Electronic Supplementary Material (ESI) for Dalton Transactions.

Tuning of *para*- position of pyridyl ligands impacts the electrical properties of a series of Cd(II) ladder polymers

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Supporting Information

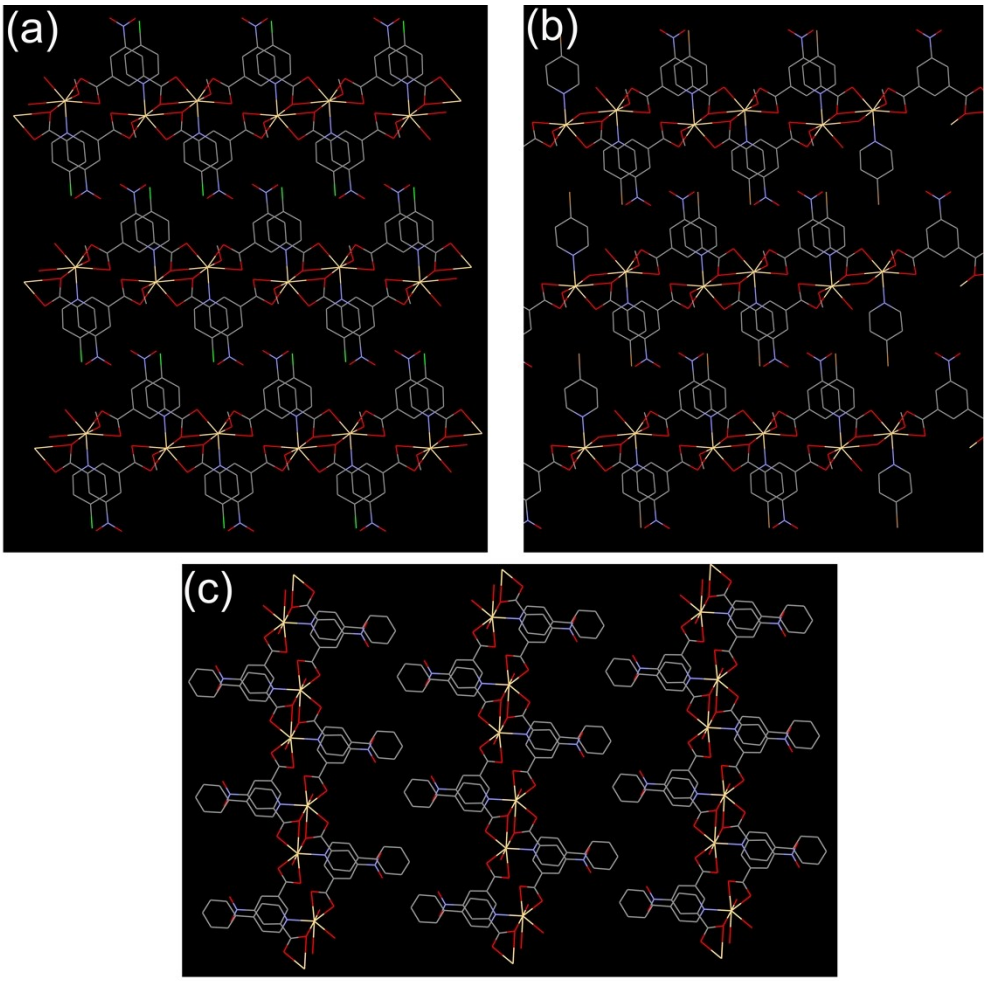

Fig. S1. Packing of compound (a) **1**, (b) **2** and (c) **3** along *a*-axis.

Table S1 Crystal data and refinement parameters for compound **1–3**

Formula	$C_{14}H_{11}CdClN_2O_7$	$C_{14}H_{11}BrCdN_2O_7$	$C_{22}H_{18}CdN_3O_{11}$
fw	467.11	511.56	612.80
crystsyst	triclinic	triclinic	triclinic
space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a (Å)	7.8063(3)	7.8129(3)	7.6232(10)
b (Å)	9.7610(4)	9.7506(4)	9.9666(13)
c (Å)	11.7162(5)	11.6897(4)	16.928(2)
α(deg)	83.121(2)	83.522(2)	89.741(4)
β(deg)	79.771(2)	80.158(2)	84.003(4)
γ (deg)	69.765(2)	69.809(2)	69.226(3)
V (Å^3)	822.68(6)	822.10(6)	1195.2(3)
Z	2	2	2
D_{calcd}(g/cm^3)	1.886	2.067	1.703
μ(mm^{-1})	1.530	3.799	0.981
λ(Å)	0.71073	0.71073	0.71073
data[$I > 2\sigma(I)$]/params	2872/231	2873/231	4024/336
GOF on F^2	1.009	0.802	1.183
final R indices[$I > 2\sigma(I)$][a,b]	$R1$ = 0.0222 $wR2$ = 0.0575	$R1$ = 0.0366 $wR2$ = 0.1100	$R1$ = 0.1201 $wR2$ = 0.3090

[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**

Cd01-O1	2.260(2)	Cd01-N1	2.316(2)
Cd01-O3_b	2.6429(19)	O1-Cd01-O2	53.52(7)
Cd01-O2	2.5774(19)	O1-Cd01-C7	26.54(7)
Cd01-O4_b	2.284(2)	O1-Cd01-O3_c	89.23(8)
Cd01-O7	2.311(3)	O2-Cd01-C7	26.99(7)
Cd01-O3_c	2.388(2)	O2-Cd01-O3_c	94.53(7)
O7-Cd01-O3_b	102.57(9)	N1-Cd01-O3_b	84.68(6)
N1-Cd01-C7	115.36(7)	C7-Cd01-O3_b	156.72(7)
N1-Cd01-O3_c	87.78(8)	O3_b-Cd01-O4_b	52.55(7)
C7-Cd01-O3_c	92.51(7)	Cd01-O1-C7	99.41(16)
O4_b-Cd01-O3_c	100.65(7)	Cd01-O7-C14	128.6(2)
Cd01-N1-C13	122.00(19)	Cd01-C7-C1	171.61(17)
Cd01-C7-O2	68.65(14)	O1-Cd01-N1	141.53(7)
O1-Cd01-O7	97.03(9)	O1-Cd01-O4_b	86.80(8)
O1-Cd01-O3_b	131.39(7	O2-Cd01-N1	88.52(7)
O2-Cd01-O7	86.22(9)	O2-Cd01-O4_b	137.29(7)
O2-Cd01-O3_b	168.33(7)	O7-Cd01-C7	91.44(9)
O7-Cd01-N1	84.96(8)	O7-Cd01-O3_c	172.68(8)
O7-Cd01-O4_b	83.54(9)	N1-Cd01-O4_b	131.39(8)
Cd01-O2-C7	84.37(15)	C7-Cd01-O4_b	112.00(7)
Cd01_a-O3-Cd01_c	104.23(8)	O3_b-Cd01-O3_c	75.77(7)
Cd01-N1-C9	121.15(19)	Cd01-C7-O1	54.05(14)

Symmetry Code: b = 1+x, -1+y, z; c = -x, 1-y, 1-z

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

Cd01-O1	2.263(4)	C7-Cd01-O6_c	92.77(13)
Cd01-O5_b	2.285(4)	O6_b-Cd01-O6_c	75.51(12)
Cd01-O2	2.569(4)	Cd01_a-O6-Cd01_c	104.49(13)
Cd01-O6_b	2.656(4)	Cd01-N2-C13	121.3(3)
Cd01-O7	2.312(5)	Cd01-C7-O2	68.3(3)
Cd01-O6_c	2.379(4)	Cd01-O7-H2M	130(7)
Cd01-N2	2.307(4)	O1-Cd01-O7	96.72(15)
O1-Cd01-O2	53.74(12)	O1-Cd01-O5_b	86.66(13)
O1-Cd01-C7	26.73(13)	O2-Cd01-O7	86.46(15)
O1-Cd01-O6_c	89.77(13)	O2-Cd01-O5_b	137.62(12)
O2-Cd01-C7	27.02(12)	O7-Cd01-N2	84.79(15)
O2-Cd01-O6_c	94.38(13)	O7-Cd01-O6_b	102.73(14)
O7-Cd01-O5_b	83.70(15)	N2-Cd01-O5_b	131.30(14)
N2-Cd01-C7	115.29(13)	C7-Cd01-O5_b	112.14(13)
O5_b-Cd01-O6_b	52.22(12)	O2-Cd01-O6_b	168.09(11)
Cd01-O1-C7	99.0(3)	O7-Cd01-C7	91.36(16)
Cd01-O7-C14	128.6(4)	O7-Cd01-O6_c	172.48(14)
Cd01-C7-C1	171.9(3)	N2-Cd01-O6_b	84.99(12)
O2-Cd01-N2	88.38(12)	C7-Cd01-O6_b	156.51(12)
O5_b-Cd01-O6_c	100.52(13)	Cd01-N2-C9	121.0(3)
Cd01-O2-C7	84.7(3)	Cd01-C7-O1	54.3(2)

Symmetry Code: a = -1+x, 1+y, z b = 1+x, -1+y, z; c = 1-x, 2-y, 1-z

Table S4 Selected bond lengths and bond angles in **3**

Cd(1)-O(5)	2.537(11)	O(14)-Cd(1)-O(4)b	83.3(5)
Cd(1)-O(3)b	2.721(11)	N(4')-Cd(1)-O(4)b	133.9(5)
Cd(1)-O(6)	2.316(12)	O(3)b-Cd(1)-O(3)c	72.1(4)
Cd(1)-O(4)b	2.243(12)	Cd(1)-O(5)-C(12)	86.9(9)
Cd(1)- O(14)	2.307(16)	Cd(1)-N(4')-C(5)	120.1(11)
Cd(1)-O(3)c	2.412(12)	O(5)-Cd(1)-N(4')	86.6(4)
Cd(1)-N(4')	2.281(14)	O(5)-Cd(1)-O(3)c	101.0(4)
O(5)-Cd(1)-O(6)	53.9(4)	O(6)-Cd(1)-O(3)b	131.4(4)
O(5)-Cd(1)-O(3)b	170.5(4)	O(14)-Cd(1)-N(4')	86.6(6)
O(6)- Cd(1)-O(14)	96.8(5)	O(14)-Cd(1)-O(3)c	171.8(5)
O(6)-Cd(1)-O(4)b	86.4(4)	N(4')-Cd(1)-O(3)c	88.6(5)
O(14)-Cd(1)-O(3)b	101.0(5)	O(4)b-Cd(1)-O(3)c	95.3(4)
N(4')-Cd(1)-O(3)b	86.7(4)	Cd(1)a-O(3) -Cd(1)c	107.9(5)
O(3)b-Cd(1)-O(4)b	51.9(4)	Cd(1)-O(6)-C(12)	97.3(10)
Cd(1)-N(4')-C(1)	120.3(11)	O(6)-Cd(1)-O(3)c	91.2(4)
O(5)-Cd(1)-O(14)	85.3(5)	O(6)-Cd(1)-N(4')	139.6(5)
O(5)-Cd(1)-O(4)b	136.8(4)		

Symmetry Code: b = 1+x,-1+y, z; c = 1-x, 1-y, 1-z

Table S5 π···π interaction parameters in **1-3**

	Cg →Cg	**Cg-Cg (Å)**	**π rings are:**
Compound **1**	Cg1 -> Cg2	3.8144(19)	Cg(1)= N1->C9-> C10 ->C11->C12-> C13 Cg(2)= C1->C2->C3 ->C4->C5 ->C6
Compound **2**	Cg1 -> Cg2	3.815(3)	Cg(1)= N2-> C9-> C10 -> C11->C12->C13 Cg(2)= C1->C2->C3-> C4->C5 ->C6
Compound **3**	Cg(2)-> Cg(4)	3.780(10)	Cg(2)= N4'->C1->C2->C3 ->C4->C5 Cg(4)= C(13) -> C(14) -> C(15) -> C(16)-> C(18) ->C(17)

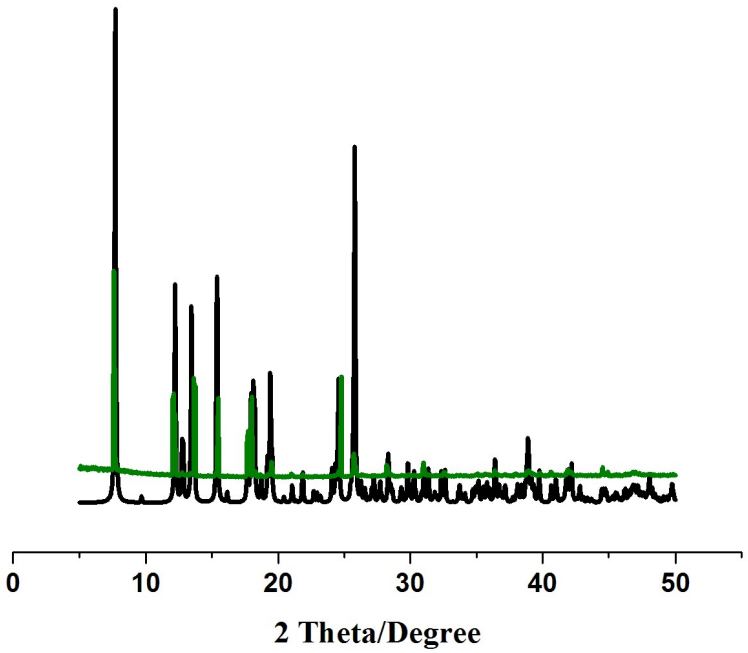

Fig. S1. PXRD patterns of (a) simulated **1** (black) and (b) as-synthesized **1** (olive).

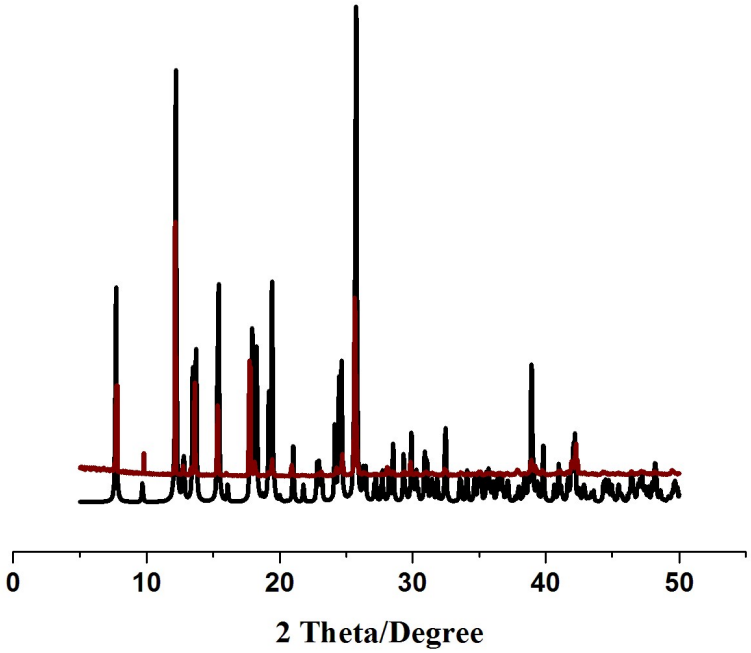

Fig. S2. PXRD patterns of (a) simulated **2** (black) and (b) as-synthesized **2** (wine).

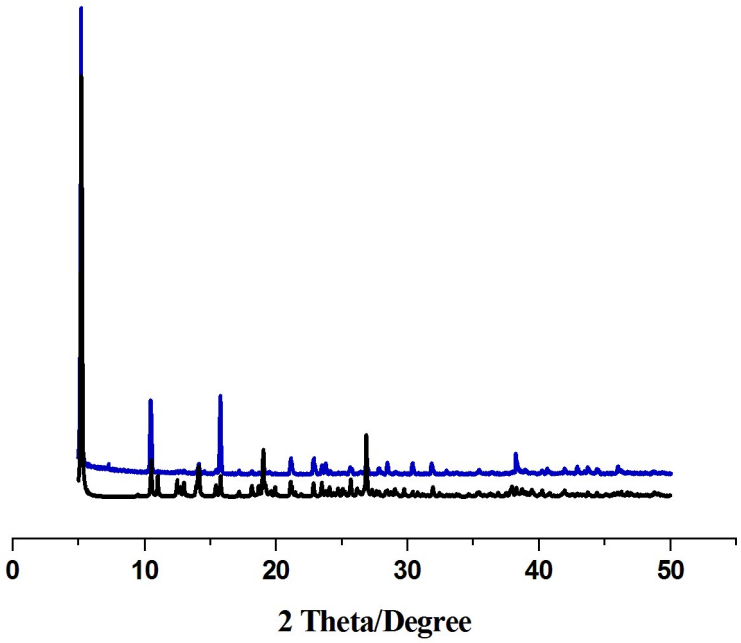

Fig. S3. PXRD patterns of (a) simulated **3** (black) and (b) as-synthesized **3** (blue).

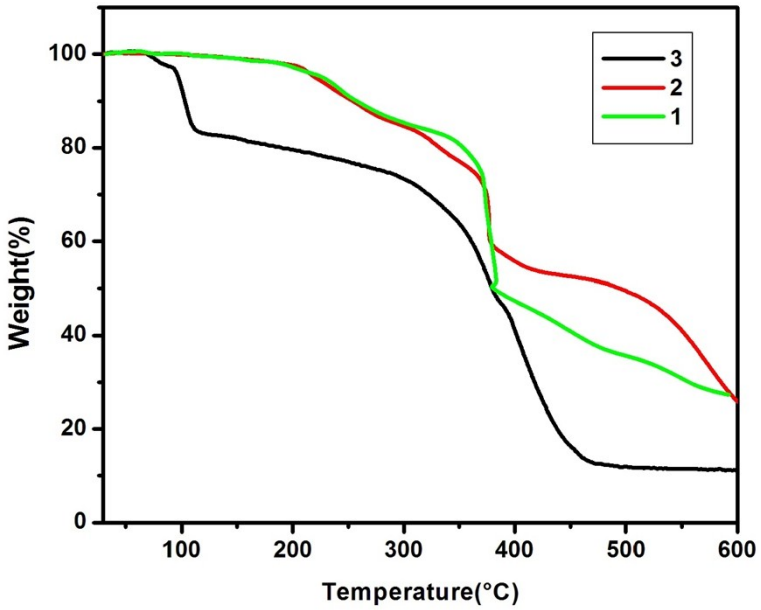

Fig. S4. TGA plots of **1** (green) and **2** (red) and **3** (black).

Table S5 Comparison of electrical conductivity data of some selected CPs

Compound	**Band Gap**	**Electrical Conductivity (S m−1)**	**References**
[Cd(2,2'-dsb)(4-nvp)(DMF)(H_2O)]	3.28 eV	6.60×10^{-4}	1
[Cd(adc)(4-nvp)$_2$(H_2O)]$_n$	3.33 eV	1.83×10^{-3}	2
[Cd(adc)(4-nvp)-(rctt-4-pncb)$_{1/2}$(H_2O)]$_n$	3.21 eV	3.91×10^{-3}	2
{[Cd(azbpy)(suc)]·$_2$(H_2O)}$_n$	2.00	3.2×10^{-3}	3
{[Cd(azbpy)-(msuc)]·2.5(H_2O)}$_n$	1.90	2.64×10^{-3}	3
{[Cd(azbpy)(mglu)]·5(H_2O)}$_n$	1.95	1.29×10^{-3}	3
{[Cd$_{1.5}$(azbpy)$_2$(glu)]·(NO_3)·MeOH}$_n$	1.92	2.07×10^{-3}	3
[Cd(4-bpd)($SCN)_2$]$_n$	2.25	2.90×10^{-4}	4
[Cd(quin)$_2$(rctt-4-pncb)]$_n$	4.08	8.84×10^{-6}	5

References

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