Electronic Supplementary Information

Cation dependent charge transport in linear dicarboxylate based isotypical 1D coordination polymers

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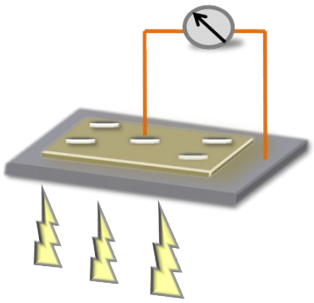

Fig. S1 The structure of Device-a (or Device-b).

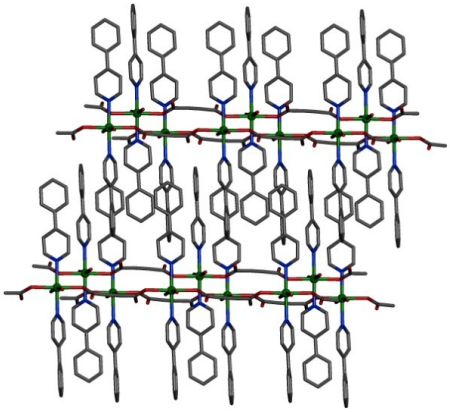

Fig. S2 A view of 3D supramolecular framework in compound **1**.

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

Formula	$C_{26}H_{22}CdN_2O_6$ (**1**)	$C_{26}H_{22}ZnN_2O_6$ (**2**)
fw	570.85	523.85
cryst syst	triclinic	monoclinic
space group	$P\bar{1}$	$C2/c$
a (Å)	9.4482(9)	9.8479(4)
b (Å)	10.0882(9)	27.7163(13)
c (Å)	14.7102(13)	9.3837(4)
α (deg)	72.942(3)	90
β (deg)	82.840(3)	114.8410(10)
γ (deg)	64.910(3)	90
V (Å^3)	1213.95(19)	2324.28(18)
Z	2	4
D_{calcd} (g/cm^3)	1.562	1.497
μ (mm^{-1})	0.944	1.103
λ (Å)	0.71073	0.71073
data [$I > 2\sigma(I)$]/params	5903/333	2833/169
GOF on F^2	1.135	1.069
final R indices [$I > 2\sigma(I)$][a,b]	R1 = 0.0575	R1 = 0.0447
	wR2 = 0.1518	wR2 = 0.1180

[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**

Cd(1)-O(3)	2.289(3)	Cd(1)-O(1)	2.306(3)
Cd(1)-O(5)a	2.292(3)	Cd(1)-N(2)	2.339(4)
Cd(1)-O(2)	2.301(3)	Cd(1)-N(1)	2.343(5)
O(3)-Cd(1)-O(5)a	178.18(11)	O(2)-Cd(1)-N(2)	84.15(14)
O(3)-Cd(1)-O(2)	90.83(12)	O(1)-Cd(1)-N(2)	83.23(14)
O(5)a-Cd(1)-O(2)	88.54(11)	O(3)-Cd(1)-N(1)	89.00(13)
O(3)-Cd(1)-O(1)	88.32(11)	O(5)a-Cd(1)-N(1)	89.38(13)
O(5)-Cd(1)-O(1)	92.67(12)	O(2)-Cd(1)-N(1)	96.41(13)
O(2)-Cd(1)-O(1)	167.32(14)	O(1)-Cd(1)-N(1)	96.23(13)
O(3)-Cd(1)-N(2)	91.87(14)	N(2)-Cd(1)-N(1)	178.96(14)
O(5)a-Cd(1)-N(2)	89.76(14)		

Symmetry Code: a = x, -1+y, z

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

Zn(1)-O(1)	2.104(2)	Zn(1)-O(2)a	2.139(2)
Zn(1)-O(1)a	2.104(2)	Zn(1)-N(1)	2.131(3)
Zn(1)-O(2)	2.139(2)	Zn(1)-N(2)	2.150(3)
O(1)-Zn(1)-O(2)	90.55(7)	N(1)-Zn(1)-O(1)a	93.36(5)
O(1)-Zn(1)-O(1)a	173.28(8)	N(2)-Zn(1)-O(2)a	89.79(5)
O(2)-Zn(1)-N(2)	89.79(5)	O(1)-Zn(1)-N(2)	86.64(5)
N(1)-Zn(1)-N(2)	180.00(3)	O(2)-Zn(1)-N(1)	90.21(5)
N(2)-Zn(1)-O(1)a	86.64(5)	O(2)-Zn(1)-O(2)a	179.59(7)
O(1)-Zn(1)-N(1)	93.36(5)	N(1)-Zn(1)-O(2)a	90.21(5)
O(1)-Zn(1)-O(2)a	89.42(7)	O(1)b-Zn(1)-O(2)a	90.55(7)
O(2)-Zn(1)-O(1)a	89.42(7)		

Symmetry Code: a = 1-x, y, 3/2-z

Table S4 Intermolecular hydrogen bonding interactions in **1** and **2**.

	D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	<D-H···A (°)	Symmetry
Compound 1	O(1)-H(1A)···O(5)	1.00(8)	1.69(8)	2.688(6)	173(8)	1-x,1-y,1-z
	O(2)-H(2B)···O(3)	1.00(7)	1.72(7)	2.712(6)	178(8)	-x,1-y,1-z
Compound 2	O(1)-H(1B)···O(2)	0.88(4)	1.85(4)	2.727(3)	175(5)	-1/2+x,3/2-y,-1/2+z

Table S5 C-H···π interactions in **1** and **2**.

	C-H→ ring(j)	H···R distance (Å)	C-H···R angle(deg)	C···R distance (Å)
Compound 1	C(12)-H(12)→R(1)	3.375	157.27	4.248
	C(16)-H(16)→R(1)	3.306	151.36	4.146
	C(7)-H(7)→R(2)	3.188	151.81	4.031
	C(8)-H(8)→R(3)	3.506	159.05	4.388
	C(10)-H(10)→R(3)	3.382	152.12	4.225
	C(11)-H(11)→R(2)	3.410	160.41	4.300
Compound 2	C(8)-H(8)→R(4)	3.251	155.02	4.112
	C(5)-H(5)→R(5)	3.169	154.16	4.026
	C(6)-H(6)→R(6)	3.409	155.52	4.272

R(j) denotes the j-th ring: R(1) = N(1)/C(1)/C(2)/C(3)/C(4)/C(5); R(2)= C(17)/C(18)/C(19)/C(20)/C(21)/C(22); R(3) = N(2)/C(12)/C(13)/C(14)/C(15)/C(16); R(4)= N(1)/C(1)/C(2)/C(3)/C(2)/C(1); R(5) = C(11)/C(12)/C(13)/C(14)/C(13)/C(12); R(6) = C(10)/C(9)/C(8)/N(2)/C(8)/C(9)

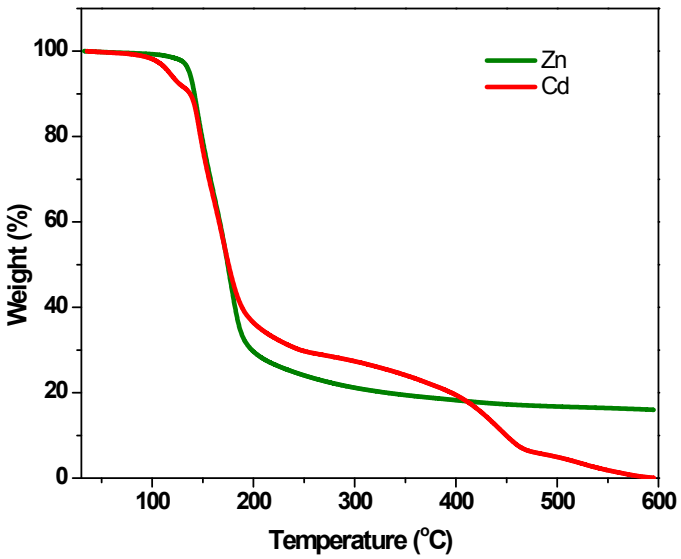

Fig. S3 TGA plots of compounds **1** (red) and **2** (green) measured under N_2 atmosphere.

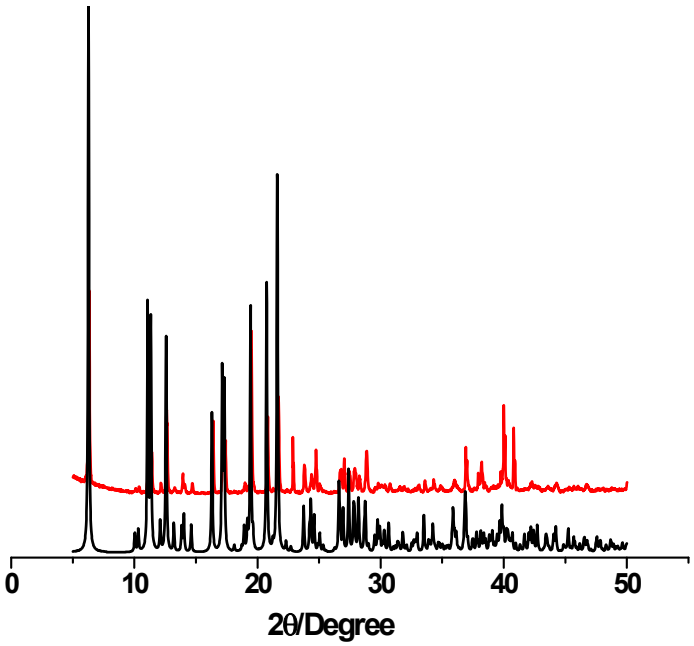

Fig. S4 Powder X-ray diffraction patterns of simulated **1** (black) and as-synthesized **1** (red).

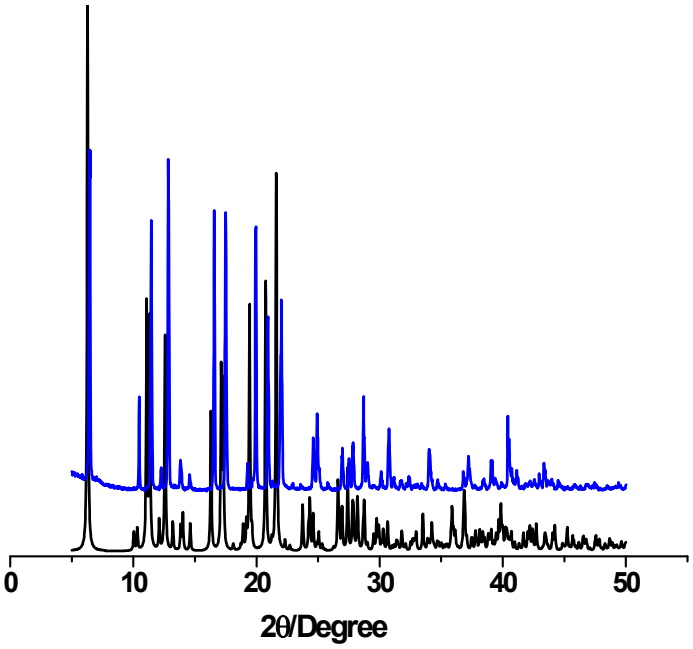

Fig. S5 Powder X-ray diffraction patterns of simulated **2** (black) and as-synthesized **2** (blue).

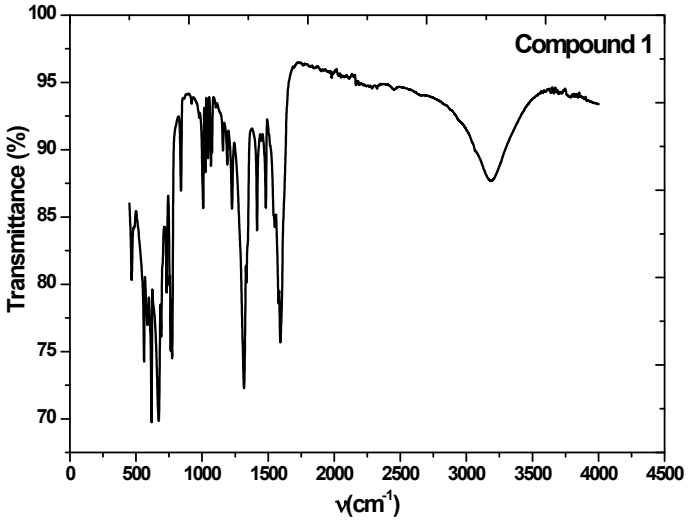

Fig. S6 FT-IR spectra of compound **1**.

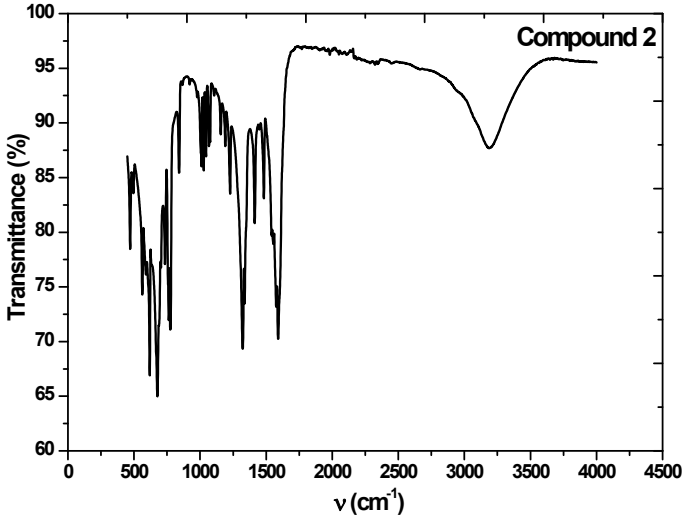

Fig. S7 FT-IR spectra of compound **2**.