Electronic Supplementary Information

Two isostructural linear coordination polymers: Size of metal ion impacts the electrical conductivity

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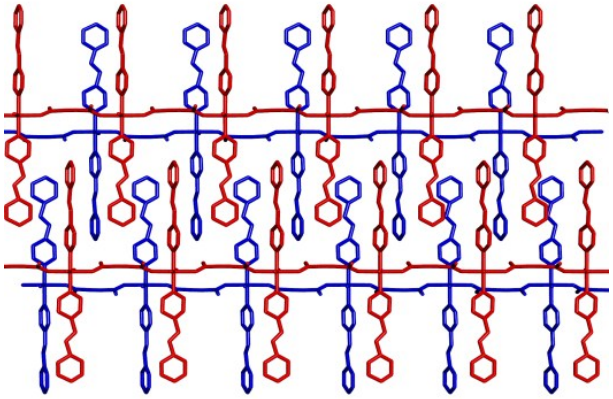

Fig. S1 A view of 3D supramolecular aggregate in compound **1** via hydrogen bonding and C-H···π interactions.

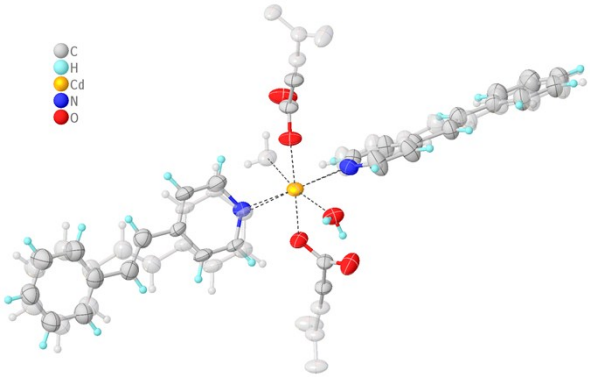

Fig. S2 A view of coordination environment of Cd(II) in **2** showing disorder 4-spy ligands.

Table S1 Crystal data and refinement parameters for compound **1**and **2**

Formula	$C_{30}H_{26}N_2O_6Zn$ (**1**)	$C_{30}H_{26}N_2O_6Cd$ (**2**)
fw	575.90	622.93
cryst syst	monoclinic	monoclinic
space group	*C*2/*c*	*C*2/*c*
a (Å)	9.8300(5)	10.0651(3)
b (Å)	32.8664(17)	33.3266(12)
c (Å)	9.1401(5)	9.1584(3)
α(deg)	90	90
β(deg)	115.385(2)	115.529(1)
γ (deg)	90	90
V (Å^3)	2667.8(2)	2772.12(16)
Z	4	4
D_{calcd}(g/cm^3)	1.434	1.493
μ(mm^{-1})	0.968	0.833
λ(Å)	0.71073	0.71073
GOF on F^2	1.112	1.077
final *R* indices [$I > 2\sigma(I)$][a,b]	$R1 = 0.0337$ $wR2 = 0.0831$	$R1 = 0.0276$ $wR2 = 0.0688$

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b] $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths and bond angles in **1**

Zn(1)-O(1)	2.0999(14)	*N(2)-Zn(1)-O(1)b	90.9(3)
Zn(1)-O(1)b	2.0999(14)	*N(2)-Zn(1)-*N(2)b	4.6(4)
Zn(1)-O(2)	2.1357(15)	O(1)b-Zn(1)- *N(2)b	95.0(3)
Zn(1)-O(2)b	2.1357(15)	*N(1)b-Zn(1)- *N(2)b	178.1(4)
Zn(1)-*N(1)	2.1481(18)	O(1)-Zn(1)-*N(1)	83.7(2)
Zn(1)-*N(1)b	2.1481(18)	O(1)-Zn(1)-O(2)b	90.11(6)
Zn(1)-*N(2)	2.1397(18)	O(2)-Zn(1)-*N(1)	89.2(3)
Zn(1)-*N(2)b	2.1397(18)	O(2)-Zn(1)-O(2)b	179.01(6)
O(1)-Zn(1)-O(2)	89.84(6)	*N(1)-Zn(1)-*N(2)	178.1(4)
O(1)-Zn(1)-O(1)b	174.17(6)	*N(1)-Zn(1)- *N(1)b	6.9(3)
O(1)-Zn(1)-*N(2)b	90.9(3)	*N(2)-Zn(1)-O(2)b	91.5(3)
O(2)-Zn(1)-O(1)b	90.11(6)	O(1)b-Zn(1)-O(2)b	89.84(6)
O(2)-Zn(1)-*N(2)b	91.5(3)	O(2)b-Zn(1)- *N(1)b	89.2(3)
*N(1)-Zn(1)-O(2)b	89.8(3)	O(1)-Zn(1)-*N(2)	95.0(3)
O(1)-Zn(1)-*N(1)b	90.5(2)	O(2)-Zn(1)-*N(1)b	89.8(3)
O(2)-Zn(1)-*N(2)	89.5(3)	*N(1)-Zn(1)-O(1)b	90.5(2)
*N(1)-Zn(1)-*N(2)b	174.5(4)	*N(2)-Zn(1)- *N(1)b	174.5(4)
O(1)b-Zn(1)-*N(1)b	83.7(2)	O(2)b-Zn(1)- *N(2)b	89.5(3)

Symmetry transformations used to generate equivalent atoms: a = -x, y, 3/2-z; b = 1-x, y, 3/2-z

* Disordered atoms

Table S3 Selected bond lengths and bond angles in **2**

Cd(1)-O(1)	2.2987(16)	*N(2)-Cd(1)-O(1)b	93.6(4)
Cd(1)-O(1)b	2.2987(16)	*N(2)-Cd(1)-*N(2)b	4.8(5)
Cd(1) -O(2)	2.2963(18)	O(1)b-Cd(1)-*N(2)b	98.3(4)
Cd(1)-O(2)b	2.2963(18)	*N(1)b-Cd(1)-*N(2)b	179.3(5)
Cd(1)-*N(1)	2.332(2)	*N(1)b-Cd(1)-*N(2)b	179.3(5)
Cd(1)-*N(1)b	2.332(2)	*N(1)-Cd(1)-*N(1)b	5.6(3)
Cd(1)-*N(2)	2.317(2)	*N(2)-Cd(1)-O(2)b	90.0(4)
Cd(1)-*N(2)b	2.317(2)	O(1)b-Cd(1)-O(2)b	92.50(6)
O(1)-Cd(1)-O(2)	92.50(6)	O(2)b-Cd(1)-*N(1)b	90.6(3)
O(1)-Cd(1)-O(1)b	168.12(7)	O(1)-Cd(1)-*N(2)	98.3(4)
O(1)-Cd(1)-*N(2)b	93.6(4)	O(1)-Cd(1)-*N(1)b	86.9(2)
O(2)-Cd(1)-O(1)b	87.61(6)	O(2)-Cd(1)-*N(2)	88.9(4)
O(2)-Cd(1)-*N(2)b	90.0(4)	O(2)-Cd(1)-*N(1)b	90.5(3)
*N(1)-Cd(1)-O(2)b	90.5(3)	*N(1)-Cd(1)-O(1)b	86.9(2)
*N(1)-Cd(1)-*N(2)b	174.8(4)	*N(2)-Cd(1)-*N(1)b	174.8(4)
O(1)b-Cd(1)-*N(1)b	81.3(2)	O(2)b-Cd(1)-*N(2)b	88.9(4)

Symmetry transformations used to generate equivalent atoms: a = -x, y, 3/2-z; b =1-x, y, 3/2-z

* Disordered atoms

Table S4 DFT table for compound **1** and **2**

Compound **1**				Compound **2**			
MO	Energy (eV)	Zn	Ligand	MO	Energy (eV)	Cd	Ligand
LUMO+10	-0.43	0	100	LUMO+10	-0.62	0	100
LUMO+9	-0.58	0	100	LUMO+9	-0.63	0	100
LUMO+8	-0.59	0	100	LUMO+8	-0.79	0	100
LUMO+7	-0.83	0	100	LUMO+7	-0.83	0	100
LUMO+6	-0.89	0	100	LUMO+6	-1.07	0	100
LUMO+5	-1.75	0	100	LUMO+5	-1.23	0	100
LUMO+4	-1.76	1	99	LUMO+4	-1.25	1	99
LUMO+3	-2.23	0	100	LUMO+3	-1.72	0	100
LUMO+2	-2.23	0	100	LUMO+2	-1.73	0	100
LUMO+1	-2.29	0	100	LUMO+1	-2.31	0	100
LUMO	-2.3	0	100	LUMO	-2.5	0	100
HOMO	-6.28	0	100	HOMO	-6.32	0	100
HOMO-1	-6.29	0	100	HOMO-1	-6.49	0	100
HOMO-2	-7.23	0	100	HOMO-2	-7.15	1	99
HOMO-3	-7.24	0	100	HOMO-3	-7.23	0	100
HOMO-4	-7.61	3	97	HOMO-4	-7.28	0	100
HOMO-5	-7.64	0	100	HOMO-5	-7.43	0	100
HOMO-6	-7.7	0	100	HOMO-6	-7.53	2	98
HOMO-7	-7.78	0	100	HOMO-7	-7.61	0	100
HOMO-8	-7.91	2	98	HOMO-8	-7.63	1	99
HOMO-9	-7.99	0	100	HOMO-9	-7.69	0	100
HOMO-10	-8.04	0	100	HOMO-10	-7.86	0	100
Key transition for both the compounds: HOMO-1→LUMO, Nature of transition: ILCT ILCT: Intra ligand charge transfer transition							

Table S5 Calculated transitions and their assignment for compound **1**

Excitation energy (eV)	Wavelength Thro. (nm)	Oscillation frequency(f)	Key Transitions	Nature of transitions
3.7170	333.56	0.0676	(39%) HOMO-1→LUMO	ILCT
3.739	331.6	0.0218	(60%) HOMO→LUMO+2	ILCT
4.7005	263.77	0.0296	(72%) HOMO-4→LUMO+1	ILCT
5.0393	246.04	0.0307	(23%) HOMO-5→LUMO+1	ILCT

Table S6 Calculated transitions and their assignment for compound **2**

Excitation energy (eV)	Wavelength Thro. (nm)	Oscillation frequency(f)	Key Transitions	Nature of transitions
3.7986	326.39	2.1531	(62%) HOMO-1→LUMO	ILCT
3.8716	320.24	0.0546	(62%) HOMO→LUMO+1	ILCT
5.0825	243.94	0.0550	(32%) HOMO-12→LUMO	ILCT
5.0921	243.48	0.0382	(29%)HOMO→LUMO+7	ILCT

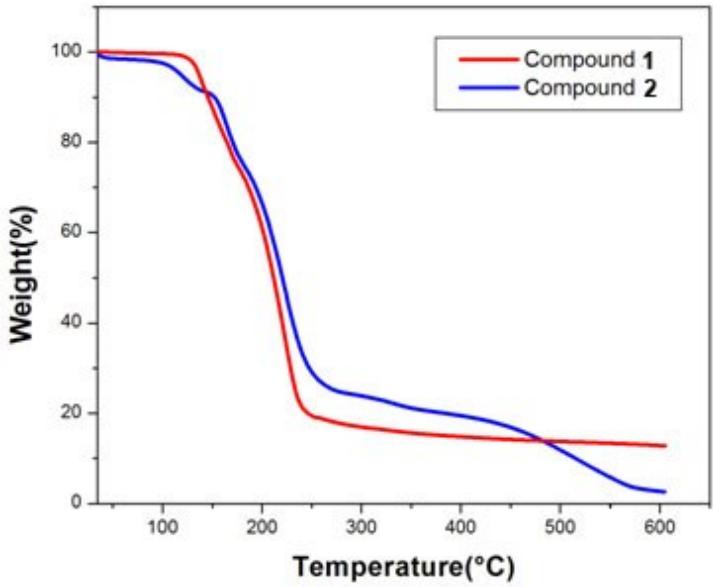

Fig. S3 TGA plots of compound **1**and **2** measured under N_2 atmosphere.

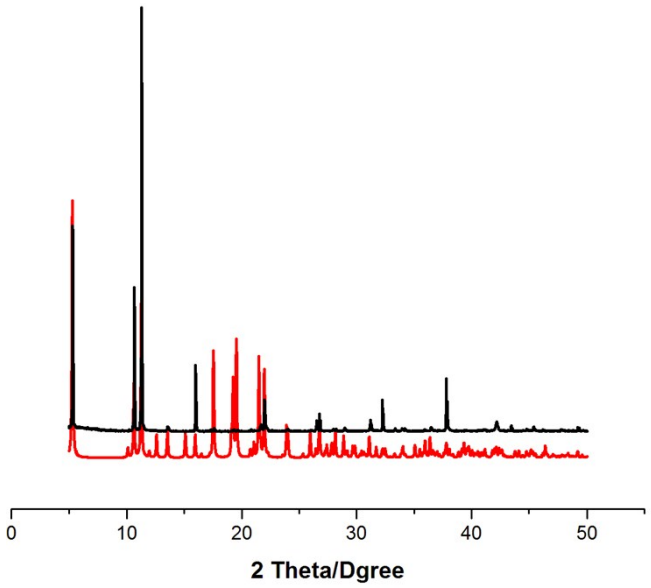

Fig. S4 Powder X-ray diffraction patterns of simulated **1** (red) and as-synthesized **1** (black).

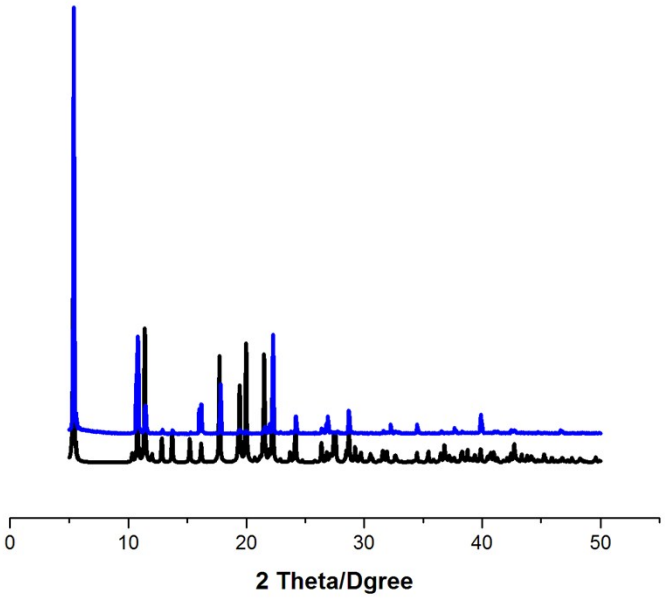

Fig. S5 Powder X-ray diffraction patterns of simulated **2** (black) and as-synthesized **2** (blue).