Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Materials

Structural Transformations in Cobalt(II) Coordination Polymers Constructed from Flexible *N,N'*-Bis(3-pyridylmethyl)sebacoamide and benzene-1,3,5-tricarboxylic acid

Ji-Hong Hu, Yuan-Chin Liu, Yu-Hsiang Liu and Jhy-Der Chen*

Fig. S1. (a) Simulated and (b) experimental PXRD patterns of **1**.

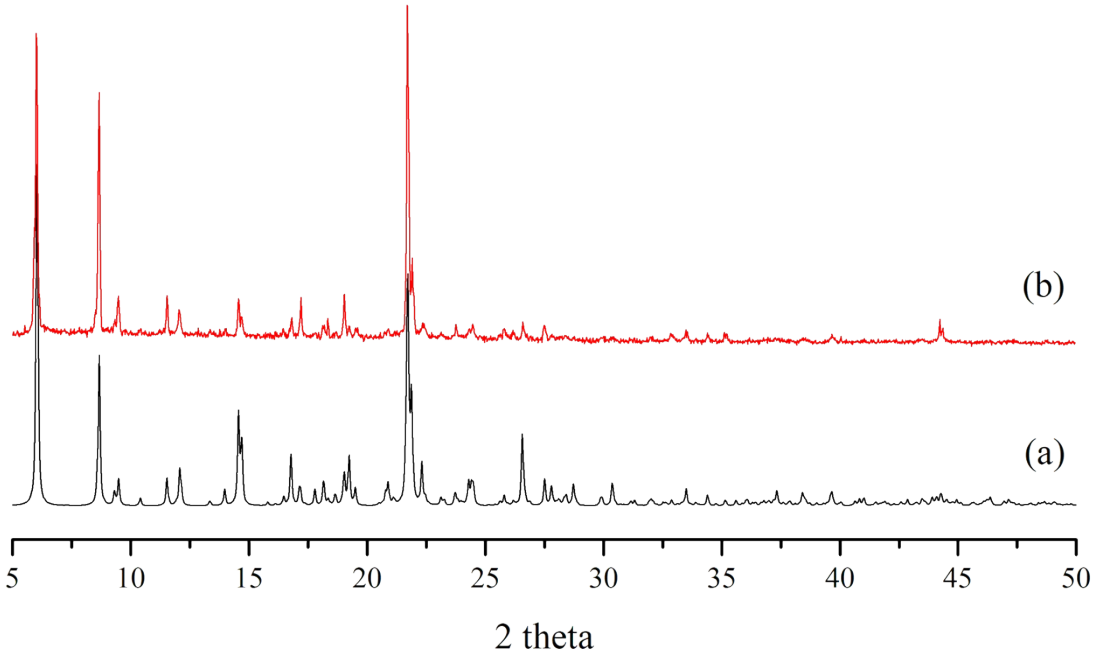


Fig. S2. (a) Simulated and (b) experimental PXRD patterns of **2**.

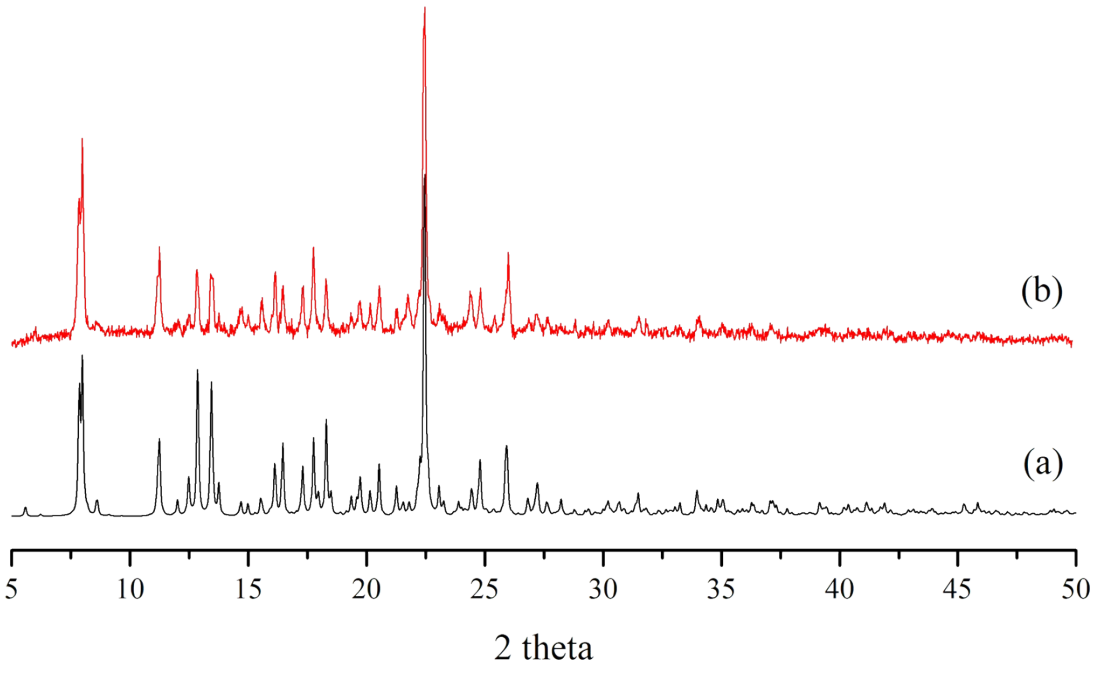


Fig. S3. (a) Simulated and (b) experimental PXRD patterns of **3**.

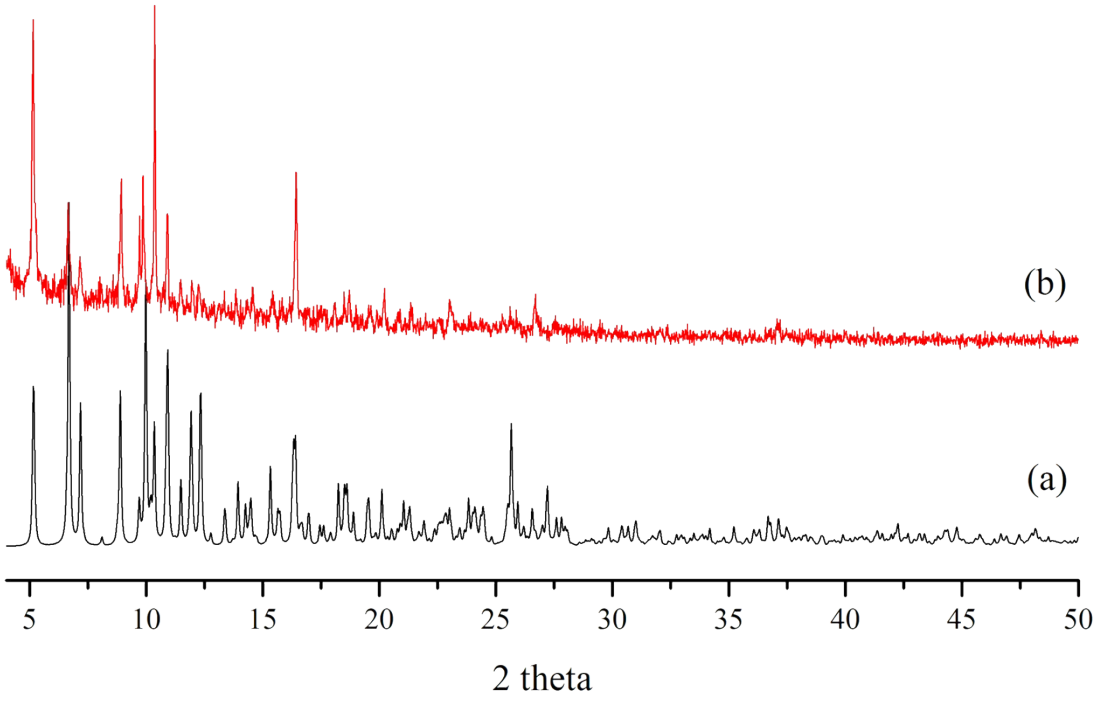


Fig. S4. (a) Simulated and (b) experimental PXRD patterns of **4**.

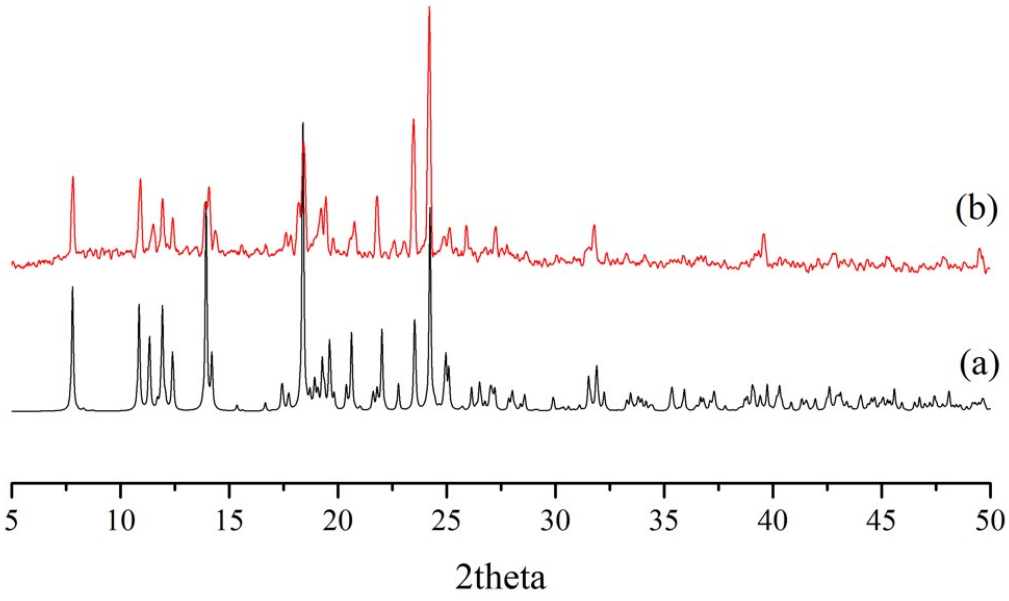


Table S1. H---O distances (Å) of hydrogen bonds with angles (°) in parenthesis for **1** – **4**.

Complex	**1**	**2**	**3**	**4**
[a]N-H---O			2.04 (176), 2.10 (177)	
[b]N-H---O	2.46 (134)	2.07 - 2.42 (132 – 166)		
[c]N-H---O	2.03 (169)			
[d]O-H---O	1.82 (161)	1.75 (172), 1.89 (167)		
[e]O-H---O	2.14 (160), 2.24 (145)	1.87 – 2.23 (120 – 169)		2.25 (136)
[f]O-H---O		2.31 (179), 2.46 (179)		
[g]O-H---O		2.28 (155), 2.53 (162)		2.60 (118)
[h]O-H---O		1.91 - 2.27 (134 – 178)		
[i]O-H---O		1.79 – 2.51 (111 – 165)		1.87 – 2.64 (118 -173)
[j]O-H---O		1.82 - 2.04 (171 – 177)		2.11 (129)
[k]O-H---O			1.77 - 2.33 (113 – 165)	
[l]O-H---O			1.75 (155), 1.95 (130)	
[m]O-H---O			1.97 (139)	
[n]O-H---O			2.26 (117)	
[o]O-H---O			2.44 (111)	
[p]O-H---O			2.11 (136)	
[q]O-H---O				1.88 (156)
[r]N-H---O				2.40 (146)

a from the amine hydrogen atoms of **L** to the carboxylate oxygen atoms.

b from the amine hydrogen atoms of **L** to the cocrystallized water oxygen atoms.

c from the amine hydrogen atoms of **L** to the amide oxygen atoms.

d from the carboxylate hydrogen atoms of 1,3,5-$HBTC^{2-}$ to the cocrystallized water molecules.

e from the cocrystallized water molecules to the carboxylate oxygen atoms.

f from the cocrystallized water molecules to the amide oxygen atoms.

g from the cocrystallized water molecules to the coordinated water molecules.

h from the cocrystallized water molecules to the cocrystallized water molecules

i from the coordinated water molecules to the carboxylate oxygen atoms.

j from the coordinated water molecules to the amide oxygen atoms.

k from the coordinated methanol molecules to the cocrystallized methanol molecules.

l from the coordinated methanol molecules to the carboxylate oxygen molecules.

m from the cocrystallized methanol molecules to the carboxylate oxygen molecules.

n from the cocrystallized methanol molecules to the amide oxygen molecules.

o from the cocrystallized methanol molecules to coordinated methanol oxygen atoms.

p from the cocrystallized methanol molecules to cocrystallized methanol oxygen atoms.

q from the coordinated water molecules to the cocrystallized water molecules.

r from the amine hydrogen atoms of **L** to the coordinated methanol molecules.

Fig. S5. Packing diagram for **1.**

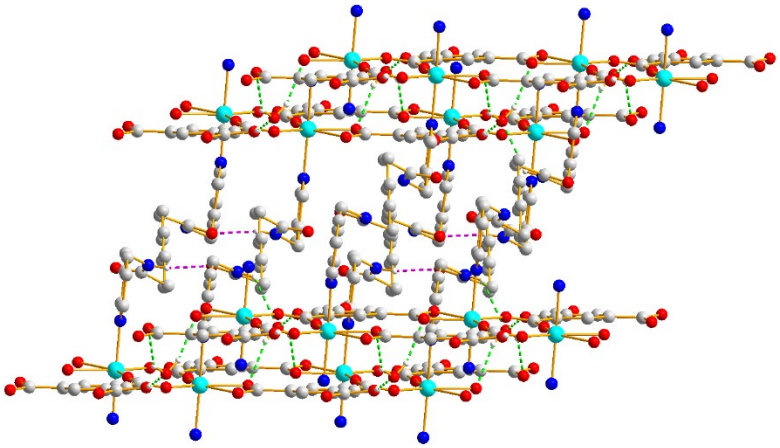


Fig. S6. Packing diagram for **2.**

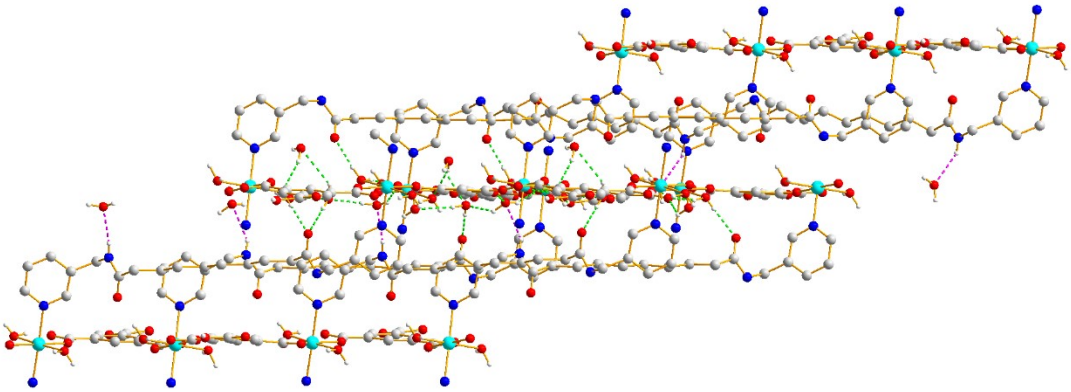


Fig. S7. Packing diagram for **3.**

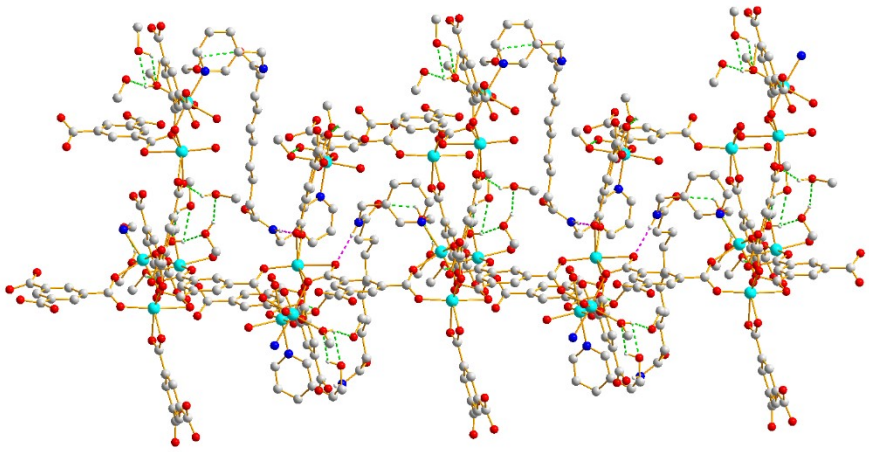


Fig. S8. Packing diagram for **4.**

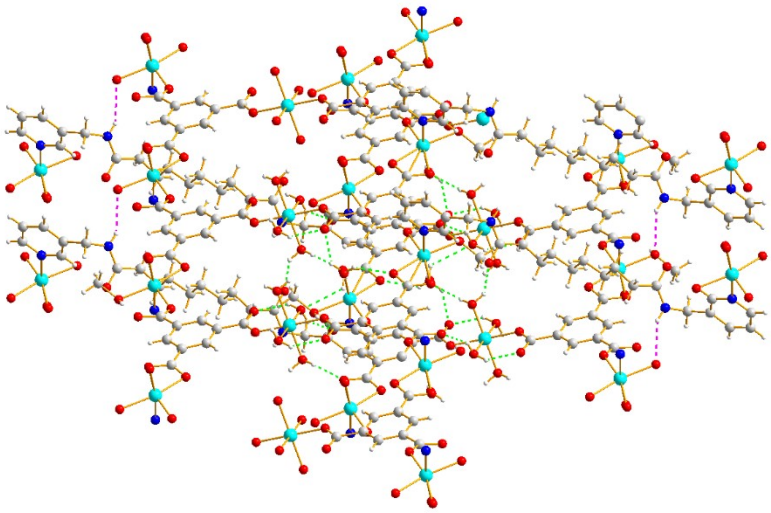
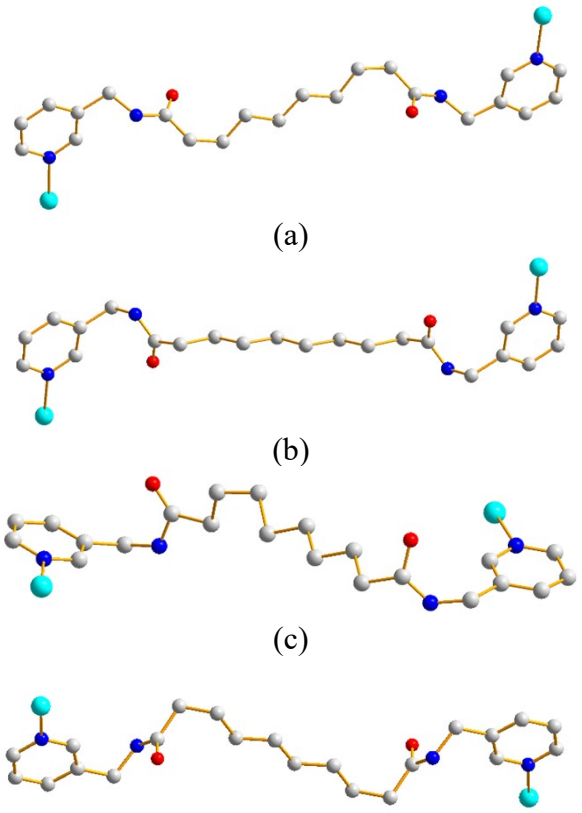


Fig. S9. Drawings showing the (a) GAAAAAG *trans anti-anti*, (b) AAAAAAA *trans syn-syn*, (c) AGAAAAA *cis anti-syn* conformations and (d) GAAAAAG *trans anti-anti* for the **L** ligands in **1** – **4**, respectively.



(a)

(b)

(c)

(d)

Fig. S10. The TGA curve for complex **1**.

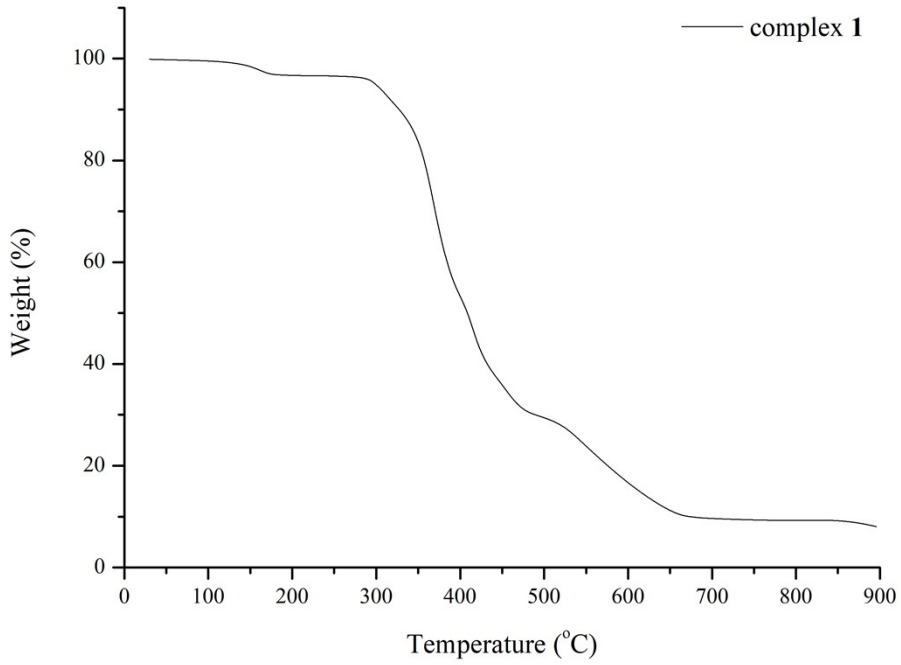


Fig. S11. The TGA curve for complex **2**.

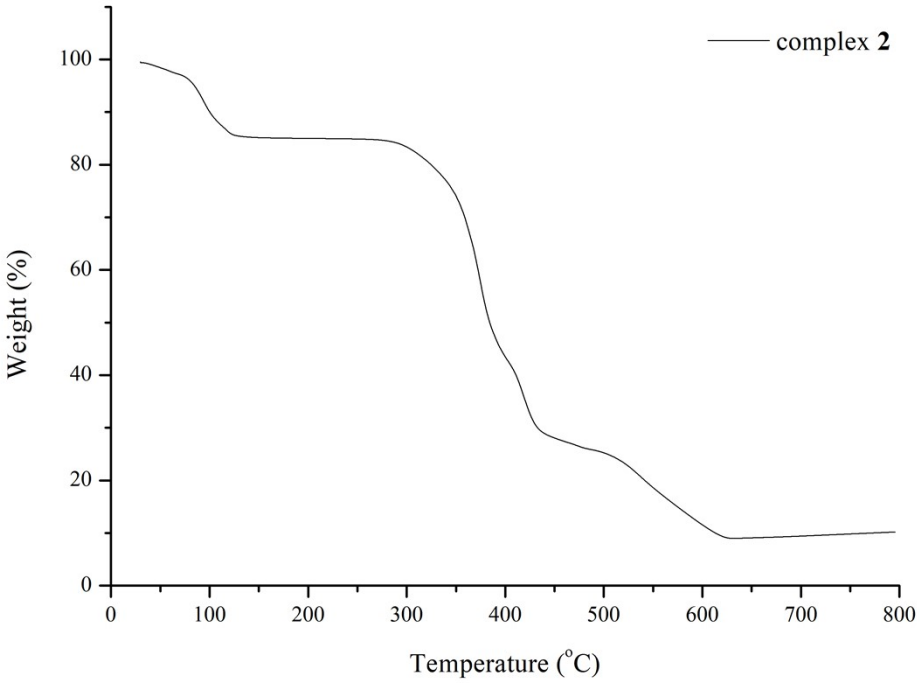


Fig. S12. The TGA curve for complex **3'**.

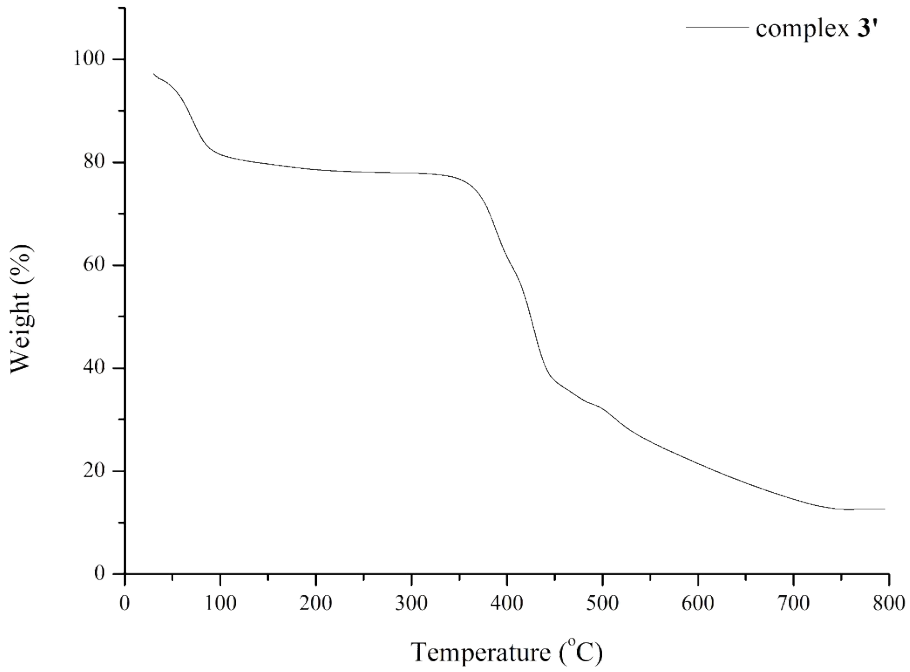


Fig. S13. The TGA curve for complex **4**.

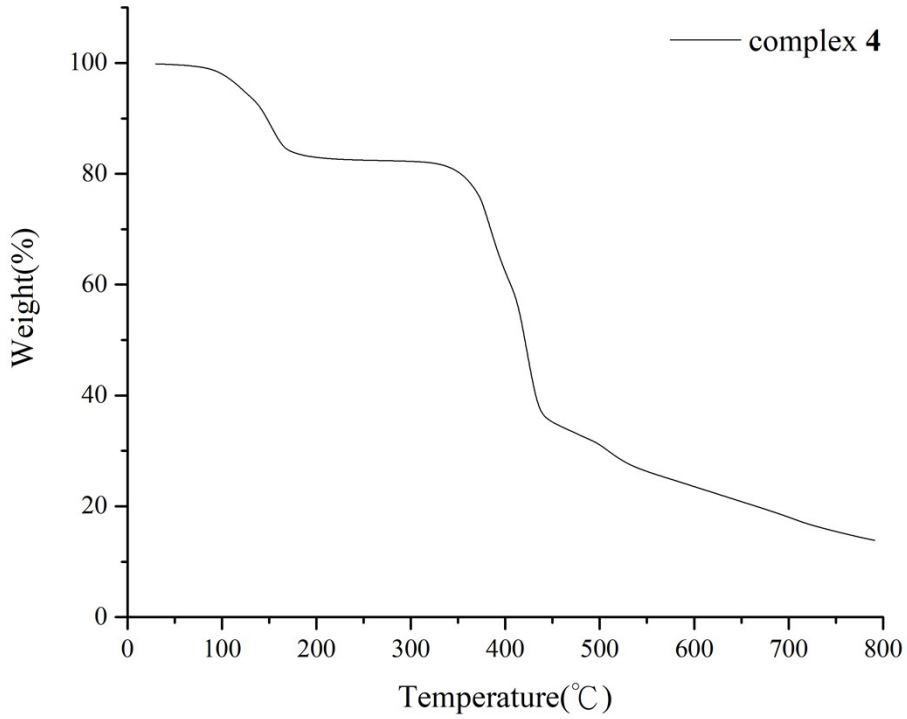


Fig. S14. PXRD patterns for transformation from **3** to **3'**. (a) simulation of **3**, (b) **3** kept in CH_3OH then exposed to air for (c) 8 min, (d) 16 min, (e) 24 min and (f) 3 h.

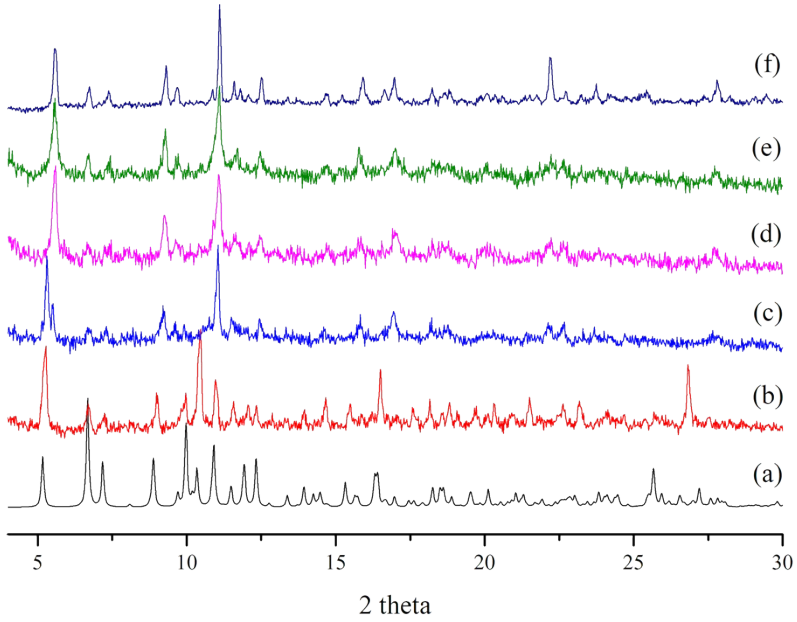


Figure S15. PXRD patterns of (a) as-synthesized of **3'**, (b) complex **3'** under vacuum for 20 minutes and (c) then immersed in MeOH for 1 h and (d) simulation of **3**.