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Pseudopolymorphism based on 1D metallacyclic chains constructed from angular zwitterionic ionic ditopic diacid organic linker

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Table S1 Distances(Å) and angles (°) of hydrogen bonds for **1α** and **1β**[a]

D-H···A	Distance (D···A)	D-H-A	Angle (D-H-A)
1α			
O(6W)-H(6WB)···O(4)#1	2.8252(7)	O(6W)-H(6WB)-O(4)#1	174
O(6W)-H(6WA)···O(3)	2.9476(3)	O(6W)-H(6WA)-O(3)	167
C(1)-H(1A)···O(6W)#2	3.1765(7)	C(1)-H(1A)-O(6W)#2	153
C(5)-H(5A)···O(2)#1	3.0076(7)	C(5)-H(5A)-O(1)#1	128
C(5)-H(5A)···O(1)#3	3.0194(7)	C(5)-H(5A)-O(1)#3	134
C(13)-H(13A)···O(6W)#2	3.4364(8)	C(13)-H(13A)-O(6W)#2	152
1β			
O(1W)-H(1WA)···O(1)#4	2.8640(10)	O(1W)-H(1WA)-O(1)#4	176
O(1W)-H(1WB)···O(4)	2.9771(11)	O(6W)-H(6WA)-O(3)	172
C(9)-H(9A)···O(1W)#5	3.3955(12)	C(9)-H(9A)-O(1W)#5	157
C(12)-H(12A)···O(4)#6	3.2950(12)	C(12)-H(12A)-O(4)#6	159
C(13)-H(13A)···O(2)#7	3.1986(11)	C(13)-H(13A)-O(2)#7	167

[a] Symmetry transformations used to generate equivalent atoms: #1 1/4-x, 1/4+y, 1/4+z; #2 1/2-x, -y, -1/2+z; #3 1/4+x, -1/4-y, 1/4+z; #4; #5 x, 1-y, -1/2+z; #6 1/2-x, 3/2-y, 1/2-z; #7 -1/2+x, 1/2-y, z.

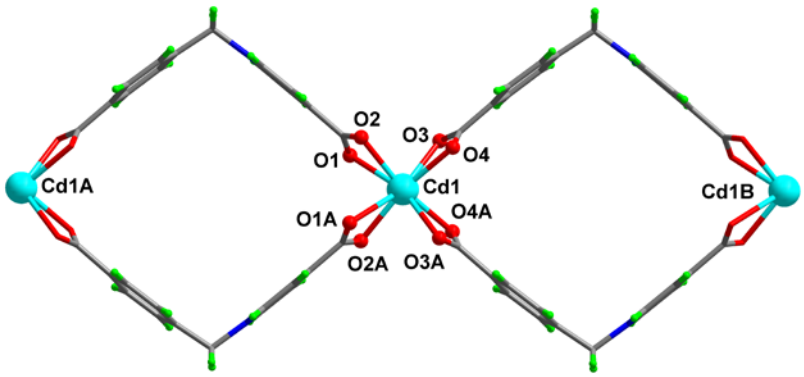

Fig. S1 Partial structure in**1α** and **1β** showing the coordination environment of Cd(II) ion.

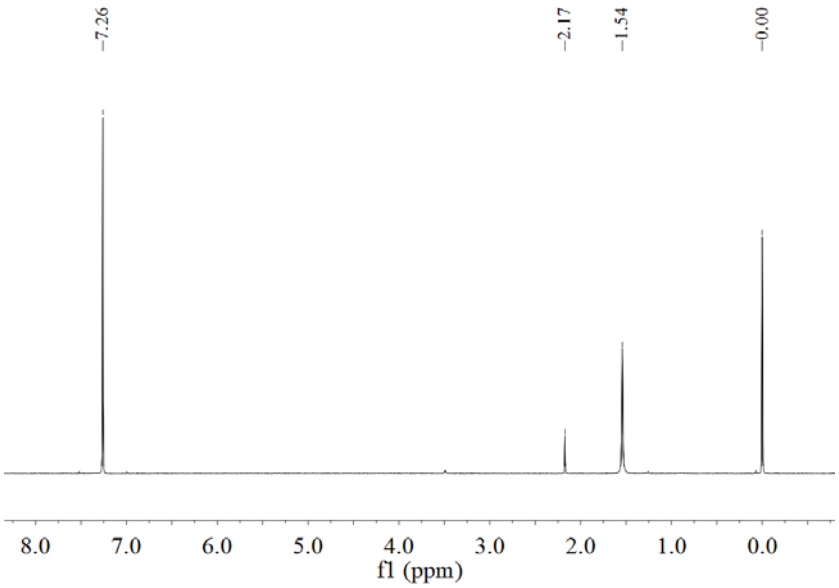

Fig. S2 The ^{1}H NMR spectrum of complex **1α**.

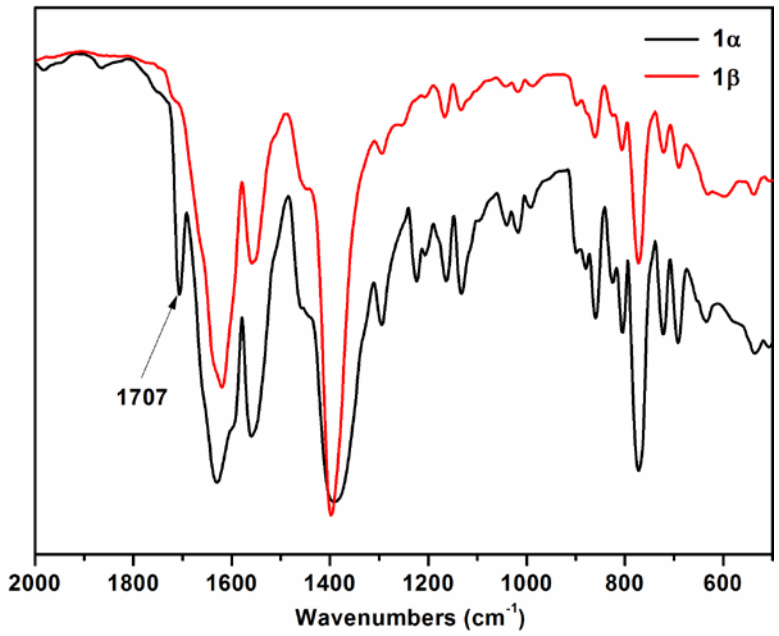

Fig. S3. The IR spectra of complexes **1α** and **1β**.

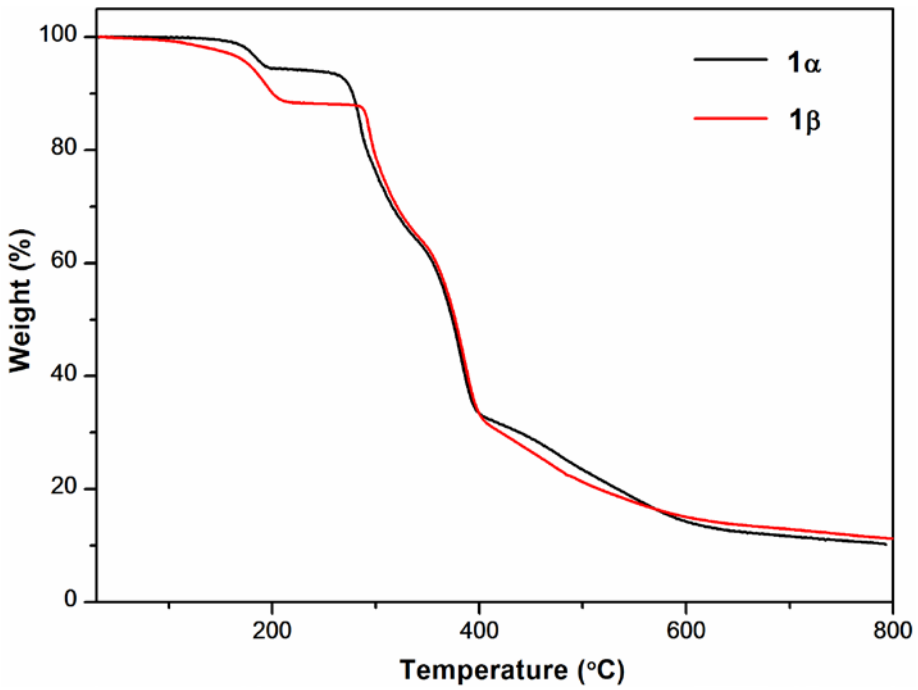

Fig. S4 TGA plots of complexes **1α** and **1β** under a N_2 atmosphere.

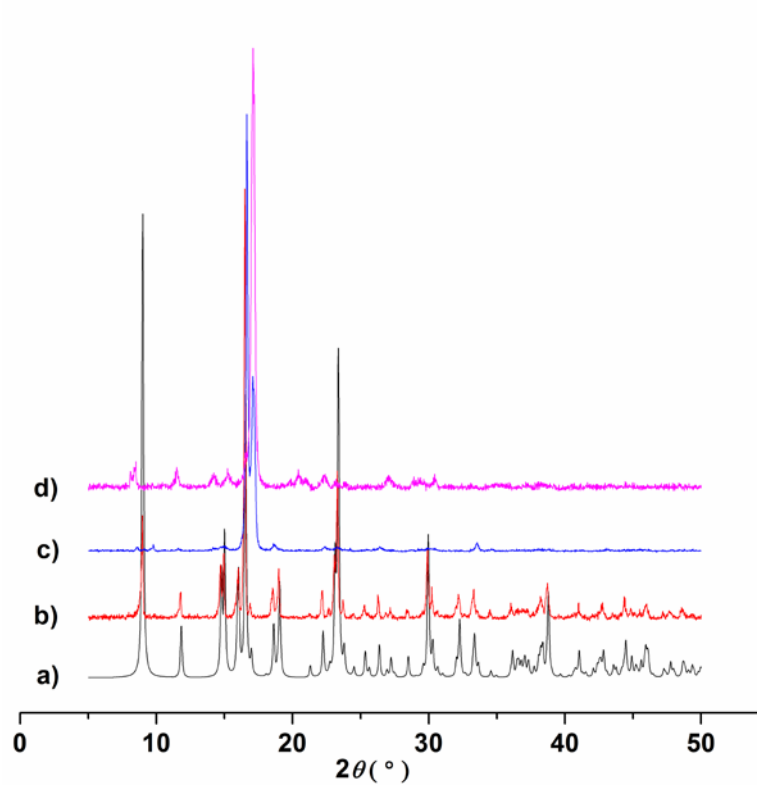

Fig. S5 Powder X-ray diffraction (PXRD) pattern of complex **1α**. a): calculated from single crystal data; b): experimental; c) heated at 180 °C for 3 days; d) the desolvated **1α´** were soaked in acetone for 3 days.

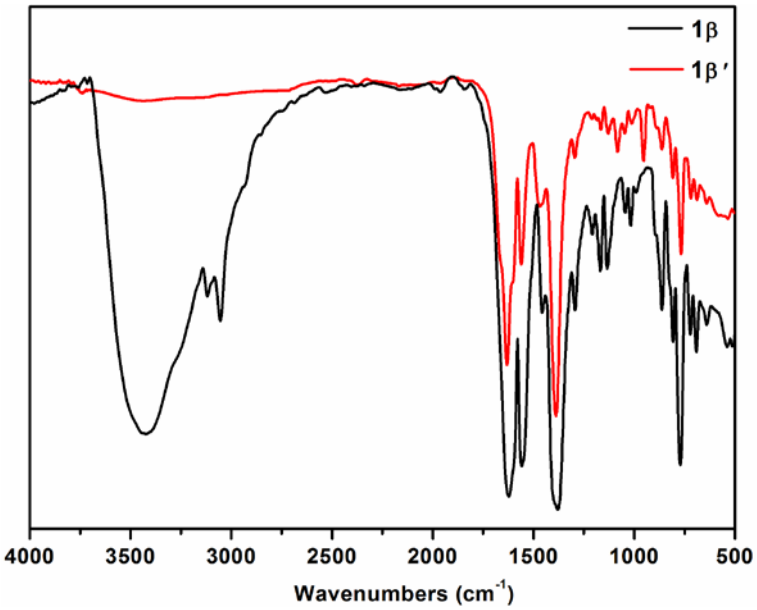

Fig. S6 The IR spectra of complexes **1β** and **1β´**.

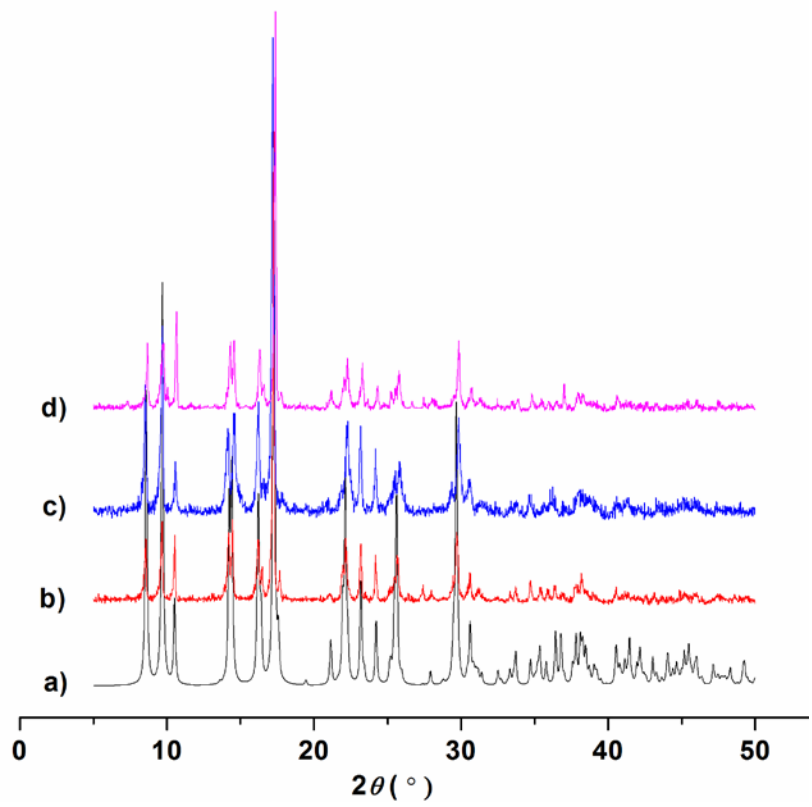

Fig. S7 Powder X-ray diffraction (PXRD) pattern of complex **1β**. a): calculated from single crystal data; b): experimental; c) heated at 180 °C for 1 days; d) the desolvated **1β´** were soaked in water for 3days.

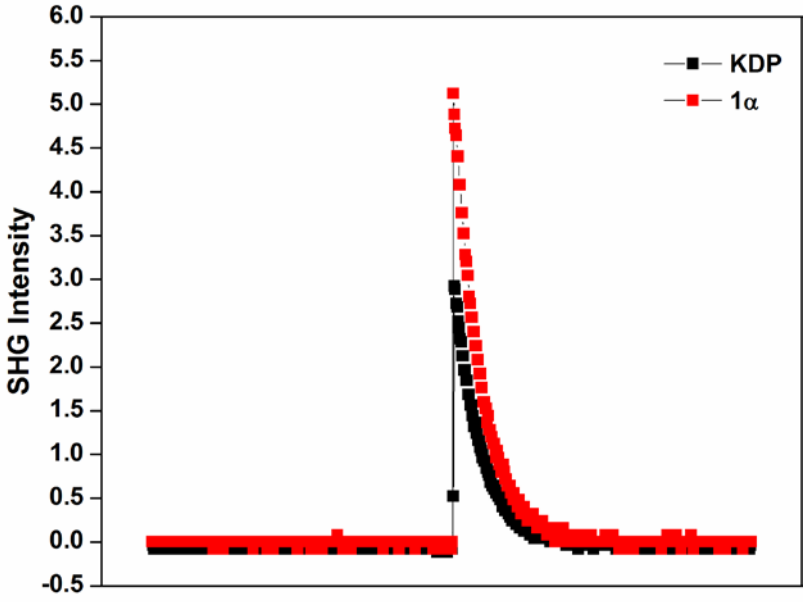

Fig. S8 Curves of the measured SHG signals of KDP and complex **1α**.