Linear dicarboxylate based pyridyl appended cobalt(II) coordination polymers in search of opto-electronic properties

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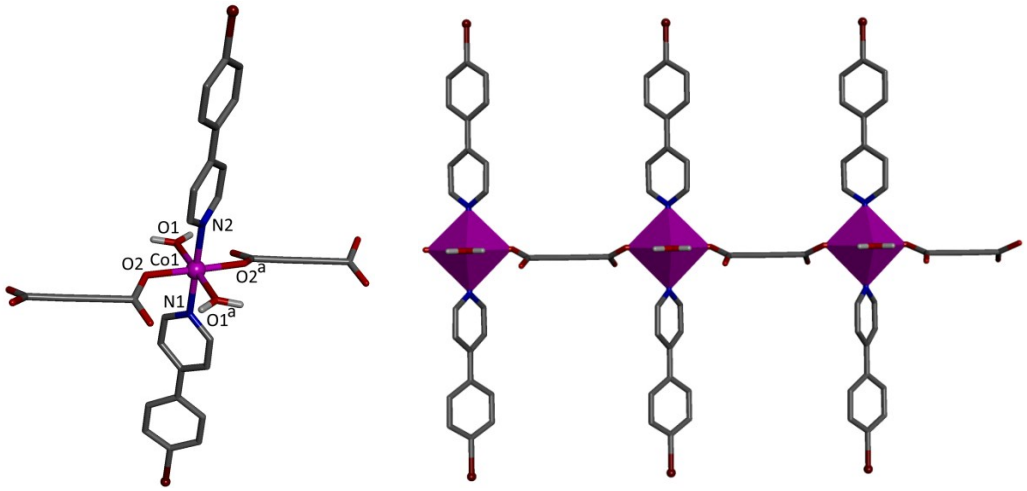
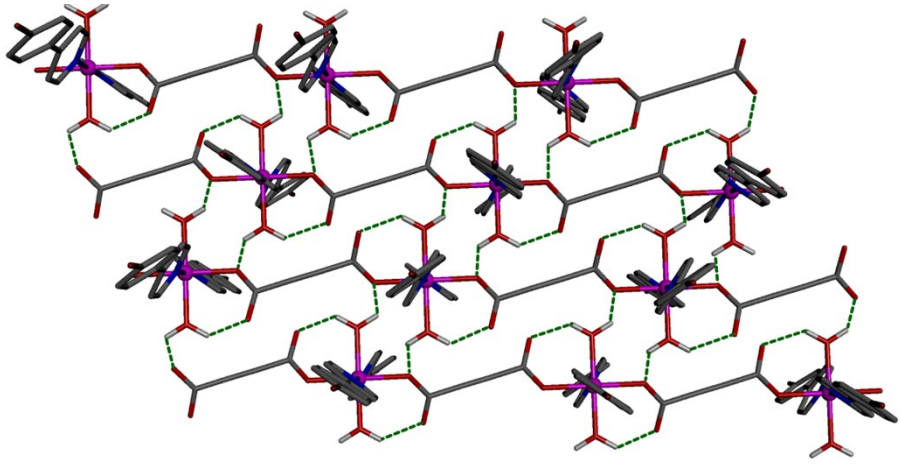
Supporting Information



(a) (b)



(c)

Fig. S1 (a) Basic unit of compound **2**. (b) A portion of 1D CP of **2**. (c) View of 2D sheet formed by hydrogen bonding interactions in **2**. Symmetry related a = 1-x, y, 3/2-z.

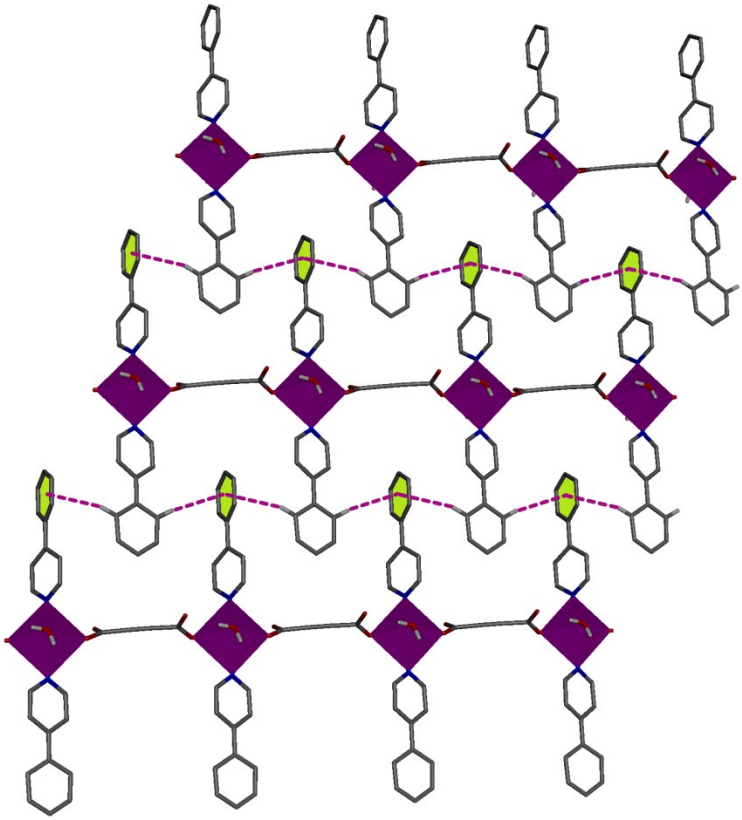


Fig. S2 C-H···π interactions among the pyridyl ligands with edge-to-face distance 3.70 Å in **1** forming 2D layer.

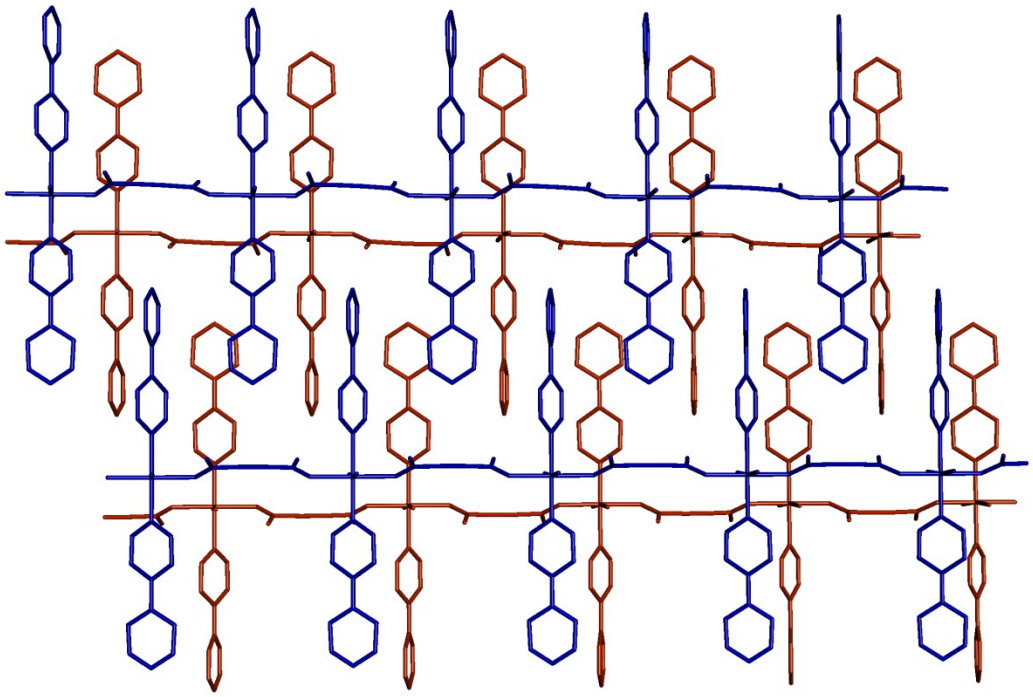


Fig. S3 A view of 3D supramolecular aggregate in compound **1** via hydrogen bonding and CH···π interactions.

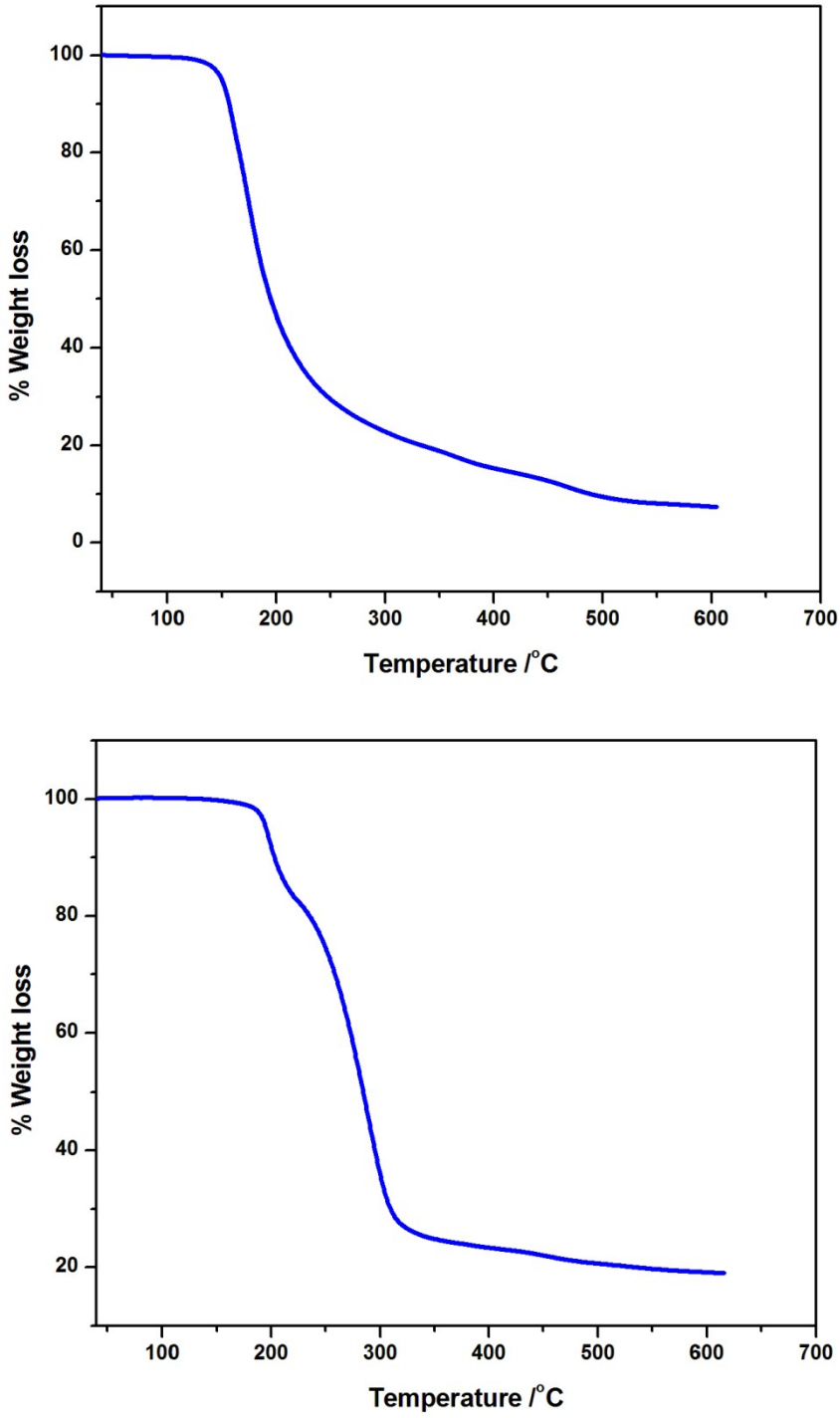


Fig. S4 TGA plot of compound **1** (above) and **2** (below) measured under N_2 atmosphere.

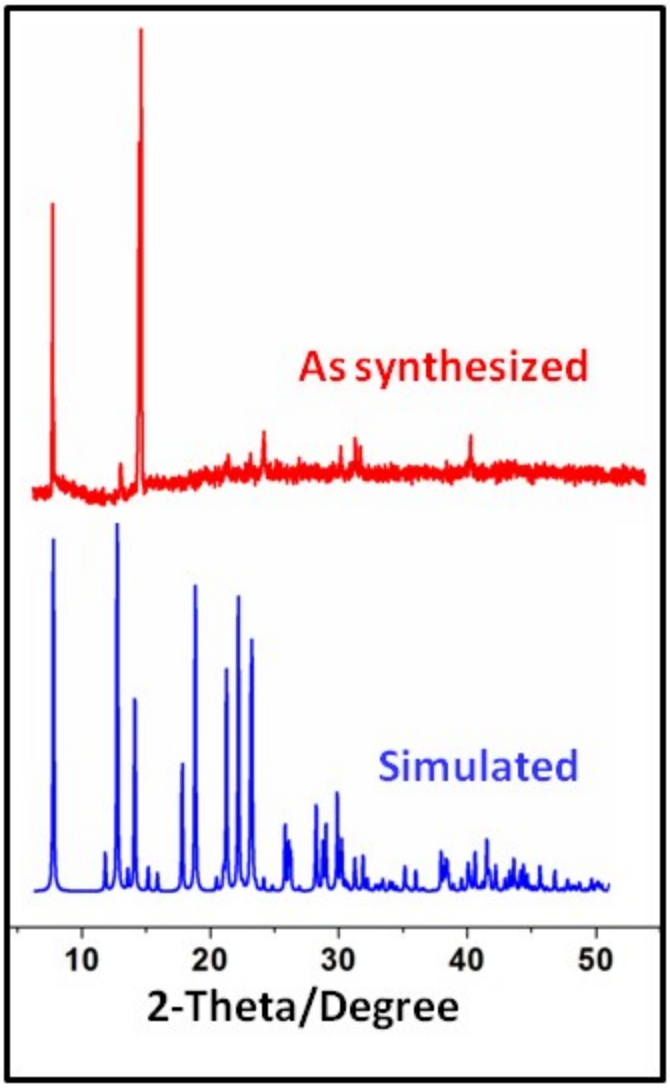


Fig. S5 PXRD patterns of simulated **1** (blue) and as-synthesized **1** (red).

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

Formula	$C_{26}H_{22}CoN_2O_6$ (**1**)	$C_{26}H_{20}Br_2CoN_2O_7$ (**2**)
Fw	517.39	691.19
cryst syst	Monoclinic	Monoclinic
space group	*C 2/c*	*C 2/c*
a (Å)	9.8195(3)	9.3188(6)
b (Å)	27.7518(10)	33.926(2)
c (Å)	9.3876(3)	9.8051(6)
α(deg)	90	90
β(deg)	115.091(1)	117.483(3)
γ (deg)	90	90
V (Å^3)	2316.80(13)	2750.1(3)
Z	4	4
D_{calcd}(g/cm^3)	1.483	1.669
μ(mm^{-1})	0.787	3.576
λ(Å)	0.71073	0.71073
data[$I > 2\sigma(I)$]/params	2028/167	2422/178
GOF on F^2	1.071	1.077
final *R* indices[$I > 2\sigma(I)$][a,b]	$R1 = 0.0762$	$R1 = 0.0778$
	$wR2 = 0.2022$	$wR2 = 0.2630$

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

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

bond lengths (Å)			
Co(1)-O(1)	2.097(3)	Co(1)-O(2)	2.119(3)
Co(1)-N(1)	2.141(6)	Co(1)-N(2)	2.144(6)
Co(1)-O(1)^{b}	2.097(3)	Co(1)-O(2)^{b}	2.119(3)
bond angles (°)			
O(1) -Co(1)-O(2)	90.32(15)	O(1)-Co(1) -N(1)	93.35(10)
O(1) -Co(1)-N2	86.65(10)	O(1) -Co(1) -O(1)^{b}	173.31(15)
O(1)-Co(1) -O(2)^{b}	89.65(15)	O(2) -Co(1)-N(1)	90.25(9)
O(2)-Co(1)-N(2)	89.75(9)	O(1)b-Co(1)-O(2)	89.65(15)
O(2)-Co(1)-O(2)^{b}	179.51(14)	N(1)-Co(1)-N(2)	179.98(3)
O(1)b-Co(1)-N(1)	93.35(10)	O(2)b-Co(1)-N(1)	90.25(9)
O(1)b-Co(1)-N(2)	86.65(10)	O(2)b-Co(1)-N(2)	89.75(9)
O(1)b-Co(1)-O(2)^{b}	90.32(15)		

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

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

bond lengths (Å)			
Co(1) -O(1)	2.103(5)	Co(1) -O(2)	2.108(4)
Co(1) -N(1)	2.126(10)	Co(1) -N(2)	2.149(7)
Co(1) -O(1) [b]	2.103(5)	Co(1)-O(2) [b]	2.108(4)
bond angles (°)			
O(1) -Co(1) -O(2)	89.51(19)	O(1) -Co(1)-N(1)	91.35(13)
O(1) -Co(1) -N(2)	88.65(13)	O(1)-Co(1) -O(1)[b]	177.3(2)
O(1) Co(1) -O(2)[b]	90.5(2)	O(2) -Co(1) -N(1)	89.32(13)
O2-Co(1) –N(2)	90.68(13)	O(1)[b] -Co(1) -O(2)	90.52(19)
O(2)-Co(1)-O(2) [b]	178.6(2)	N(1)-Co(1)-N(2)	180.00(1)
O(1)b -Co(1)-N(1)	91.35(13)	O(2)[b] -Co(1) -N(1)	89.32(13)
O1(b) -Co(1) -N(2)	88.65(13)	O(2)[b]-Co(1)-N(2)	90.68(13)
O(1)b-Co(1)-O(2) [b]	89.51(19)		

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

Table S4 Hydrogen bonding interactions of compound **1** and **2**.

Compound	D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	<D-H···A (°)
1	O(1) – H(1A)···O(2)	0.8800	1.9800	2.731(5)	144.00
	O(1)--H(1B) ···O(3)	0.8700	1.9400	2.712(6)	146.00
2	O(1)—H(1B)···O(2)	0.9300	2.3500	2.778(7)	108.00
	O(1) – H(1B)···N(1)	0.9300	2.6100	3.540(4)	176.00
	O(1)—H(2A)···O(3)	0.9300	2.0400	2.718(7)	129.00

Table S5: The values of simulated parameters of impedance analysis for **1** and **2**.

Compound	**R_s (Ω)**	**R_P (Ω)**	**C_P (F)**
1	13.54	3391.54	1.71×10^{-11}
2	38.69	20097.5	1.63×10^{-11}