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Electronic Supplementary Information (ESI)

Supramolecular Structural Diversities in the MOFs Derived from Pyridylamide Ligands: Studying the Effects of Ligating Topologies, Hydrogen Bonding Backbone of the Ligands and Counter Anions

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$[\{(CH_3COO)(\mu\text{–}OOCH_3)Zn\}_2(\mu\text{–}L1)_2]_n$ 1: FT-IR (cm^{-1}): 3292w, 3256m, 3191b, 3137w, 3082s, 2924w, 2526b, 1989w, 1944w, 1894w, 1674vs, 1575b, 1552s, 1481vs, 1418b, 1329vs, 1301vs, 1265m, 1226m, 1190s, 1117b, 1056s, 1029s, 963m, 927m, 893s, 848m, 816vs, 705vs, 664s, 646m, 617s, 591m, 531b, 479b, 442m, 415s

$[\{(H_2O)_2Zn\}(\mu\text{–}L1)_2\}BF_4]_n$ 2: FT-IR (cm^{-1}): 3358s, 3253b, 3195m, 3134b, 2930w, 2523b, 2361m, 2048b, 1696vs, 1639m, 1576vs, 1545vs, 1495m, 1468vs, 1403vs, 1344m, 1303vs, 1073b, 889m, 805vs, 727vs, 703w, 681s, 620s, 578vs, 528m, 475m, 419m

$[\{(Cl)_2Zn\}(\mu\text{–}L1)]_n$ 3: FT-IR (cm^{-1}): 3654w, 3325s, 3080b, 2365w, 1957w, 1924w, 1856b, 1786b, 1682vs, 1613vs, 1585vs, 1527s, 1486vs, 1428vs, 1332vs, 1290s, 1246s, 1193s, 1123s, 1102m, 1058s, 1031m, 920b, 899m, 862s, 826m, 805vs, 736s, 721vs, 693vs, 652vs, 605m, 577b, 490m, 415b.

$[\{(NO_3)_2$~~Zn~~Cd$(\mu\text{–}L1)_2\}$.nitrobenzene$]_n$ 4: FT-IR (cm^{-1}): 3272b, 3075m, 2855w, 2471b, 2361b, 1983w, 1764m, 1680vs, 1606vs, 1550vs, 1524m, 1487s, 1431s, 1305b, 1235m, 1198s, 1123s, 1045s, 938m, 893vs, 849s, 817vs, 730w, 699vs, 641vs, 591m, 409m.

$[\{Cl_2Zn(\mu\text{–}L2)\}]_n$ 5: FT-IR (cm^{-1}): 3908w, 3698w, 3270s, 3158w, 3094m, 3039m, 2918w, 2847b, 2678w, 2457w, 2336w, 2007w, 1963m, 1869w, 1685vs, 1613vs, 1549vs, 1487vs, 1424s, 1335s, 1302vs, 1232s, 1193m, 1134m, 1109m, 1062s, 1026s, 944w, 899s, 870w, 842w, 821s, 759m, 696vs, 648m, 631w, 600m, 520s, 413s.

$[\{(NO_3)_2Cd\}(\mu\text{–}L2)_2]_n$ 6: FT-IR (cm^{-1}): 3263s, 3206b, 3140m, 3082b, 2840m, 2451m, 2353w, 1976m, 1924w, 1855m, 1754s, 1683vs, 1607vs, 1590vs, 1555vs, 1482s, 1430b, 1293b, 1217m, 1191m, 1136s, 1109m, 1048s, 1014s, 935m, 925w, 898vs, 857s, 837s, 812vs, 753vs, 701vs, 688s, 660m, 636s, 596vs, 526s, 506vs, 419s

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Hydrogen Bonding Parameters for 1-6

D–H···A	D–H(Å)	H···A(Å)	D···A(Å)	D–H···A(^{0})	Symmetry operation for A
1					
N(7)–H(7)···O(22)	0.86	2.09	2.932(4)	166	-x, 1-y, 1-z
C(6)–H(6)···O(22)	0.93	2.48	3.274(5)	143	-x, 1-y, 1-z
C(13)–H(13)···O(18)	0.93	2.56	3.117(5)	119	-x, 1-y, 2-z
C(15)–H(15)···O(22)	0.93	2.31	3.180(5)	156	-x, 1-y, 1-z
2					
N(7)–H(7)···F(19)	0.86	2.09	2.896(11)	157	1-x, 1/2+y, 1/2-z
O(16)–H(16A)···F(18)	1.00	1.95	2.943(8)	175	1+x, y, z
O(16)–H(16B)···O(9)	0.88	1.83	2.702(8)	170	2-x, 1/2+y, 1/2-z
C(2)–H(2)···F(19)	0.93	2.29	3.084(12)	143	1-x, 1-y, 1-z
C(6)–H(6)···F(19)	0.93	2.42	3.150(13)	136	1-x, 1/2+y, 1/2-z
C(11)–H(11)···F(18)	0.93	2.38	2.936(11)	118	x, y, z
3					
N(7A)–H(7)···Cl(16)	0.90(16)	2.48(14)	3.205(13)	138(1)	-x, 1-y, -z
4					
N(7)–H(7)···O(37)	0.88	2.04	2.900(10)	167	1+x, 1/2-y, 1/2+z
N(22)–H(22)···O(38)	0.88	2.23	3.015(8)	148	1-x, -y, -z
C(15)–H(15)···O(37)	0.95	2.47	3.056(9)	120	1+x, 1/2-y, 1/2+z
C(17)–H(17)···O(33)	0.95	2.47	3.327(10)	150	1-x, -y,- 1-z
C(17)–H(17)···O(34)	0.95	2.60	3.393(10)	141	1-x, -y,- 1-z
C(21)–H(21)···O(38)	0.95	2.44	3.222(9)	139	1-x, -y, -z
C(30)–H(30)···O(35)	0.95	2.48	3.202(12)	133	1-x, -y, -z
C(30)–H(30)···O(38)	0.95	2.46	3.400(11)	168	1-x, -y, -z
5					
N(7)–H(7) ..Cl(17)	0.77(3)	2.72(3)	3.454(3)	160(3)	3/2-x, -1/2+y, 1/2-z
C(12)–H(12) ..O(9)	0.94(3)	2.24(3)	3.161(3)	169(2)	3/2-x, -1/2+y, -1/2-z
6					
N(7)–H(7)···O(16)	0.78(4)	2.55(4)	3.168(3)	137(4)	x, y, -1+z
N(7)–H(7)···O(18)	0.78(4)	2.20(4)	2.965(3)	165(4)	x, y, -1+z
C(4)–H(4)···O(18)	0.96(3)	2.46(3)	3.284(4)	144(3)	x, y, -1+z
C(12)–H(12)···O(19)	0.89(4)	2.53(4)	3.152(4)	128(4)	-x, -y, 1-z
C(14)–H(14)···O(18)	0.94(3)	2.56(3)	3.237(3)	129(2)	x, 1+y, -1+z

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XRPD Plots for 1-6

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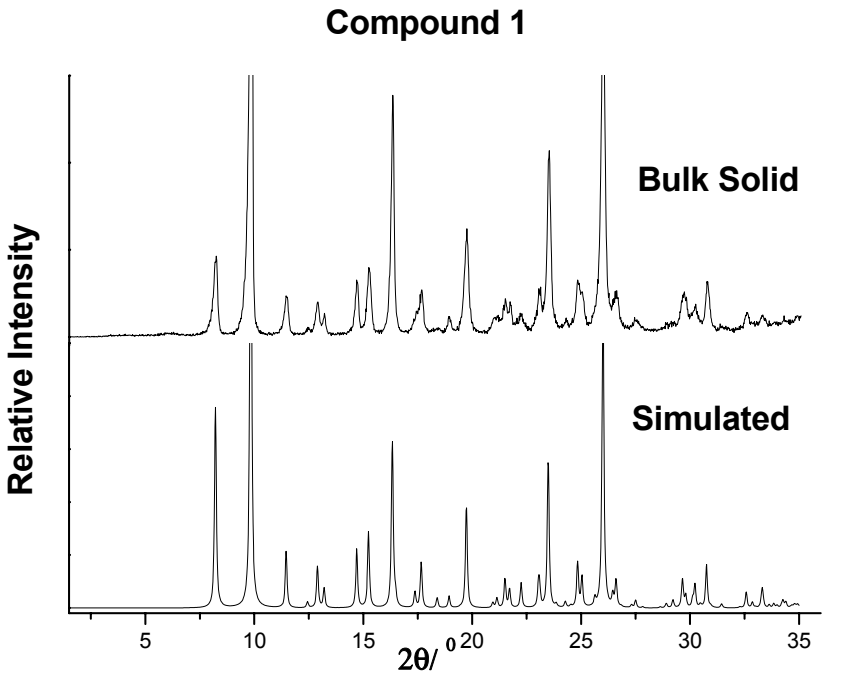

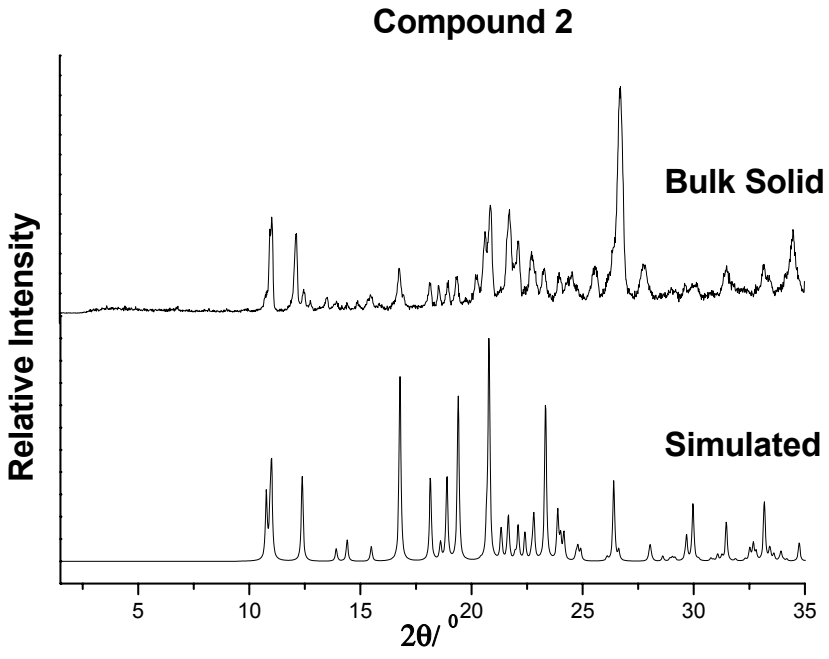

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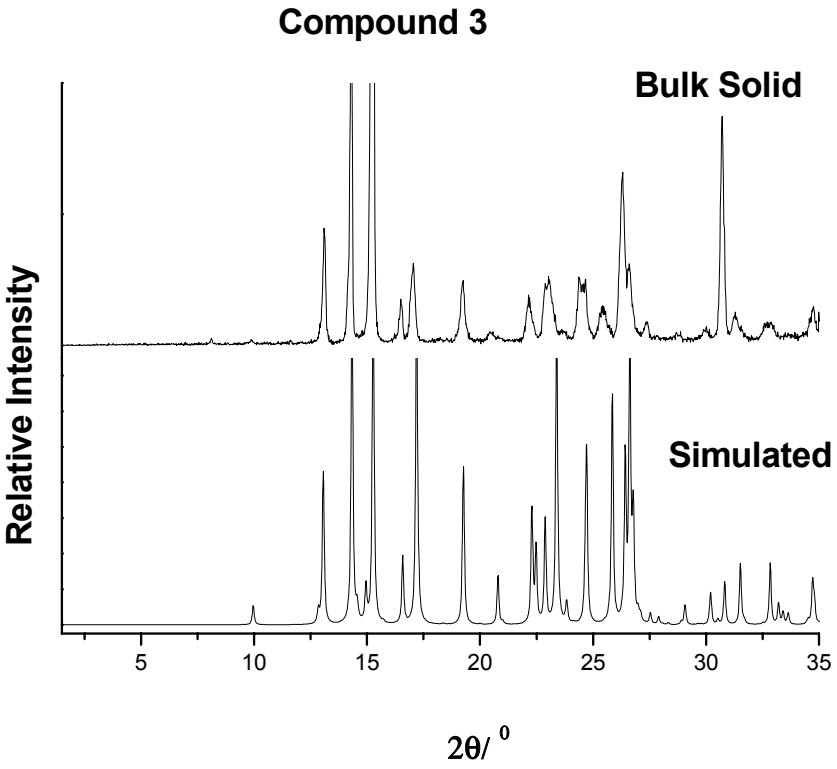

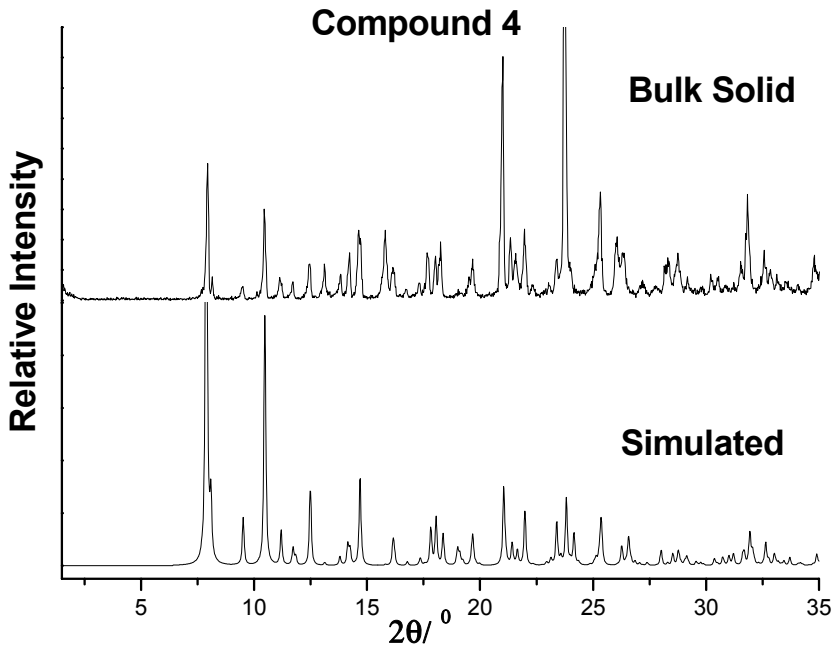

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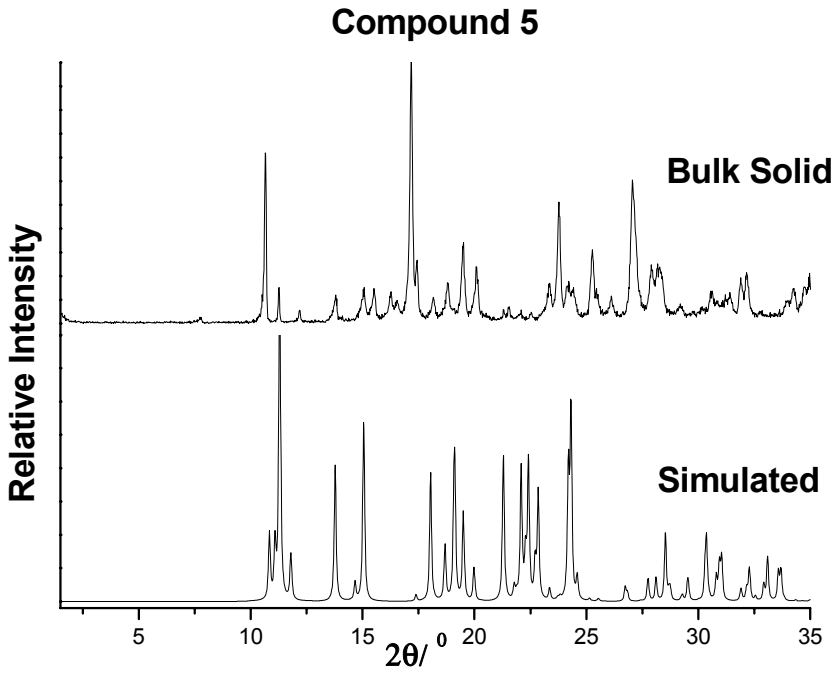

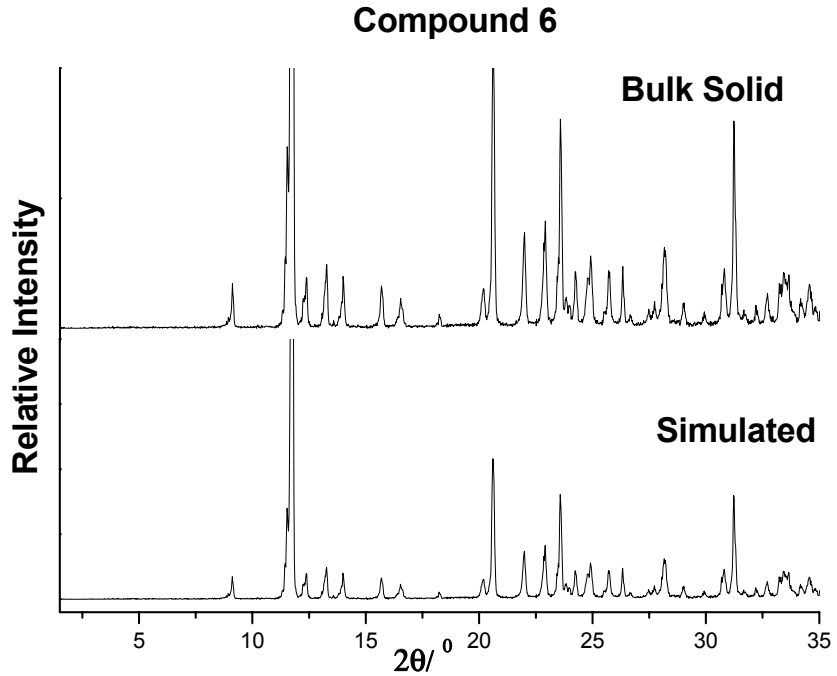

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