Electronic Supplementary Information

1D Ladder and 2D bilayer coordination polymers constructed from a new T-shaped ligand: Luminescent, magnetic and CO₂ gas adsorption properties

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1		2		3		4	
Mn(1)-N(1)#2	2.3119(18)	Cd(1)-Cl(1)	2.2560(12)	Co(1)-N(1)	2.252(4)	Ni(1)-N(1)	2.152(2)
Mn(1)-N(2)#2	2.2975(19)	Cd(1)-N(1)#4	2.3753(11)	Co(1)-N(2)#8	2.151(4)	Ni(1)-N(2)#6	2.095(2)
Mn(1)-O(1)	2.1337(17)	Cd(1)-N(2)#2	2.3892(12)	Co(1)-O(1)	2.006(3)	Ni(1)-O(1)	2.0291(17)
Mn (1)-O(3)#2	2.1824(16)	Cd(1)-O(1)	2.2924(11)	Co(1)-O(3)#4	2.077(4)	Ni(1)-O(5)	2.0551(16)
Mn (1)-O(5)	2.2098(17)	Cd(1)-O(2)	2.4173(11)	Co(1)-O(4)#4	2.296(4)	Ni(1)-O(9)	2.085(2)
Mn (1)-O(6)	2.1889(17)	Cd(1)-O(4)#4	2.2455(10)	Co(1)-O(5)	2.059(3)	Ni(1)-O(10)	2.1078(19)
N(1)#2-Mn(1)-N(2)#2	93.72 (6)	Cl(1)-Cd(1)-N(1)#4	107.13(4)	N(1)-Co(1)-N(2)#8	168.43(16)	N(1)-Ni(1)-N(2)#6	168.76(8)
N(1)#2-Mn(1)-O(1)	117.06(7)	Cl(1)-Cd(1)-N(2)#2	93.10(5)	N(1)-Co(1)-O(1)	79.67(14)	N(1)-Ni(1)-O(1)	79.52(7)
N(1)#2-Mn(1)-O(3)#2	73.05(6)	Cl(1)-Cd(1)-O(1)	97.99(4)	N(1)-Co(1)-O(3)#4	98.60(15)	N(1)-Ni(1)-O(5)	102.47(7)
N(1)#2-Mn(1)-O(5)	156.01(7)	Cl(1)-Cd(1)-O(2)	153.55(4)	N(1)-Co(1)-O(4)#4	84.44(14)	N(1)-Ni(1)-O(9)	94.28(8)
N(1)#2-Mn(1)-O(6)	83.60(7)	Cl(1)-Cd(1)-O(4)#4	100.80(4)	N(1)-Co(1)-O(5)	92.25(14)	N(1)-Ni(1)-O(10)	88.50(8)
N(2)#2-Mn(1)-O(1)	89.76(7)	N(1)#4-Cd(1)-N(2)#2	149.56(4)	N(2)#8-Co(1)-O(1)	89.16(16)	N(2)#6-Ni(1)-O(1)	89.54(8)
N(2)#2-Mn(1)-O(3)#2	86.28(7)	N(1)#4-Cd(1)-O(1)	106.65(4)	N(2)#8-Co(1)-O(3)#4	90.52(16)	N(2)#6-Ni(1)-O(5)	88.66(8)
N(2)#2-Mn(1)-O(5)	92.93(7)	N(1)#4-Cd(1)-O(2)	85.23(4)	N(2)#8-Co(1)-O(4)#4	94.13(15)	N(2)#6-Ni(1)-O(9)	88.64(8)
N(2)#2-Mn(1)-O(6)	176.17(7)	N(1)#4-Cd(1)-O(4)#4	71.98(4)	N(2)#8-Co(1)-O(5)	92.53(16)	N(2)#6-Ni(1)-O(10)	89.45(8)
O(1)-Mn(1)-O(3)#2	169.42(7)	N(2)#2-Cd(1)-O(1)	92.60(8)	O(1)-Co(1)-O(3)#4	157.20(15)	O(1)-Ni(1)-O(5)	174.56(8)
O(1)-Mn(1)-O(5)	85.98(7)	N(2)#2-Cd(1)-O(2)	86.32(5)	O(1)-Co(1)-O(4)#4	97.50(14)	O(1)-Ni(1)-O(9)	91.98(8)
O(1)-Mn(1)-O(6)	89.03(7)	N(2)#2-Cd(1)-O(4)#4	82.21(4)	O(1)-Co(1)-O(5)	99.33(14)	O(1)-Ni(1)-O(10)	92.72(8)
O(3)#2-Mn(1)-O(5)	84.43(7)	O(1)-Cd(1)-O(2)	55.68(4)	O(3)#4-Co(1)-O(4)#4	59.79(13)	O(5)-Ni(1)-O(9)	82.85(7)
O(3)#2-Mn(1)-O(6)	95.52(6)	O(1)-Cd(1)-O(4)#4	160.68(4)	O(3)#4-Co(1)-O(5)	103.46(14)	O(5)-Ni(1)-O(10)	92.40(7)
O(5)-Mn(1)-O(6)	90.61(7)	O(2)-Cd(1)-O(4)#4	105.30(4)	O(4)#4-Co(1)-O(5)	161.98(13)	O(9)-Ni(1)-O(10)	174.91(7)

Table S1 Selected bond distances (Å) and angles (°) for 1-4.^a

^{*a*} Symmetry code for 1: #2= -x, -y, -z; symmetry code for 2: #2= -x, y, -z+1/2, #4= - x+1/2, y+1/2, -z+1/2; symmetry code for 3: #4= x+1/2, -y+1/2, -z, #8= -x-1/2, y-1/2, z; symmetry code for 4: #6= x-1/2, y, -z-1/2.



Scheme S1 The synthesis procedure for H₂L ligand.



5 10 15 20 25 30 35 40 45 50 2-Theta (°)

Fig. S2 Powder XRD profiles of 2 and activated 2.



Fig. S3 Powder XRD profiles of 3.



Fig. S4 Powder XRD profiles of 4 and activated 4.



Fig. S5 The alternating rhombic grids with a view down the b axis in 2, showing the guest water molecules locate in the large grids.



Fig. S6 The alternating rhombic grids with a view down the *a* axis in 3.



Fig. S7 (a) The rhombic grid motif in 4. (b) The wave-like layers and 3D supramolecular framework in 4.



Fig. S8 Solid-state excitation spectra of H_2L ligand and coordination polymers 1–4.