Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Construction of Cu(II) Coordination Polymers based on Semi-rigid Tetrahedral Pyridine Ligand

Table S1 Selected bonds and angles for compounds **1 - 3**.

1			
Cu(1)-O(2)	1.9536(14)	Cu(1)-O(4)#1	1.9766(14)
Cu(1)-O(5)	1.9653(14)	Cu(1)-N(1)	2.1795(17)
Cu(1)-O(3)#1	1.9737(15)		
O(2)-Cu(1)-O(5)	168.96(7)	O(3)#1-Cu(1)-O(4)#1	165.89(7)
O(2)-Cu(1)-O(3)#1	90.26(7)	O(2)-Cu(1)-N(1)	95.54(6)
O(5)-Cu(1)-O(3)#1	88.36(7)	O(5)-Cu(1)-N(1)	95.49(6)
O(2)-Cu(1)-O(4)#1	88.81(7)	O(3)#1-Cu(1)-N(1)	98.97(6)
O(5)-Cu(1)-O(4)#1	89.87(7)	O(4)#1-Cu(1)-N(1)	95.13(6)
Symmetry code: #1 -x+3/2, -y+1/2, z.			
2			
Cu(1)-O(10)	1.939(3)	Cu(2)-O(7)	1.960(4)
Cu(1)-O(11)	1.950(3)	Cu(2)-O(5)	1.983(3)
Cu(1)-N(3)	2.004(4)	Cu(2)-O(8)#3	2.316(4)
Cu(1)-N(4)#1	2.014(4)	Cu(2)-N(1)	2.024(4)
		Cu(2)-N(2)#2	2.012(4)
O(10)-Cu(1)-O(11)	161.47(15)	O(5)-Cu(2)-N(2)#2	86.63(16)
O(10)-Cu(1)-N(3)	92.14(15)	O(7)-Cu(2)-N(1)	93.60(16)
O(11)-Cu(1)-N(3)	89.75(16)	O(5)-Cu(2)-N(1)	87.94(15)
O(10)-Cu(1)-N(4)#1	90.02(16)	N(2)#2-Cu(2)-N(1)	176.90(18)
O(11)-Cu(1)-N(4)#1	90.15(16)	O(7)-Cu(2)-O(8)#3	109.30(16)

N(3)-Cu(1)-N(4)#1	173.51(17)	O(5)-Cu(2)-O(8)#3	87.84(14)
O(7)-Cu(2)-O(5)	162.72(17)	N(2)#2-Cu(2)-O(8)#3	91.28(16)
O(7)-Cu(2)-N(2)#2	86.63(16)	N(1)-Cu(2)-O(8)#3	91.57(16)
Symmetry code: #1 -x+1, -y+2, -z+1; #2 x-1, y, z; #3 -x, -y+1, -z+2.			

3

Cu(1)-N(1)	2.024(2)	Cu(1)-N(1)#3	2.024(2)
Cu(1)-N(1)#1	2.024(2)	Cu(1)-O(1W)#2	2.488(3)
Cu(1)-N(1)#2	2.024(2)	Cu(1)-O(1W)	2.488(3)
N(1)#1-Cu(1)-N(1)#2	88.45(13)	N(1)#3-Cu(1)-O(1W)#2	88.09(10)
N(1)#1-Cu(1)-N(1)#3	91.68(13)	N(1)-Cu(1)-O(1W)#2	91.91(10)
N(1)#2-Cu(1)-N(1)#3	176.2(2)	N(1)#1-Cu(1)-O(1W)	88.09(10)
N(1)#1-Cu(1)-N(1)	176.2(2)	N(1)#2-Cu(1)-O(1W)	91.91(10)
N(1)#2-Cu(1)-N(1)	91.68(13)	N(1)#3-Cu(1)-O(1W)	91.91(10)
N(1)#3-Cu(1)-N(1)	88.45(13)	N(1)-Cu(1)-O(1W)	88.09(10)
N(1)#1-Cu(1)-O(1W)#2	91.91(10)	O(1W)#2-Cu(1)-O(1W)	180.0
N(1)#2-Cu(1)-O(1W)#2	88.09(10)		
Symmetry code: #1 y-1/2, x+1/2, -z+3/2; #2 -x+1, -y+2, z; #3 -y+3/2, -x+3/2, -z+3/2.			

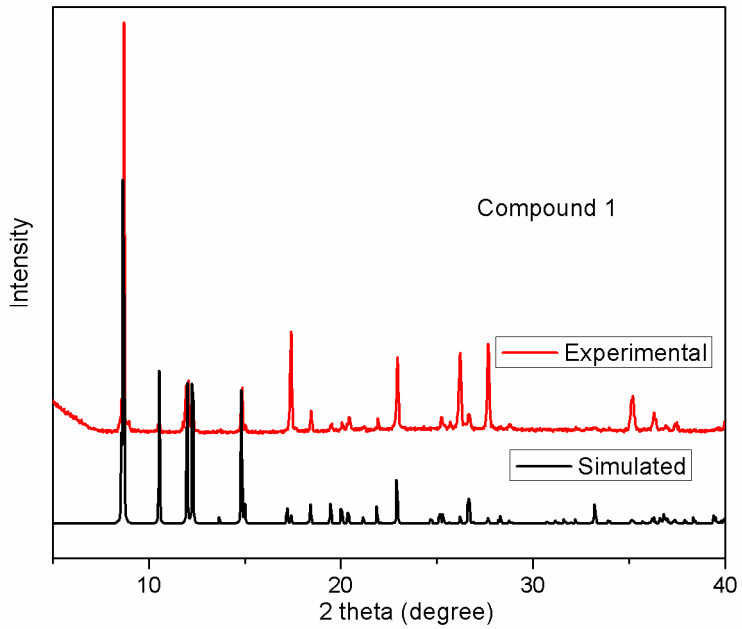

Figure S1. Simulated and experimental powder X-ray diffraction patterns of compound **1**.

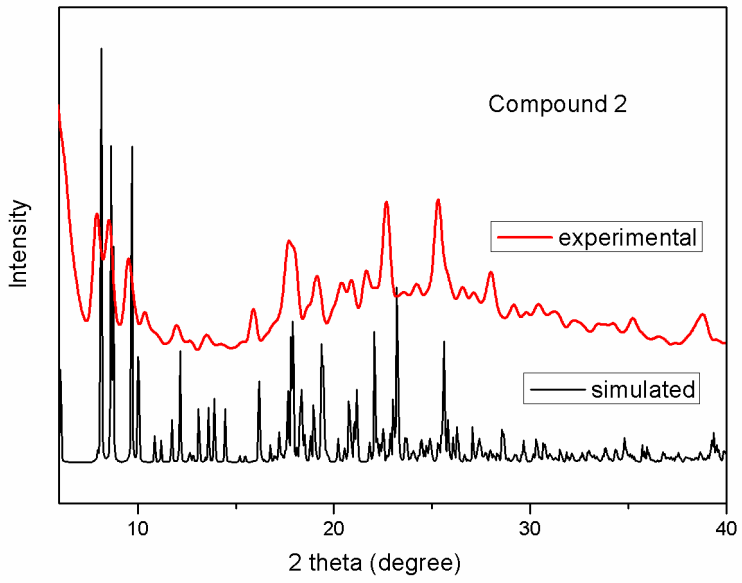

Figure S2. Simulated and experimental powder X-ray diffraction patterns of compound **2**.

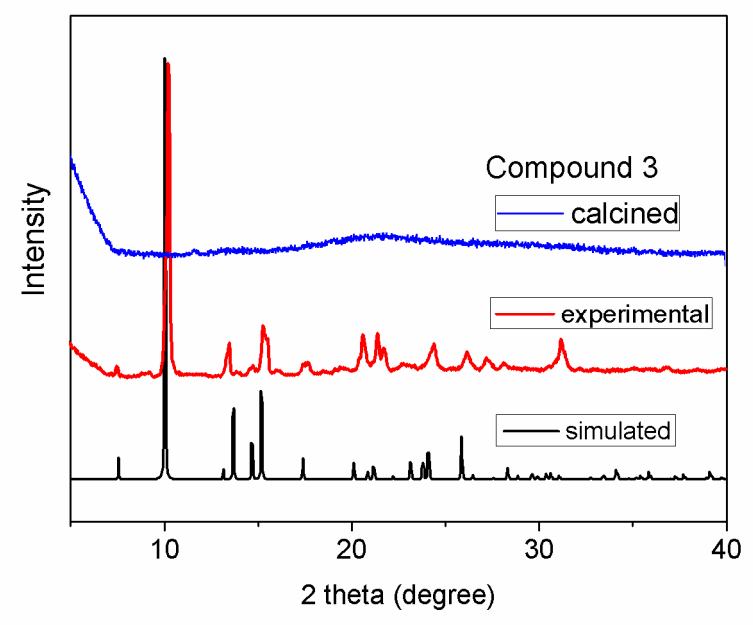

Figure S3. Simulated, experimental and calcined (at 100 °C for 2h) powder X-ray diffraction patterns of compound **3**.

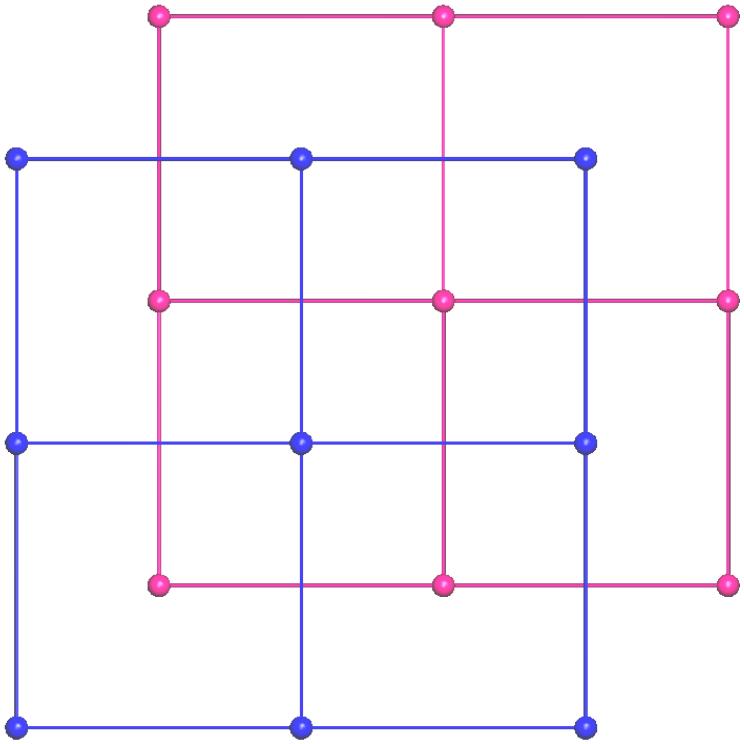

Figure S4. Simplified net of *sql* topology for compound **1**.

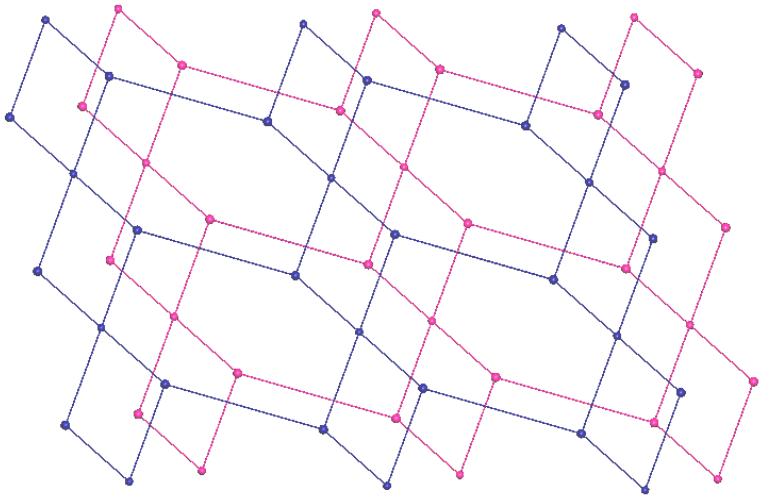

Figure S5. Simplified net of *3,4L13* topology for compound **2**.

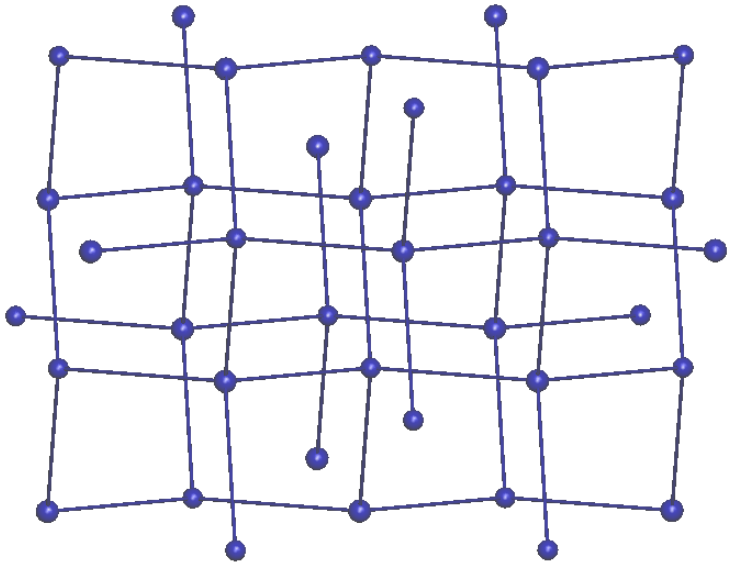

Figure S6. Simplified net of *dia* topology for compound **3**.