Four Cluster-Based Coordination Polymers Built on a Semirigid Tripod Tricarboxylate Ligand

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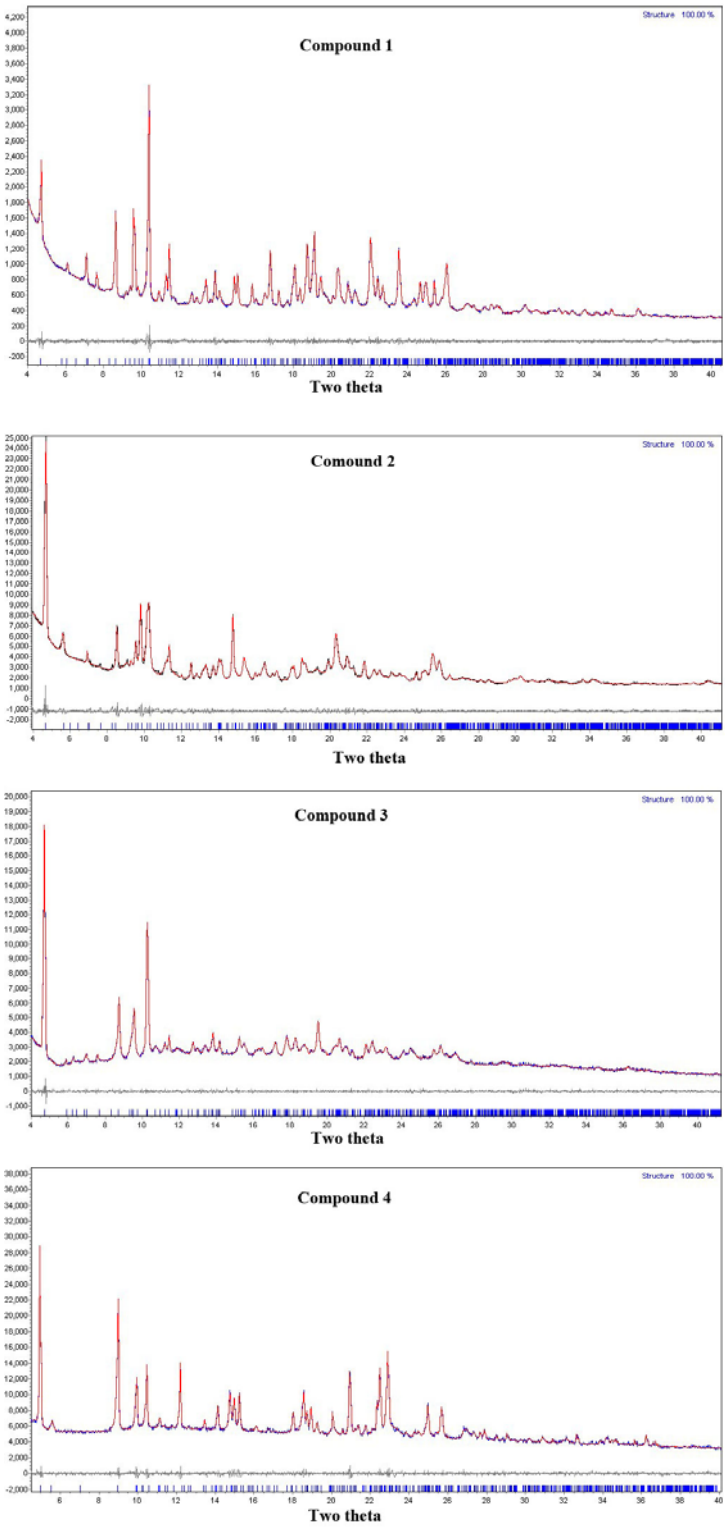
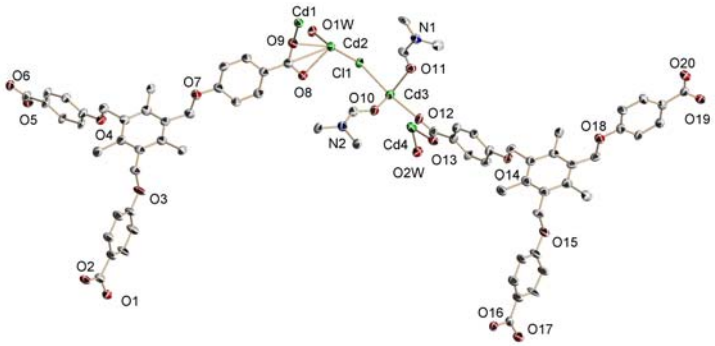
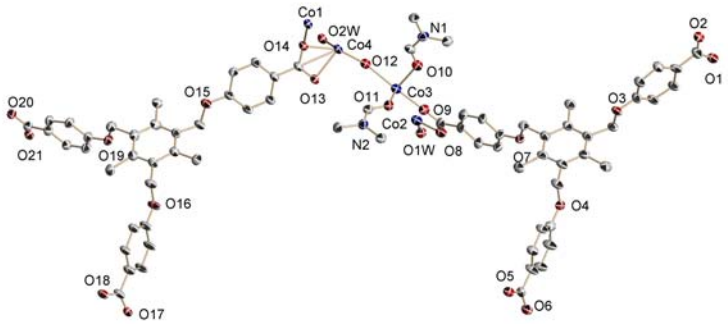


Fig. S1. X-ray powder diffraction patterns of **1-4**: the red line is the best fitted, the blue line is as-synthesized and the gray line is the difference. The best fitting results for **1**: a = 14.644 (3), b = 17.519 (9), c = 20.557 (6) Å, α = 66.78 (2), β = 77.97 (3), γ = 68.06 (2)°; for **2**: a = 14.89 (2), b = 17.94 (2), c = 20.63 (2) Å, α = 67.35 (9), β = 77.62 (10), γ = 67.75 (9) °; for **3**: a = 15.116 (5), b = 17.425 (5), c = 20.426 (8) Å, α = 67.05 (2), β = 76.33 (2), γ = 65.09 (2) °; for **4**: a = 8.600 (3), b = 35.52 (2), c = 17.857 (8) Å, β = 92.37 (4) °.



(a)



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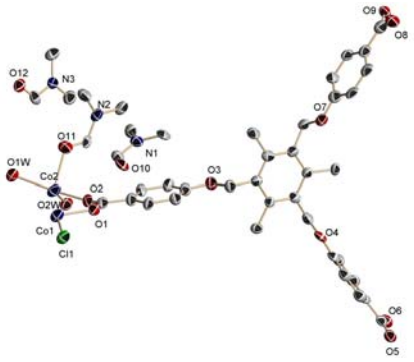

(c)

Fig. S2. ORTEP drawings of the asymmetric units of **2** (a), **3** (b) and **4** (c), respectively, at the 50% probability. The H atoms and guest water molecules are omitted for clarity.

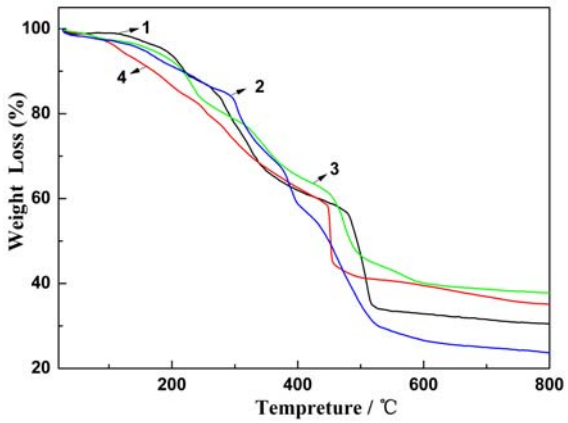

Fig. S3 TGA profiles under nitrogen for compounds **1** – **4**.

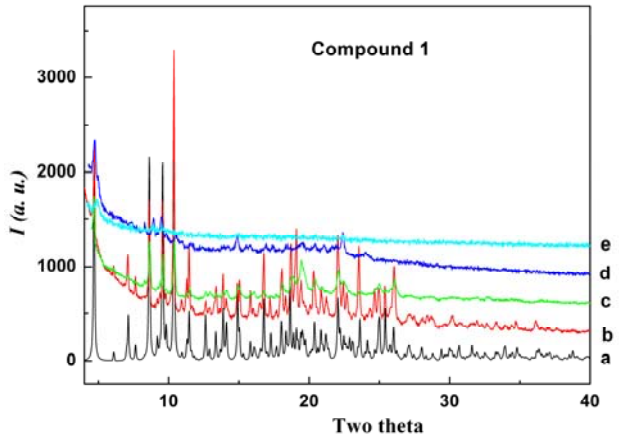

Fig. S4 XRPD patterns of **1**: (a) calculated, (b) as-synthesized and heated at (c)120 °C, (d) 200 °C and (e) 240 °C for *ca.* 0.5 h, respectively.

Table. S1. Selected bond lengths (Å) and angles (deg) for **2** and **3**.

2							
Cd1—O2^{i}	2.283(2)	Cd2—O5^{iii}	2.176(2)	Cd3—O11	2.267(2)	Cd4—O2W	2.247(2)
Cd1—O6^{iii}	2.269(2)	Cd2—O8	2.337(2)	Cd3—O12	2.210(2)	Cd4—O13	2.165(2)
Cd1—O9	2.298(2)	Cd2—O9	2.390(2)	Cd3—O16^{vii}	2.321(2)	Cd4—O16^{vii}	2.321(2)
Cd2—O1^{ii}	2.162(2)	Cd2—Cl1	2.531(1)	Cd3—O20^{vi}	2.265(2)	Cd4—O17^{vii}	2.214(2)
Cd2—O1W	2.389(2)	Cd3—O10	2.286(2)	Cd3—Cl1	2.581(1)	Cd4—O19^{vi}	2.128(2)
O2^{i}—Cd1—O2^{ii}	180.	O5^{iii}—Cd2—O9	99.94(8)	O12—Cd3—O10	86.61(8)	O2W—Cd4—O16^{vii}	149.13(8)
O2^{i}—Cd1—O6^{iii}	89.99(8)	O8—Cd2—O1W	85.40(8)	O12—Cd3—O11	87.55(9)	O13—Cd4—O2W	104.46(8)
O2^{i}—Cd1—O9	89.79(8)	O8—Cd2—O9	55.60(8)	O12—Cd3—O16^{vii}	86.48(8)	O13—Cd4—O16^{vii}	98.68(7)
O6^{iii}—Cd1—O6^{iv}	180	O9—Cd2—O1W	82.53(8)	O12—Cd3—O20^{vi}	100.29(9)	O13—Cd4—O17^{vii}	98.37(9)
O6^{iv}—Cd1—O9	87.48(8)	O1^{ii}—Cd2—Cl1	101.88(6)	O20^{vi}—Cd3—O16^{vii}	92.87(8)	O17^{vii}—Cd4—O2W	105.86(9)
O9—Cd1—O9^{v}	180	O1W—Cd2—Cl1	84.66(6)	O20^{vi}—Cd3—O11	170.20(9)	O17^{vii}—Cd4—O16^{vii}	49.94(8)
O1^{ii}—Cd2—O1W	80.39(8)	O5^{iii}—Cd2—Cl1	93.62(6)	O20^{vi}—Cd3—O10	81.42(8)	O19^{vi}—Cd4—O2W	92.35(9)
O1^{ii}—Cd2—O5^{iii}	97.83(8)	O8—Cd2—Cl1	99.70(6)	O10—Cd3—Cl1	96.72(6)	O19^{vi}—Cd4—O16^{vii}	102.14(8)
O1^{ii}—Cd2—O8	152.82(8)	O9—Cd2—Cl1	152.91(6)	O11—Cd3—Cl1	86.60(6)	O19^{vi}—Cd4—O13	103.02(8)
O1^{ii}—Cd2—O9	99.37(8)	O10—Cd3—O16^{vii}	170.11(8)	O12—Cd3—Cl1	173.42(6)	O19^{vi}—Cd4—O17^{vii}	147.40(9)
O5^{iii}—Cd2—O1W	177.19(8)	O11—Cd3—O10	93.29(8)	O16^{vii}—Cd3—Cl1	90.88(5)		
O5^{iii}—Cd2—O8	97.09(8)	O11—Cd3—O16^{vii}	93.48(8)	O20^{vi}—Cd3—Cl1	85.84(6)		
3							
Co1—O14	2.175(2)	Co2—O6^{vii}	1.921(2)	Co3—O10	2.098(2)	Co4—O13	2.153(1)
Co1—O18^{i}	2.056(2)	Co2—O8	1.934(2)	Co3—O11	2.060(2)	Co4—O14	2.146(2)
Co1—O20^{iii}	2.064(2)	Co3—O2^{vi}	2.035(2)	Co3—O1W	2.270(2)	Co4—O17^{ii}	1.979(1)
Co2—O1^{vi}	1.914(2)	Co3—O5^{vii}	1.996(1)	Co4—O2W	2.015(2)	Co4—O21^{iii}	1.997(2)
Co2—O12	2.006(2)	Co3—O9	1.989(2)	Co4—O1W	2.247(2)		
O14—Co1—O14^{v}	180	O8—Co2—O1W	110.67(7)	O9—Co3—O11	90.92(6)	O17^{ii}—Co4—O2W	85.28(6)
O18^{i}—Co1—O18^{ii}	180	O2^{vi}—Co3—O10	170.28(6)	O9—Co3—O12	177.34(6)	O17^{ii}—Co4—O12	95.76(6)
O18^{i}—Co1—O20^{iii}	88.40(6)	O2^{vi}—Co3—O11	86.47(6)	O10—Co3—O12	88.02(6)	O17^{ii}—Co4—O13	163.18(6)
O18^{ii}—Co1—O14	88.67(6)	O2^{vi}—Co3—O12	84.95(6)	O11—Co3—O10	86.71(6)	O17^{ii}—Co4—O14	104.00(6)
O20^{iv}—Co1—O14	94.37(6)	O5^{vii}—Co3—O2^{vi}	98.36(6)	O11—Co3—O12	89.09(6)	O17^{ii}—Co4—O21^{iii}	96.01(6)
O20^{iii}—Co1—O20^{iv}	180	O5^{vii}—Co3—O10	88.19(6)	O2W—Co4—O12	83.47(6)	O21^{iii}—Co4—O2W	173.85(6)
O1^{vi}—Co2—O1W	100.05(7)	O5^{vii}—Co3—O11	174.60(6)	O2W—Co4—O13	86.01(5)	O21^{iii}—Co4—O12	90.41(6)
O1^{vi}—Co2—O6^{vii}	121.89(7)	O5^{vii}—Co3—O12	88.92(6)	O2W—Co4—O14	84.16(6)	O21^{iii}—Co4—O13	94.18(5)
O1^{vi}—Co2—O8	115.25(7)	O9—Co3—O2^{vi}	97.70(6)	O13—Co4—O12	97.51(6)	O21^{iii}—Co4—O14	101.31(6)
O6^{vii}—Co2—O1W	95.54(7)	O9—Co3—O5^{vii}	90.84(6)	O14—Co4—O12	155.68(5)		
O6^{vii}—Co2—O8	110.35(7)	O9—Co3—O10	89.32(6)	O14—Co4—O13	60.75(5)		

Symmetry transformations: for **2**: (i) 2-x, 2-y, -z; (ii) x, -1+y, 1+z; (iii) x, y, 1+z; (iv) 2-x, 1-y, -z; (v) 2-x, 1-y, 1-z; (vi) x, y, -1+z; (vii) x, -1+y, z; (viii) x, 1+y, -1+z; (ix) x, 1+y, z; for **3**: (i) 2-x, 2-y, -z; (ii) x, -1+y, 1+z; (iii) x, y, 1+z; (iv) 2-x, 1-y, -z; (v) 2-x, 1-y, 1-z; (vi) x, y, -1+z; (vii) x, -1+y, z; (viii) x, 1+y, z; (ix) x, 1+y, -1