Supplementary information

Isostructural coordination polymers of tethering naphthalene anchored bis(2-methylpyridinecarboxamide) ligand: Single crystal, XPS, EDS and theoretical studies

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Table of contents

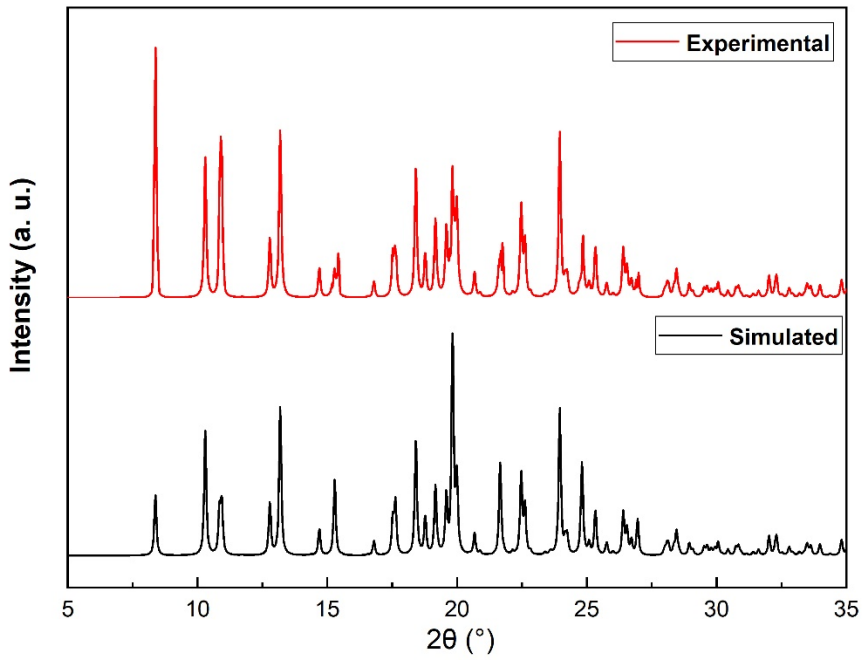

Figure S1 Shows the comparison of powder patterns of compound **1**.

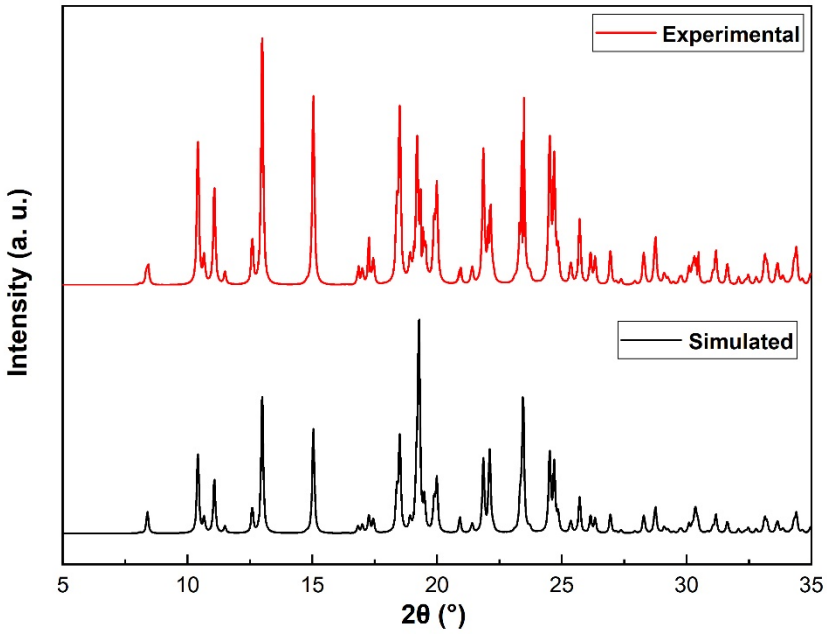

Figure S2 Shows the comparison of powder patterns of compound **2**.

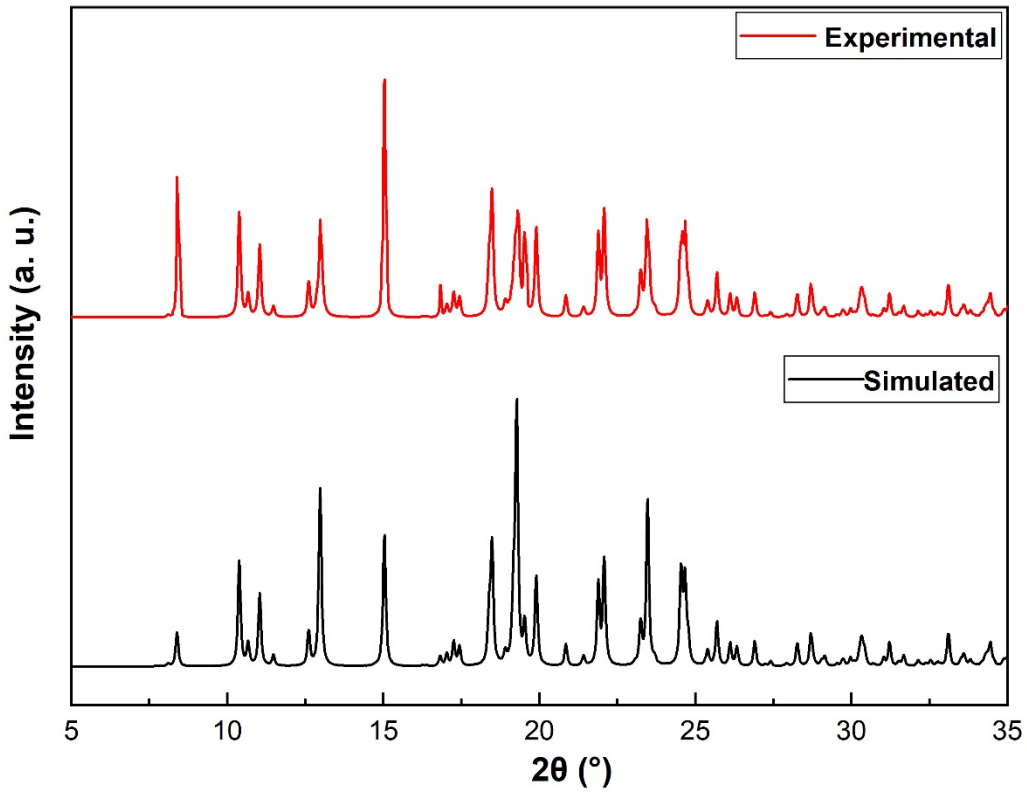

Figure S3 Shows the comparison of powder patterns of compound **3**.

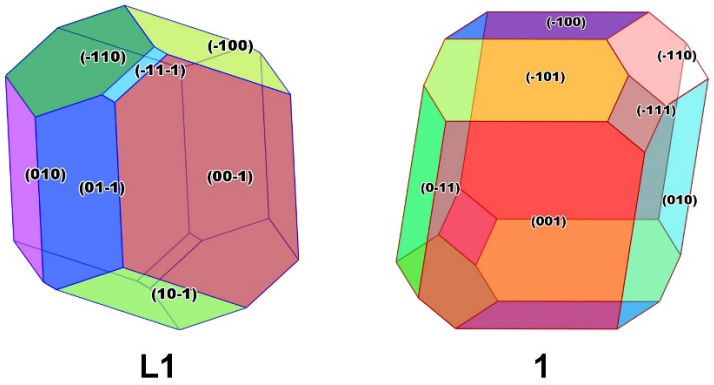

Figure S4 BFDH morphologies of **L1** and compound **1**.

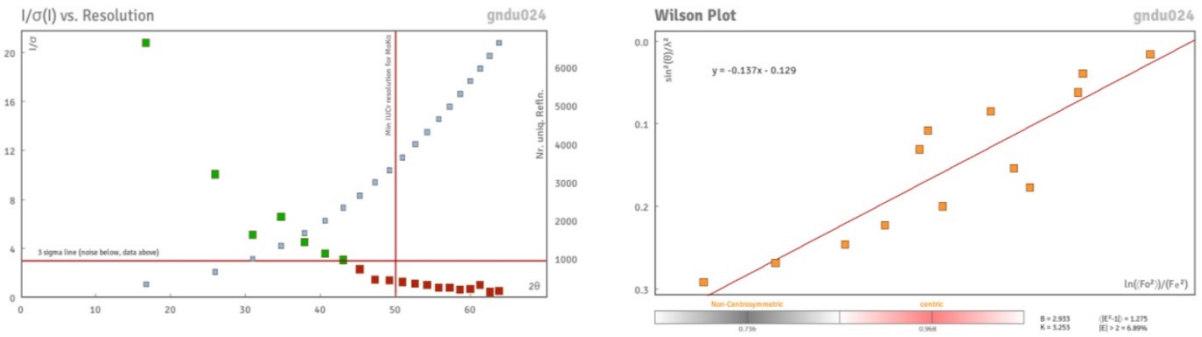

Figure S5 Diffraction data plots showing noise at higher angles (I/σ(I) vs resolution plot) and poor quality of data (large deviation from straight line in Wilson plot).

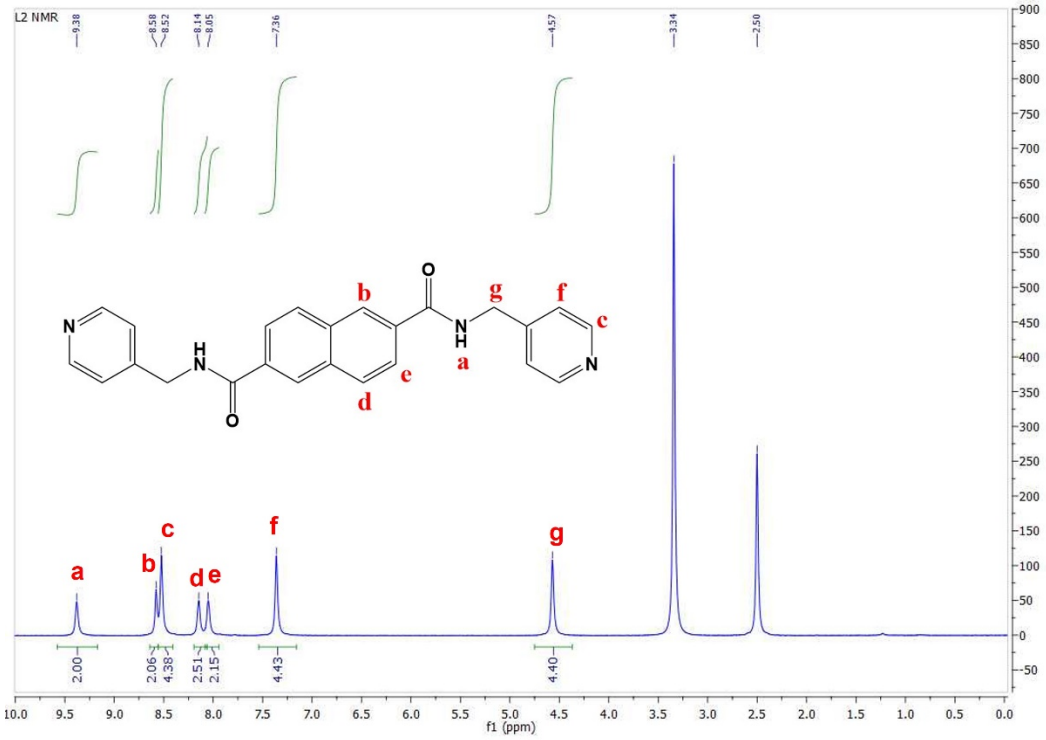

Figure S6 ^{1}H-NMR of **L1**.

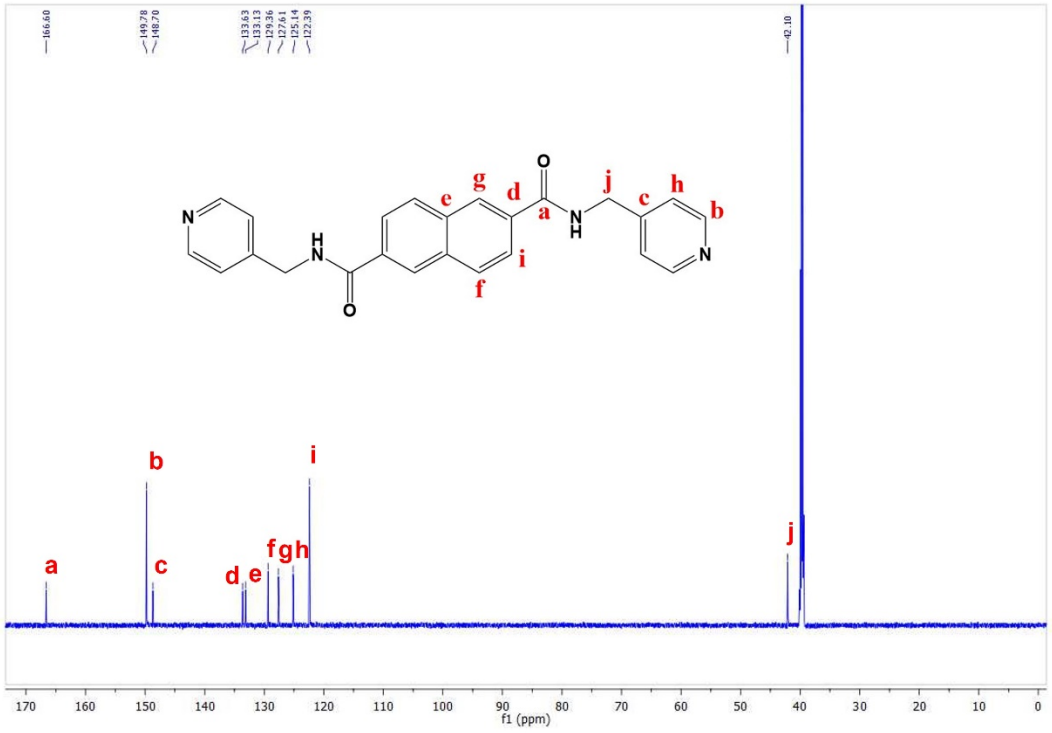

Figure S7 ^{13}C-NMR of **L1**.

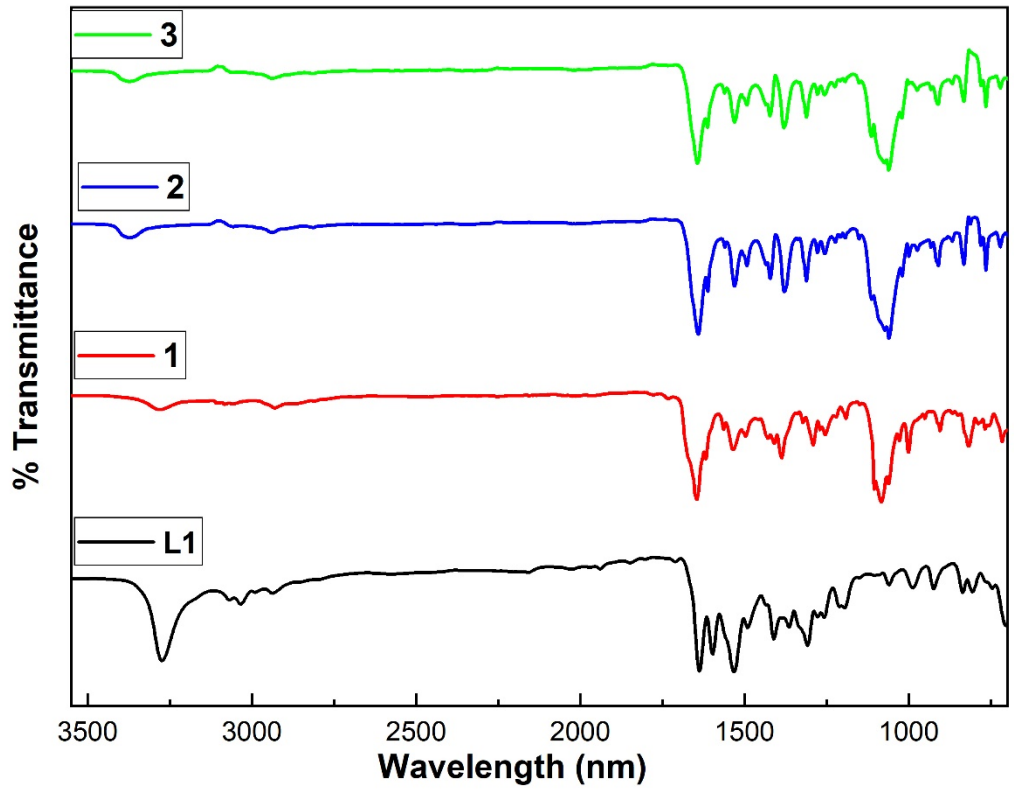

Figure S8 IR spectra comparison involving **L1** and compounds **1**, **2**, and **3**.

Table S1 – Characterstic IR peaks for **L1** and compounds **1**, **2**, and **3**.

Complex	Group	Functionality	Wavenumber (cm^{-1})
L1	ν $(O\text{-}H)_{Stretching}$	Water	3272 (s)
	ν $(N\text{-}H)_{Stretching}$	Amide	3068 (w,b)
	ν (C=O)	Amide	1639 (s)
	ν (C=N)	Pyridine	1597 (s)
	ν (C=C)	Pyridine	1533 (b)
	ν $(C\text{-}H)_{Stretching}$	Methylene	2937(m)
	ν (C=C)	Naphthalene	1487 (w)
1	ν (N-H)	Amide	3076 (w)
	ν (C=O)	Amide	1645 (s)
	ν (C=N)	Pyridine	1615 (w)
	ν (C=C)	Pyridine	1532 (m, b)
	ν $(C\text{-}H)_{Stretching}$	Methylene	2932 (vw)
	ν (C=C)	Naphthalene	1494 (w)
	ν (Cl-O)	Perchlorate	**1060 (w)**
			1081 (m)
			1105 (w)
2	ν (N-H)	Amide	3069 (w)
	ν (C=O)	Amide	1640 (s)
	ν (C=N)	Pyridine	1611 (w)
	ν (C=C)	Pyridine	1533 (s)
	ν $(C\text{-}H)_{Stretching}$	Methylene	2940 (vw)
	ν (C=C)	Naphthalene	1493 (w)
	ν (Cl-O)	Perchlorate	**1019 (w)**
			1058 (w)
			1112 (w)
3	ν (N-H)	Amide	3071 (w)
	ν (C=O)	Amide	1643 (s)
	ν (C=N)	Pyridine	1612 (w)
	ν (C=C)	Pyridine	1529 (s)
	ν $(C\text{-}H)_{Stretching}$	Methylene	2935 (vw)
	ν (C=C)	Naphthalene	1492 (w)
	ν (Cl-O)	Perchlorate	**1021 (w)**
			1061 (w)
			1114 (w)

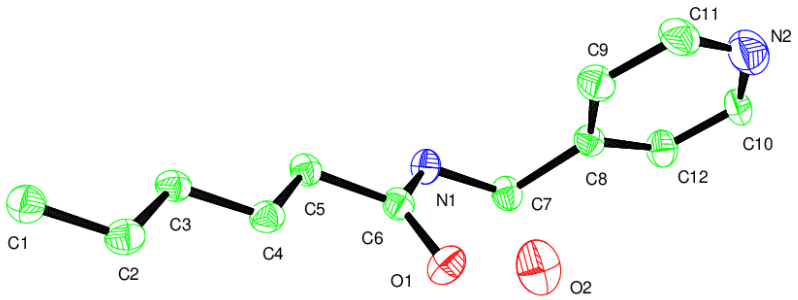

Figure S9 ORTEP diagram of **L1** drawn at 40% ellipsoidal probability (Hydrogen atoms have not been shown for clarity).

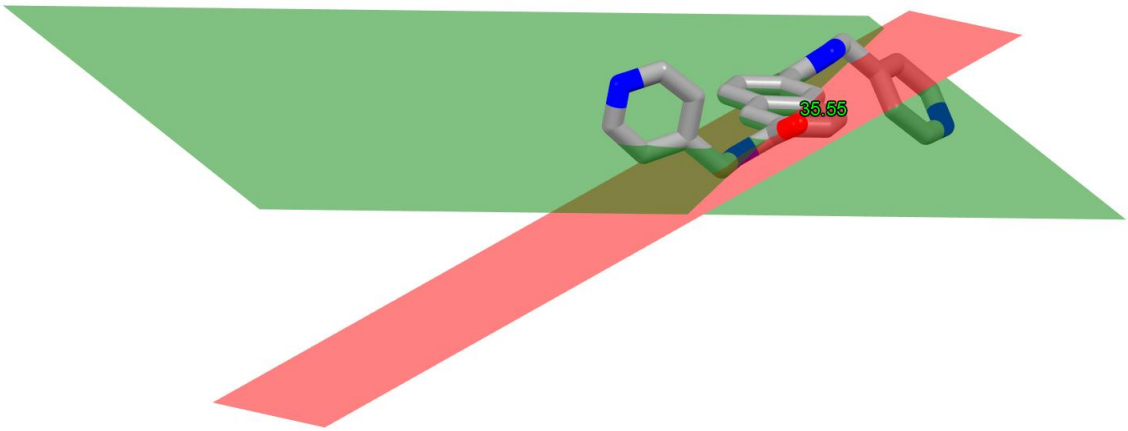

Figure S10 Showing the dihedral angle between pyridine and naphthalene ring planes of **L1**.

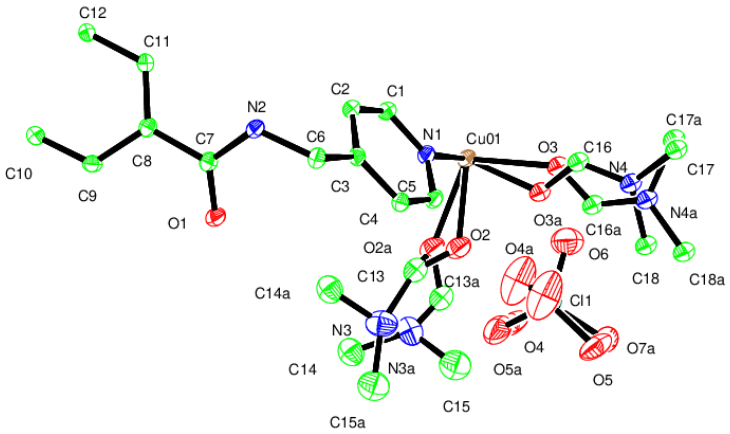

Figure S11 ORTEP diagram of compound **1** at 40% ellipsoidal probability.

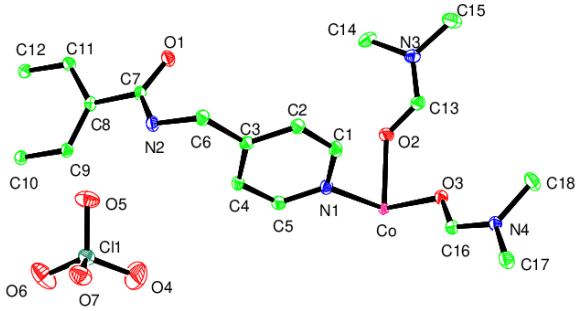

Figure S12 ORTEP diagram of compound **2** at 40% ellipsoidal probability.

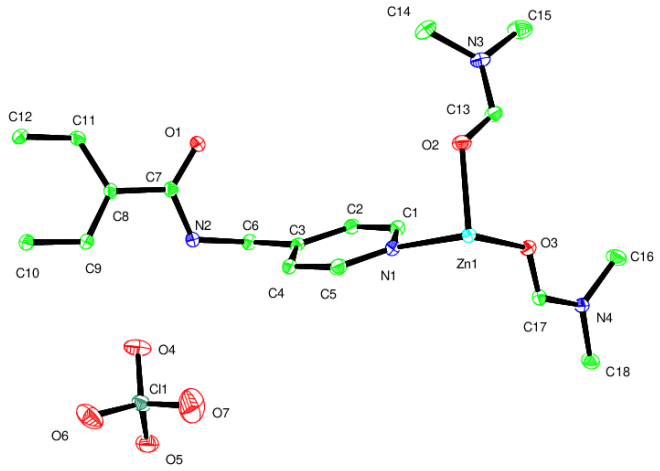

Figure S13 ORTEP diagram of compound **3** at 40% ellipsoidal probability.

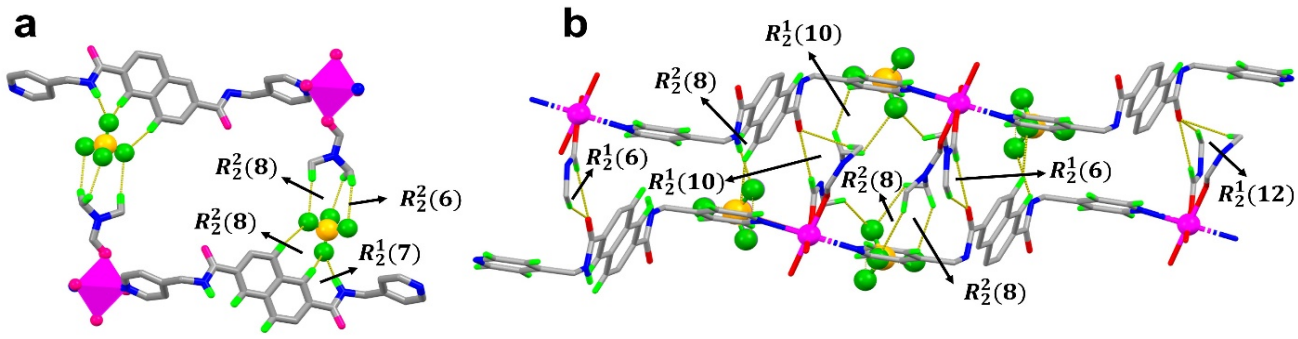

Figure S14 Supramolecular synthons generated in a 2D sheet and 3D hydrogen bonded framework of compound **1**.

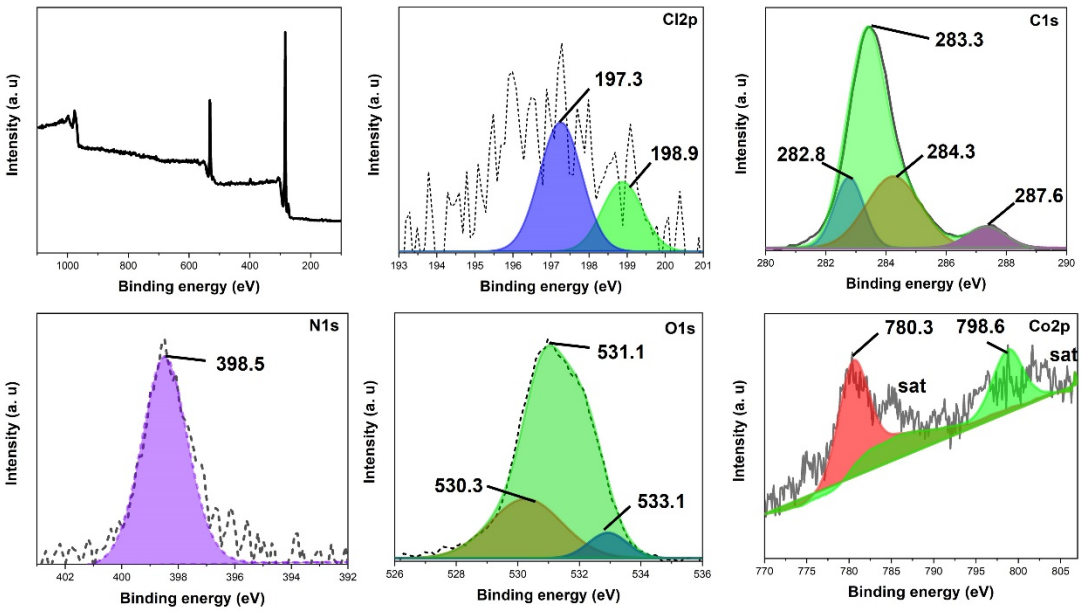

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Figure S15 XPS spectral peaks for compound **2**.

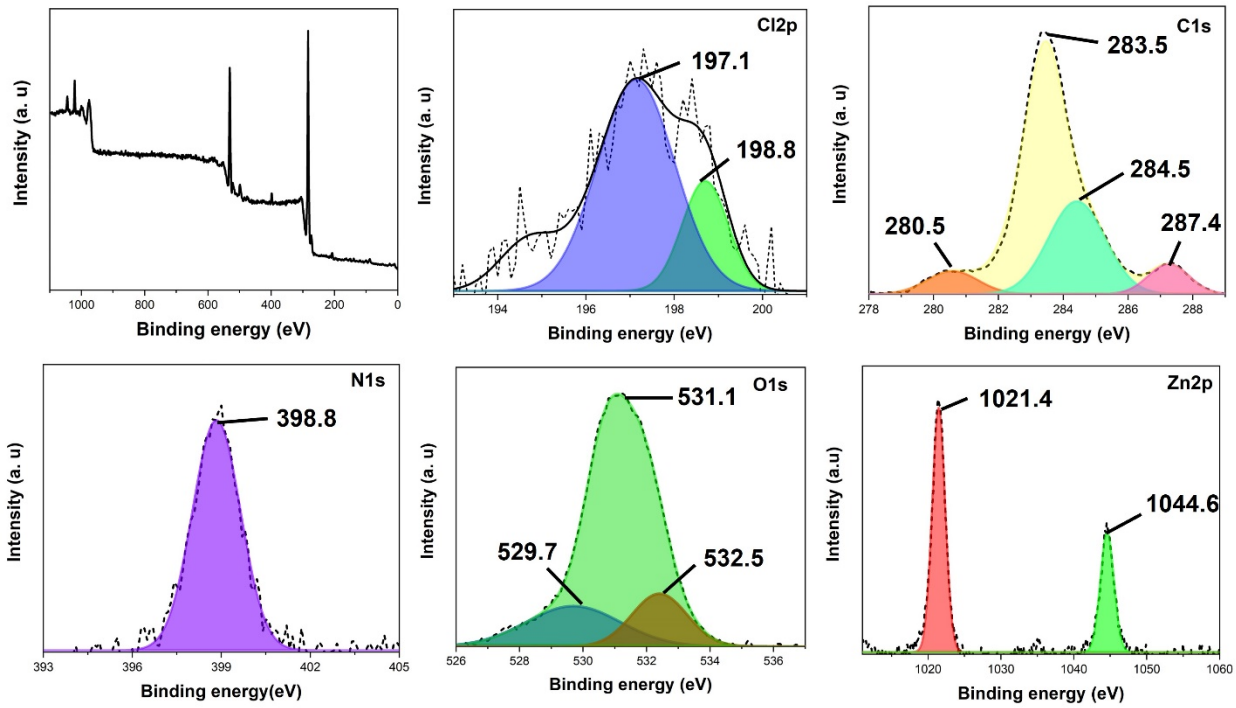

Figure S16 XPS spectral peaks for compound **3**.

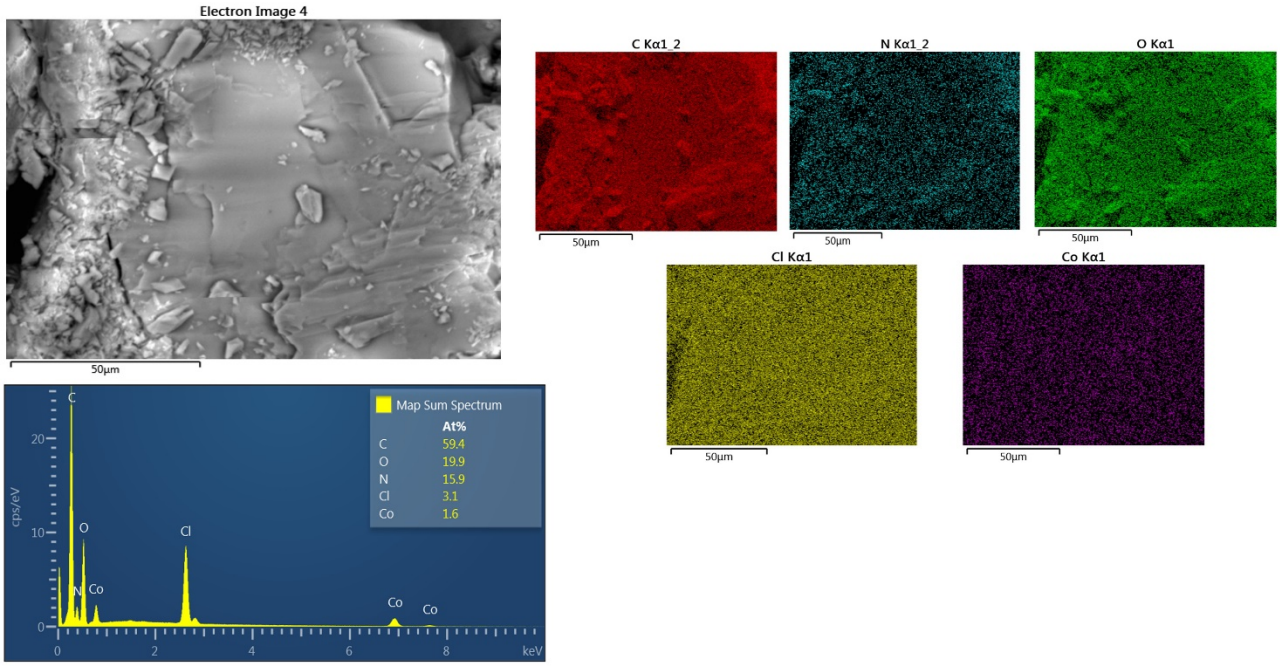

Figure S17 EDS spectra of compound **2**

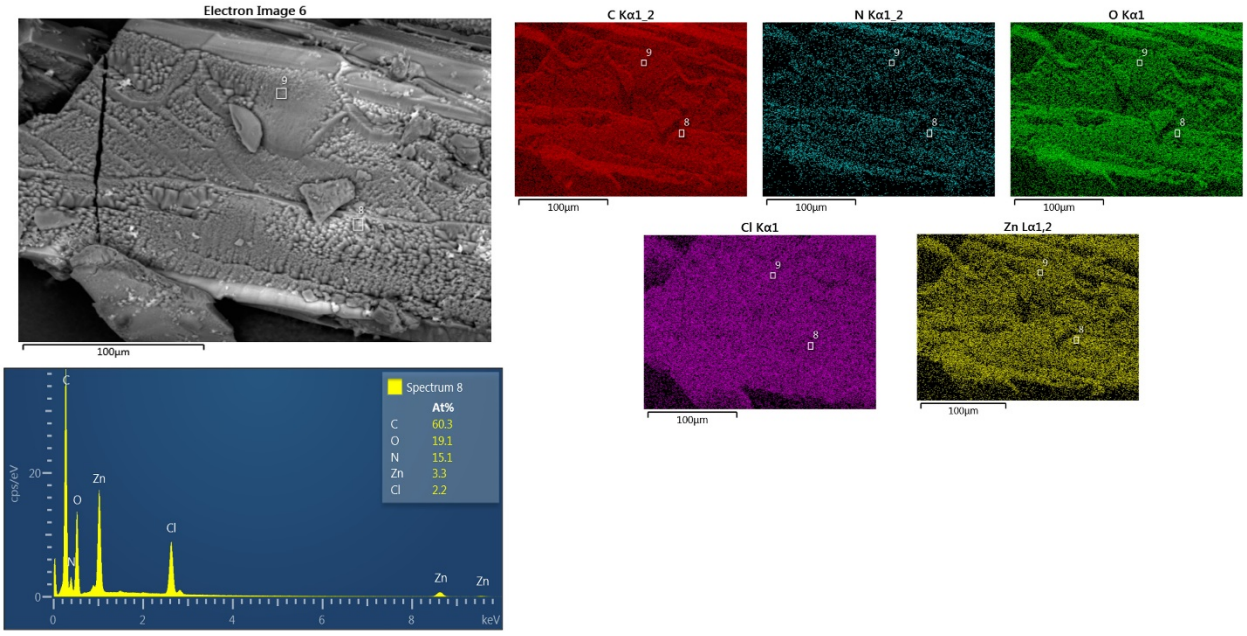

Figure S18 EDS spectra of compound **3**

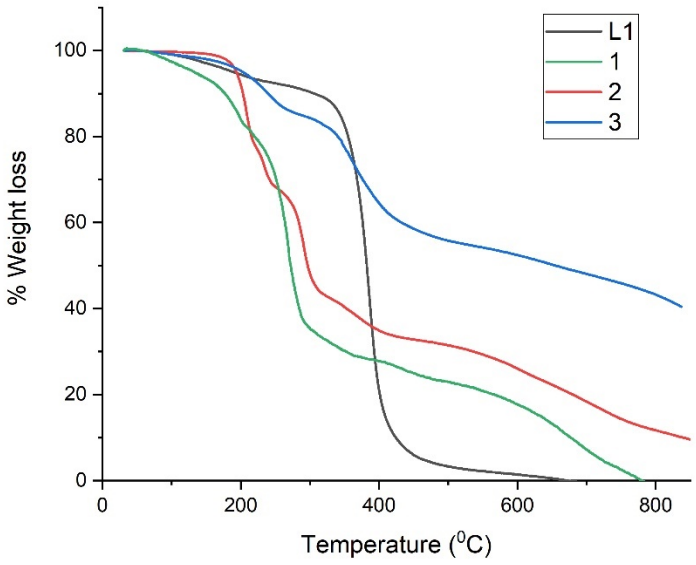

Figure S19 Thermogravimetry curves for **L1** and **1-3**.

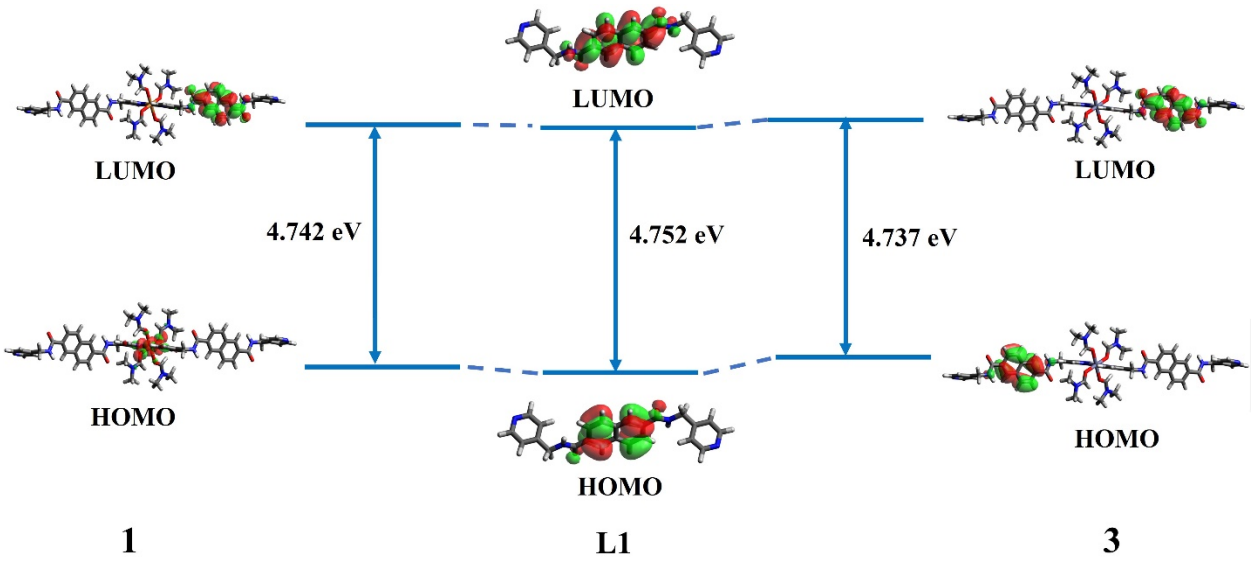

Figure S20 Variation of HOMO-LUMO energy gap in compounds **1** and **3** relative to **L1**. (Note-Tis figure is showing speculative anomaly in HOMO-LUMO energies of compounds **1** and **3** due to solvent effect of DMF. In both cases, HOMO orbitals are more affected by solvent interactions than LUMO orbitals.)

Table S2. Hydrogen bonds for **L1** [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(2)#1	0.88	2.02	2.801(4)	147.1
N(3)-H(3)...O(1)#2	0.88	2.05	2.821(4)	146.5
C(3)-H(3A)...O(2)#3	0.95	2.73	3.382(5)	126.6
C(6)-H(6)...N(2)#4	0.95	2.71	3.556(5)	149.3
C(4)-H(4)...N(2)#4	0.95	2.83	3.657(6)	145.8
C(1)-H(1A)...N(4)#5	0.95	2.68	3.538(5)	150.7
C(9)-H(9)...N(4)#5	0.95	2.86	3.681(6)	145.4
C(16)-H(16)...O(1)#6	0.95	2.84	3.640(6)	142.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1 #2 -x+1,-y+1,-z+1 #3 x+1,y,z, #4 x-1,y-1,z-1 #5 x+1,y+1,z+1 #6 -x+2,-y+2,-z+2

Table S3. Hydrogen bonds for **1** [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(3)-H(3)...O(4^a)#1	0.950	2.574	3.197	123.3
C(3)-H(3)...O(2^a)#2	0.950	2.879	3.649	137.16
C(7)-H(7b)...O(5)#3	0.990	2.989	3.590	120.21
C(9)-H(9)...O(4^a)#4	0.950	2.862	3.687	145.88
N(2)-H(2)...O(1^a)#4	0.880	2.081	2.930	160.64

C(16^b)-H(17^a)...O(2^a)#5	0.880	2.177	2.904	139.64
C(17^b)-H(17e^a)...O(3a^b)#6	0.879	2.675	3.510	159.21
C(17a^a)-H(17e^a)...O(1^a)#6	0.980	2.977	3.899	156.4
C(11)...O(11)#6	0.950	2.439	3.292	149.34
C(18b^b)-H(18a^b)...O5 #7	0.980	2.418	3.314	151.68
C(18a^b)-H(18e^a)...O5 #7	0.882	2.519	3.314	150.25
C(14a^a)-H(14c^b)...O4a^b #7	1.080	2.589	3.686	140
C(18a^a)-H(18e)...O#7	0.980	2.519	3.182	160.5
C(15a^a)-H(14b^b)...N3^b #8	1.416	2.660	3.753	131.59
C(15a^a)-H(15f^a)...N3a^a #8	0.980	2.770	3.744	172.91
C(14^b)-H(14b^b)...N3^b #8	0.980	2.660	3.631	170.66
C(15^b)-H(15c^b)...N(3a^a)#9	0.980	2.874	3.795	156.84
C(14a^a)-H(14e^b)...O(3^b)#9	0.98	2.597	3.537	160.9

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z #2 -x+1,+y,+z #3 -x+2,-y+1,-z #4 -x+1,-y,-z #5 -x+1,-y+1,-z+1 #6 x,y+1,z #7 x-1,+y,+z #8 -x,y+1,-z+1 #9 -x+1,-y,-z+1

Table S4. Hydrogen bonds for **2** [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(17)-H(17C)...O(1)#3	0.96	2.49	3.412(3)	160.0
C(16)-H(16)...O(1)#3	0.93	2.52	3.383(3)	154.6

C(4)-H(4)...O(6)#4	0.93	2.88	3.508(3)	126.2
C(5)-H(5)...O(6)#4	0.93	2.90	3.536(3)	126.4
C(1)-H(1)...O(5)#5	0.93	2.88	3.527(3)	127.5
C(1)-H(1)...O(7)#5	0.93	2.56	3.401(3)	149.9
C(2)-H(2A)...O(4)#5	0.93	2.83	3.601(4)	141.2
C(12)-H(12)...O(6)#2	0.93	2.93	3.740(4)	147.1
C(14)-H(14C)...N(4)#6	0.96	2.91	3.767(3)	149.3
C(18)-H(18B)...O(7)#7	0.96	2.58	3.283(3)	130.0
C(14)-H(14A)...O(1)#8	0.96	2.57	3.383(3)	142.4
C(14)-H(14B)...O(6)#9	0.96	2.75	3.677(4)	162.4
C(15)-H(15A)...O(7)#9	0.96	2.64	3.290(4)	125.7
C(15)-H(15B)...O(4)#9	0.96	2.84	3.628(5)	139.6

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2 #2 -x+2,-y,-z+1 #3 x-1,y,z #4 -x+1,-y,-z+1 #5 -x+1,-y+1,-z+1 #6 x+1,y,z #7 x,y+1,z+1 #8 -x+2,-y+1,-z+2 #9 x+1,y+1,z+1

Table S5. Hydrogen bonds for **3** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(17)-H(17)...O(1)#3	0.93	2.53	3.391(3)	154.4
C(18)-H(18A)...O(1)#3	0.96	2.50	3.411(3)	158.8
C(4)-H(4)...O(6)#4	0.93	2.88	3.505(3)	125.9

C(5)-H(5)...O(6)#4	0.93	2.91	3.535(3)	126.2
C(1)-H(1)...O(4)#5	0.93	2.90	3.538(3)	127.0
C(1)-H(1)...O(5)#5	0.93	2.56	3.390(3)	149.1
C(2)-H(2A)...O(7)#5	0.93	2.83	3.600(4)	140.8
C(12)-H(12)...O(6)#2	0.93	2.94	3.755(3)	147.3
C(14)-H(14A)...N(4)#6	0.96	2.89	3.769(3)	151.9
C(16)-H(16B)...O(5)#7	0.96	2.58	3.297(3)	131.1
C(14)-H(14B)...O(6)#8	0.96	2.77	3.677(4)	158.8
C(15)-H(15B)...O(7)#8	0.96	2.87	3.662(4)	140.1
C(15)-H(15C)...O(5)#8	0.96	2.64	3.283(3)	125.0
C(14)-H(14C)...O(1)#9	0.96	2.59	3.382(3)	139.6

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x,-y+2,-z+1 #3 x+1,y,z #4 -x+1,-y+2,-z+1 #5 -x+1,-y+1,-z+1 #6 x-1,y,z #7 x,y-1,z-1 #8 x-1,y-1,z-1 #9 -x,-y+1,-z