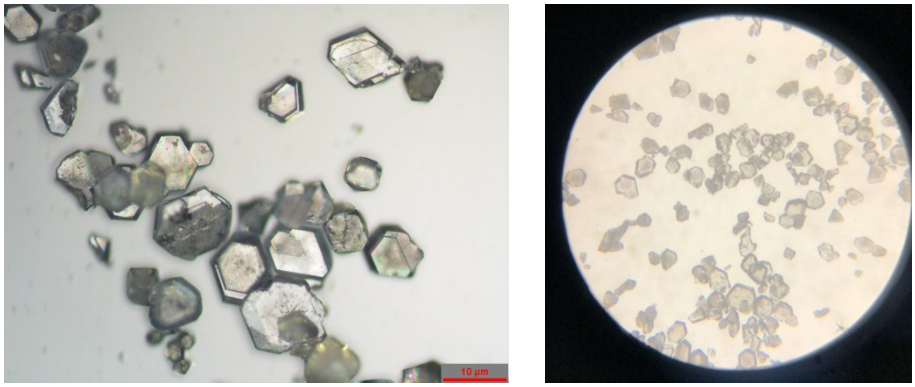
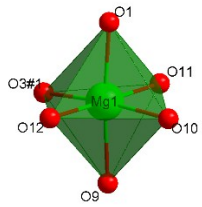


Fig. S8 Photographs of single crystals of **3**.

Table S1: Selected bond distances (Å) and angles (°) in **1–3**

CP 1



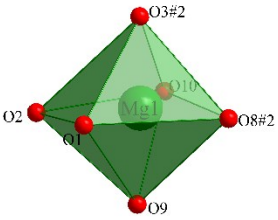
Bond lengths

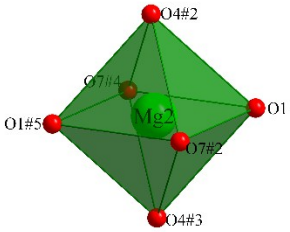
Mg1–O1	2.006(3)	Mg1–O3#1	2.070(3)	Mg1–O9	2.081(4)
Mg1–O10	2.092(3)	Mg1–O11	2.064(4)	Mg1–O12	2.055(4)

Bond angles

O12–Mg1–O11	179.21(17)	O12–Mg–O1	89.48(14)	O11– Mg1–O1	89.74(14)
O12–Mg1–O3#1	91.47(14)	O11–Mg1–O3#1	88.47(14)	O1–Mg1–O3#1	99.16(14)
O12–Mg1– O9	90.34(14)	O11–Mg1–O9	90.45(15)	O1–Mg1–O9	172.88(15)
O3#1–Mg1–O9	87.97(15)	O12– Mg1–O10	90.45(14)	O11– Mg1–O10	89.69(14)
O1–Mg1–O10	87.16(14)	O3#1– Mg1–O10	173.40(15)	O9– Mg1–O10	85.72(15)

CP 2





Bond lengths

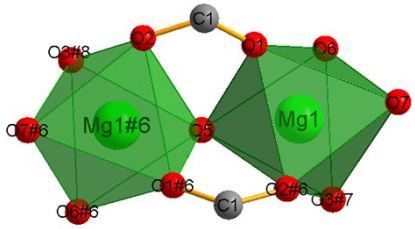
Mg1–O1	2.153(3)	Mg1–O2	2.211(3)	Mg1–O3#2	1.965(3)

Mg1–O8#2	2.013(3)	Mg1–O9	2.068(4)	Mg1–O10	2.028(3)
Mg2–O1	2.144(2)	Mg2–O1#5	2.144(2)	Mg2–O4#2	2.139(2)
Mg2–O4#3	2.139(2)	Mg2–O7#2	2.028(3)	Mg2–O7#4	2.028(3)

Bond angles

O3#2–Mg1–O8#2	92.63(15)	O3#2–Mg1–O10	90.92(13)	O8#2–Mg1–O10	96.65(14)
O3#2–Mg1–O9	177.45(16)	O8#2–Mg1–O9	89.47(17)	O10–Mg1–O9	87.41(13)
O3#2–Mg1–O1	90.47(12)	O8#2–Mg1–O1	102.05(12)	O10–Mg1–O1	161.17(13)
O9–Mg1–O1	90.47(12)	O3#2–Mg1–O2	102.05(12)	O8#2–Mg1–O2	161.17(13)
O10–Mg1–O2	101.14(12)	O9–Mg1–O2	85.46(16)	O1–Mg1–O2	60.03(10)
O7#4–Mg2–O7#2	180.00(19)	O7#4–Mg2–O4#3	92.93(10)	O7#2–Mg2–O4#3	87.07(10)
O7#4–Mg2–O4#2	87.07(10)	O7#2–Mg2–O4#2	92.93(10)	O4#3–Mg2–O4#2	180.00(18)
O7#4–Mg2–O1#5	87.28(10)	O7#2–Mg2–O1#5	92.72(10)	O4#3–Mg2–O1#5	89.95(9)
O4#2–Mg2–O1#5	90.05(9)	O7#4–Mg2–O1	92.72(10)	O7#2–Mg2–O1	87.28(10)
O4#3–Mg2–O1	90.05(9)	O4#2–Mg2–O1	89.95(9)	O1#5–Mg2–O1	180.0(3)

CP 3



Bond lengths

Mg1–O1	1.9824(19)	Mg1–O2#6	2.1060(19)	Mg1–O3#7	2.0217(19)
Mg1–O5	2.1751(15)	Mg1–O6	2.094(2)	Mg1–O7	2.0819(19)

Mg#6–O1#6	1.9824(19)	Mg#6–O2	2.1060(19)	Mg#6–O3#8	2.0217(19)
Mg#6–O5	2.1751(15)	Mg#6–O6#6	2.094(2)	Mg#6–O7#6	2.0819(19)

Bond angles

O1–Mg1–O3#7	172.750(99)	O1–Mg1–O7	95.928(88)	O3#7–Mg1–O7	91.053(87)
O1–Mg1–O6	90.464(104)	O3#7–Mg1–O6	92.018(105)	O7–Mg1–O6	85.651(88)
O1–Mg1–O2#6	91.207(90)	O3#7–Mg1–O2#6	87.261(87)	O7–Mg1–O2#6	86.481(79)
O6–Mg1–O2#6	172.084(100)	O1–Mg1–O5	86.883(64)	O3#7–Mg1–O5	86.501(65)
O7–Mg1–O5	171.129(66)	O6–Mg1–O5	85.915(73)	O2#6–Mg1–O5	101.901(64)
O1#6–Mg1#6–O3#8	172.750(99)	O1#6–Mg1#6–O7#6	95.928(88)	O3#8–Mg1#6–O7#6	91.053(87)
O1#6–Mg1#6–O6#6	90.464(104)	O3#8–Mg1#6–O6#6	92.018(105)	O7#6–Mg1#6–O6#6	85.651(88)
O1#6–Mg1#6–O2	91.207(90)	O3#8–Mg1#6–O2	87.261(87)	O7#6–Mg1#6–O2	86.481(79)
O6#6–Mg1#6–O2	172.084(100)	O1#6–Mg1#6–O5	86.883(64)	O3#8–Mg1#6–O5	86.501(65)
O7#6–Mg1#6–O5	171.129(66)	O6#6–Mg1#6–O5	85.915(73)	O2–Mg1#6–O5	101.901(64)

Symmetry transformations used to generate equivalent atoms for 1/2/3: #1=0.5-x, -0.5+y, 0.5-z; #2=-x, -0.5+y, 0.5-z; #3=x, -0.5-y, -0.5+z; #4=x, 0.5-y, 0.5+z; #5=-x, -y, -z; #6=1-x, y, 1.5-z; #7=-0.5+x, 0.5+y, z; #8=1.5-x, 0.5+y, 1.5-z.