Electronic Supplementary Material for CrystEngComm

Supporting Information

Conformation Dependent Network Structures in the Cooridnation Polymers Derived from Pyridylisonicotinamides, Carboxylates and Co(II): Entrapment of $(H_2O)_{14}$ Water Cluster of an Unprecedented Topology

D. Krishna Kumar, Amitava Das* and Parthasarathi Dastidar*[a]

[a] *Present address: Department of Organic Chemistry, Indian Association for the Cultivation of Science (IACS), Jadavpur, 2A&2B Raja S C Mullick Road, Kolkata – 700032, West Bengal, India*

Analytical Science Discipline, Central Salt & Marine Chemicals Research Institute (CSIR), G. B. Marg, Bhavnagar – 364 002, Gujarat (India) Fax: +91-278-2567562 E-mail: parthod123@rediffmail.com; ocpd@iacs.res.in *(PD);* amitava@csmcri.org *(AD)*

FT-IR for 1-4

$[\{(H_2O)_4Co(\mu\text{-}L1)_2\}.fumarate.2H_2O]_n$ 1:
FT-IR (cm^{-1}): 3275b, 1654vs, 1609vs, 1555b, 1490vs, 1432vs, 1418s, 1369s, 1337s, 1312s, 1241m, 1199s, 1132w, 1057m, 1035s, 995vs, 931s, 901s, 803s, 703vs, 672vs, 646s, 600w, 420s

$[\{(H_2O)_3(\mu\text{-fumarate})Co(\mu\text{-}L1)_2\}.fumarate.2H_2O]_n$ 2:
FT-IR (cm^{-1}): 3275b, 1653vs, 1608vs, 1553s, 1489vs, 1382s, 1312vs, 1200vs, 1132b, 1034s, 996s, 899s, 835s, 804vs, 703vs, 672vs, 598w, 420s

$[\{(H_2O)_4Co(\mu\text{-}L2)_2\}.terepthalate.3H_2O]_n$ 3:
FT-IR (cm^{-1}): 3378b, 1697s, 1599s, 1550m, 1517s, 1424w, 1383vs, 1332m, 1295s, 1207s, 1115b, 1063m, 1018s, 894m, 831b, 755vs, 694m, 591w, 544s

$[\{(H_2O)_4Co(\mu\text{-}L2)_2\}.terepthalate.10H_2O]_n$ 4:
FT-IR (cm^{-1}): 3233vb, 1699vs, 1598vs, 1515s, 1382vs, 1331m, 1295s, 1117w, 1065m, 1018s, 832b, 754s, 692s, 592m, 545vs, 506s

Hydrogen Bonding Parameters for 1–4

Electronic Supplementary Material for CrystEngComm

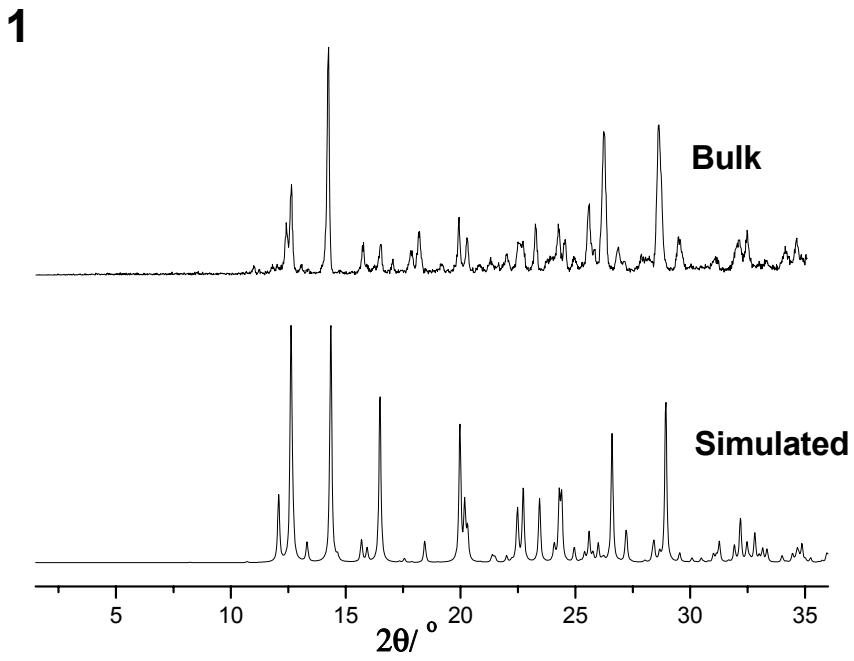
1					
D–H···A	**D–H (Å)**	**H···A (Å)**	**D···A (Å)**	**D–H···A (^{0})**	**Symmetry operation for A**
O(16)–H(16A)···O(26)	0.84	2.08	2.915(4)	169	x, y, z
O(16)–H(16B)···O(29)	0.81(6)	1.92(6)	2.716(5)	166(6)	x, –1+y, z
O(17)–H(17A)···O(27)	0.84	1.88	2.709(4)	168	1–x, –y, 1–z
O(17)–H(17B)···O(22)	0.81(5)	1.77(4)	2.571(5)	170(4)	x, 1/2–y, –1/2+z
O(18)–H(18A)···O(20)	0.84	1.89	2.715(4)	165	–1+x, 1/2–y, 1/2+z
O(18)–H(18B)···O(28)	0.79(4)	2.11(4)	2.889(4)	173(5)	–x, –1/2+y, 3/2–z
O(19)–H(19A)···O(27)	0.84	1.83	2.652(4)	164	1–x, –y, 2–z
O(19)–H(19B)···O(9)	0.73(5)	1.91(5)	2.640(4)	173(6)	x, 1/2–y, 1/2+z
O(28)–H(28A)···O(20)	0.78(5)	1.97(5)	2.742(4)	170(4)	x, y, z
O(28)–H(28B)···O(27)	0.97(5)	1.87(5)	2.753(4)	150(4)	1–x, 1/2+y, 3/2–z
O(29)–H(29A)···O(26)	0.88	1.90	2.769(5)	170	2–x, 1–y, 1–z
O(29)–H(29B)···O(20)	0.96	2.19	3.024(5)	145	x, 3/2–y, –1/2+z
2					
N(7) –H(7)···O(23)	0.88	2.04	2.874(9)	158	x, y, 1+z
O(20)–H(20A)···O(27)	0.94	1.81	2.753(6)	178	x, 1+y, z
O(20)–H(20B)···O(27)	1.00	1.78	2.700(6)	151	2–x, 1–y, 2–z
O(21)–H(21A)···O(25)	0.95	1.74	2.689(6)	171	x, y, z
O(21)–H(21B)···O(25)	0.91	1.87	2.759(6)	166	2–x, 2–y, 1–z
O(27)–H(27A)···O(23)	0.89	1.75	2.631(7)	170	2–x, 1–y, 1–z
O(27)–H(27A)···O(25)	0.89	2.54	3.177(6)	130	2–x, 1–y, 1–z
O(27)–H(27B)···O(9)	0.89	1.97	2.824(8)	161	1–x, 1–y, 2–z
O(28)–H(28A)···O(28)	0.87	1.87	2.741(9)	174	1–x, 1–y, –z
O(28)–H(28B)···O(9)	0.93	2.09	3.006(7)	168	x, y, –1+z
3					
O(16)–H(10)···O(32)	0.84	1.96	2.782(3)	167	x, y, z
O(16)–H(16A)···O(34)	0.76(4)	1.96(4)	2.712(3)	170(4)	1–x, 2–y, 1–z
O(17)–H(17A)···O(31)	0.84	2.03	2.823(3)	156	1+x, 3/2–y, 1/2+z
O(17)–H(17B)···O(33)	0.78(5)	1.87(5)	2.633(3)	168(4)	x, 3/2–y, –1/2+z
O(18)–H(18A)···O(30)	0.84	1.80	2.633(3)	171	1+x, y, z
O(18)–H(18B)···O(32)	0.87(4)	1.97(4)	2.838(3)	172(6)	1–x, –1/2+y, 1/2–z
O(19)–H(19A)···O(31)	0.84	1.90	2.738(3)	177	1+x, y, z
O(19)–H(19B)···O(20)	0.77(4)	1.96(4)	2.733(3)	175(3)	1–x, 1/2+y, 1/2–z
O(32)–H(32A)···O(22)	0.86(2)	1.90(2)	2.742(3)	165(2)	x, y, z
O(32)–H(32B)···O(32)	0.83	1.99	2.818(3)	174	1–x, 2–y, 1–z
O(33)–H(33A)···O(20)	0.88(3)	1.80(3)	2.673(3)	174(3)	x, 3/2–y, 1/2+z
O(33)–H(33B)···O(19)	0.83(5)	2.28(5)	3.008(3)	148(6)	x, y, 1+z
O(34)–H(34A)···O(22)	0.89(4)	1.83(4)	2.718(3)	177(4)	x, y, z
O(34)–H(34B)···O(30)	0.78(2)	1.93(2)	2.669(3)	158(3)	–x, 1/2+y, 1/2–z
Angular parameters are not available for the atoms for which the hydrogen atoms could not be located					
4					
N(22)–H(22)···O(72)	0.86	2.20	3.041(9)	166	x, y, z

O(31)–H(31)···O(71)	0.82	2.15	2.801(9)	136	x, –1+y, z
O(31)···O(41)			2.963(10)		x, y, z
O(32)–H(32)···O(49)	0.82	1.88	2.659(8)	158	2–x, –y, 1–z
O(32)···O(65)			2.727(8)		1+x, –1+y, z
O(33)–H(33)···O(68)	0.82	1.94	2.732(8)	161	1+x, –1+y, z
O(33)···O(53)			2.632(13)		1+x, –1+y, z
O(34)–H(34)···O(66)	0.82	1.84	2.648(12)	168	1+x, –1+y, z
O(34)···O(63)			2.719(9)		1+x, –1+y, 1+z
O(35)–H(35A)···O(70)	0.82	1.97	2.681(11)	145	x, y, z
O(35)–H(35B)···O(41)	0.93(10)	1.83(10)	2.734(10)	164(9)	x, 1+y, z
O(36)–H(36A)···O(66)	0.82	2.31	3.105(10)	164	1–x, 1–y, 2–z
O(36)–H(36B)···O(39)	1.01(7)	1.74(7)	2.747(9)	172(6)	x, 1+y, z
O(36)···O(71)			2.753(10)		x, y, z
O(37)–H(37A)···O(51)	0.79(10)	2.35(10)	2.973(14)	136(8)	x, y, z
O(37)–H(37A)···O(53)	0.79(10)	2.51(10)	3.294(13)	168(10)	x, y, z
O(37)–H(37B)···O(67)	0.97(13)	1.79(13)	2.724(11)	160(11)	x, y, z
O(38)–H(38)···O(68)	0.82	1.95	2.729(10)	158	x, y, z
O(38)–H(38A)···O(24)	0.72(9)	2.15(9)	2.797(9)	150(10)	2–x, –y, 1–z
O(63)···O(39)			2.733(8)		1–x, –y, 1–z
O(63)···O(64)			2.752(10)		x, y, –1+z
O(63)···O(71)			2.846(10)		–1+x, y, –1+z
O(64)···O(61)			2.662(9)		x, –1+y, z
O(64)···O(72)			2.819(10)		x, –1+y, z
O(64)···O(9)			2.954(10)		1–x, –y, 2–z
O(65)···O(41)			2.785(9)		–1+x, 1+y, z
O(65)···O(62)			2.727(9)		–x, 2–y, 1–z
O(65)···N(7A)			3.033(10)		1–x, 1–y, 1–z
O(65)···N(7B)			2.977(18)		1–x, 1–y, 1–z
O(66)···O(51)			2.690(15)		x, y, z
O(66)···O(37)			2.960(10)		1–x, 1–y, 2–z
O(66)···O(67)			2.785(13)		x, y, z
O(67)···O(51)			2.629(14)		1–x, 1–y, 2–z
O(67)···O(69)			2.698(11)		1–x, 1–y, 1–z
O(68)···O(50)			2.727(8)		x, y, z
O(68)···O(49)			2.724(8)		1–x, 1–y, 1–z
O(69)···O(72)			2.753(10)		x, y, –1+z
O(69)···O(50)			2.762(8)		1–x, 1–y, 1–z
O(70)···O(62)			2.632(12)		1+x, –1+y, z
O(70)···O(70)			2.854(13)		2–x,1–y,1–z
O(71)···O(61)			2.689(11)		1+x, –1+y, z
O(72)···O(72)			2.837(11)		1–x, 2–y, 2–z

Electronic Supplementary Material for CrystEngComm

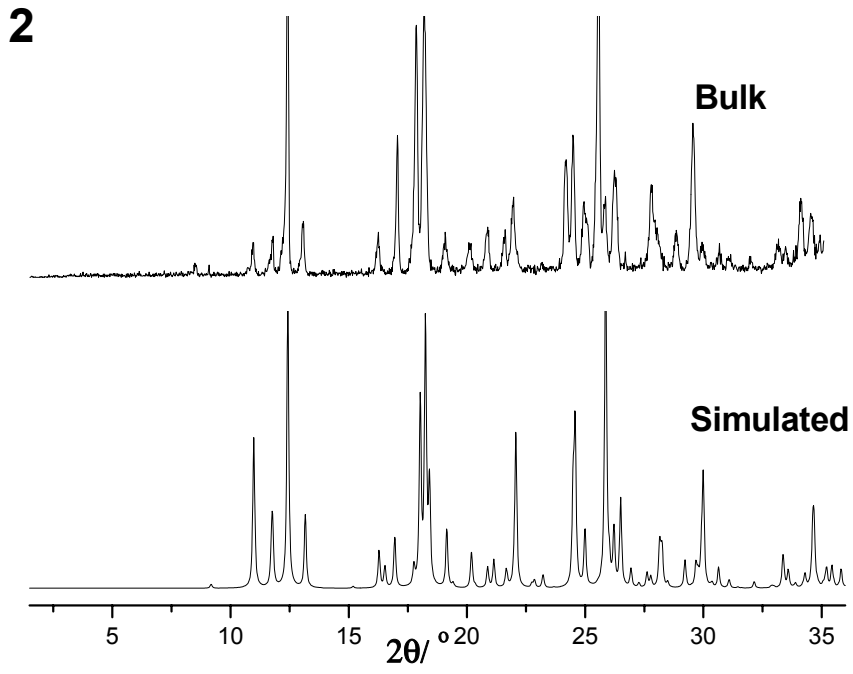
Powder X-ray diffraction comparison plots (simulated and bulk solids) for 1 and 2.

Comparison Plot for 1



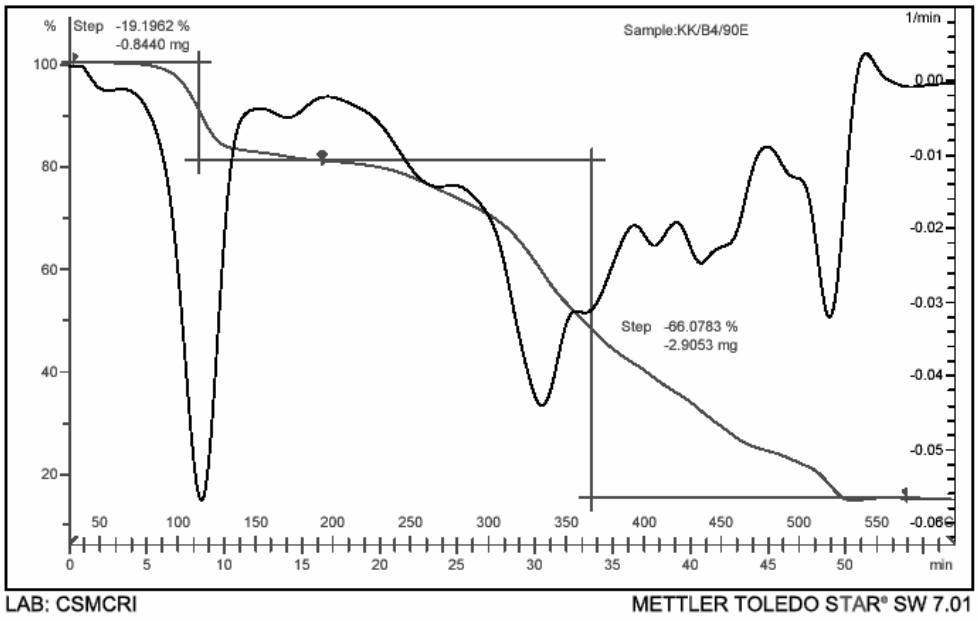
Electronic Supplementary Material for CrystEngComm

Comparison Plot for 2

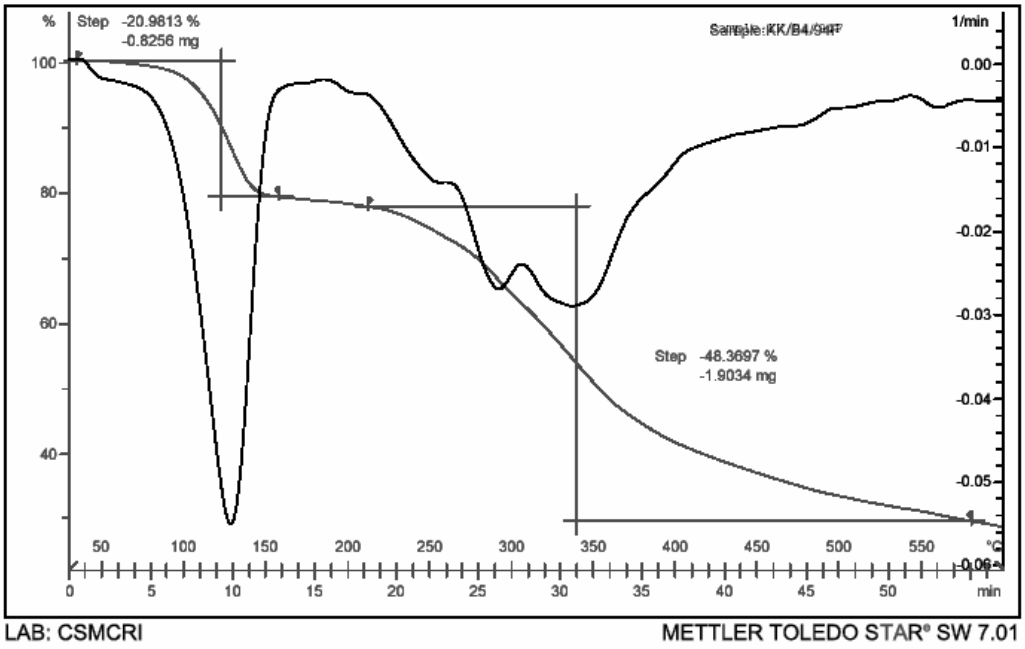


Electronic Supplementary Material for CrystEngComm

TGA plot for **1**



TGA plot for **2**



Since the coordination polymers **3** and **4** were obtained in the same pot in an agglomerated form, physical separation of these two forms was impossible and therefore, no TGA data could be obtained.