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Heterometallic Coordination Polymers Based on dipepdide Schiff base Cu(II) Metalloligand: Synthesis, Structures, and Magnetic Properties

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Electronic Supporting Information

Table S1 Selected bond lengths (Å) and angles (°) for complexes **1-3**[a]

1

Cu1-O1	1.878(3)	Cu1-N2	1.880(3)	Cu1-N1	1.934(3)
Cu1-O3	2.003(3)	Cu1-O6#2	2.611(4)	Ca1-O3	2.473(3)
Ca1-O4	2.729(3)	Ca1-O4#1	2.444(3)	Ca1-O8	2.488(3)
Ca1-O9	2.420(3)	Ca1-O10	2.442(3)	Ca1-O11	2.392(4)
Ca1-O12	2.412(3)	Cu1…Cu1#1	9.847(2)	N1-Cu1-O3	166.02(13)
O1-Cu1-N2	178.45(14)	O1-Cu1-N1	95.59(13)	N2-Cu1-N1	84.14(14)
O1-Cu1-O3	97.18(11)	N2-Cu1-O3	82.94(12)	O8-Ca1-O4	122.32(9)
O11-Ca1-O12	99.33(7)	O11-Ca1-O9	142.34(12)	O12-Ca1-O9	84.91(11)
O11-Ca1-O10	69.68(12)	O12-Ca1-O10	80.98(12)	O9-Ca1-O10	147.91(11)
O11-Ca1-O4#1	73.83(13)	O12-Ca1-O4#1	82.09(11)	O9-Ca1-O4#1	72.59(10)
O10-Ca1-O4#1	132.84(11)	O11-Ca1-O3	98.61(16)	O12-Ca1-O3	152.82(11)
O9-Ca1-O3	80.52(10)	O10-Ca1-O3	99.60(11)	O4#2-Ca1-O3	114.68(10)
O11-Ca1-O8	141.45(13)	O12-Ca1-O8	78.26(11)	O9-Ca1-O8	75.31(10)
O10-Ca1-O8	73.67(10)	O4#2-Ca1-O8	143.54(11)	O3-Ca1-O8	75.92(10)
O11-Ca1-O4	73.11(13)	O12-Ca1-O4	148.19(10)	O9-Ca1-O4	78.51(10)
O10-Ca1-O4	125.89(11)	O4#1-Ca1-O4	67.16(11)	O3-Ca1-O4	49.46(9)

2

Cu1-O1	1.876(4)	Cu1-N2	1.884(5)	Cu1- N1	1.910(4)
Cu1-O3	1.955(4)	Sr1-O2#1	2.506(4)	Sr1-O4#2	2.523(4)
Sr1-O6#3	2.544(4)	Sr1 -O5#4	2.576(4)	Sr1 -O9	2.601(4)
Sr1- O8	2.607(3)	Sr1- O3	2.647(4)	Sr1- O4	2.849(4)
O1-Cu1-N2	177.60(17)	O1-Cu1-N1	95.89(17)	N2-Cu1-N1	95.8917
O1-Cu1-O3	97.02(15)	N2-Cu1-O3	84.63(17)	N1-Cu1-O3	166.83(17)
O2#1-Sr1-O4#2	93.56(12)	O2#1-Sr1-O6#3	76.65(12)	O4#2-Sr1-O6#3	89.77(12)
O2#1-Sr1-O5#4	159.12(12)	O4#2-Sr1-O5#4	83.98(11)	O6#3-Sr1-O5#4	82.59(12)
O2#1-Sr1-O9	79.35(11)	O4#2-Sr1-O9	171.35(11)	O6#3-Sr1-O9	83.82(11)
O5#4-Sr1-O9	100.87(11)	O2#1-Sr1-O8	60.92(12)	O4#2-Sr1-O8	78.17(12)
O6#3-Sr1-O8	134.60(12)	O5#4-Sr1-O8	137.77(12)	O9-Sr1-O8	102.27(11)
O2#1-Sr1-O3	126.36(11)	O4#2-Sr1-O3	115.01(11)	O6#3-Sr1-O3	142.00(11)
O5#4-Sr1-O3	72.61(12)	O9-Sr1-O3	73.45(11)	O8-Sr1-O3	80.83(11)
O2#1-Sr1-O4	128.89(12)	O4#2-Sr1-O4	67.46(13)	O6#3-Sr1-O4	144.81(11)
O5#4-Sr1-O4	69.12(12)	O9-Sr1-O4	120.89(10)	O8-Sr1-O4	68.70(11)
O3-Sr1-O4	47.60(11)	Cu1…Cu1#2	10.082(2)		

3

Cu1-O1	1.865(3)	Cu1-N2	1.883(4)	Cu1-N1	1.923(4)
Cu1-O3	1.985(3)	Cu1-O6#4	2.430(3)	Ba1-O4#1	2.714(3)
Ba1-O5#2	2.738(3)	Ba1-O7#3	2.774(4)	Ba1-O11	2.781(4)
Ba1-O10	2.798(4)	Ba1-O9	2.831(4)	Ba1-O3	2.893(3)
Ba1-O8	2.933(4)	Ba1-O4	2.949(4)	Cu1…Cu1#1	10.341(2)
O1-Cu1-N2	178.08(18)	O1-Cu1-N1	95.48(15)	N2-Cu1-N1	84.52(16)
O1-Cu1-O3	95.67(14)	N2-Cu1-O3	84.03(15)	N1-Cu1-O3	165.71(15)
O1-Cu1-O6#4	93.97(15)	N2-Cu1-O6#4	87.91(15)	N1-Cu1-O6#4	101.04(15)
O3-Cu1-O6#4	87.07(14)	O4#1-Ba1-O5#	271.09(10)	O4#1-Ba1-O7#3	93.68(11)
O5#2-Ba1-O7#3	75.68(11)	O4#1-Ba1-O11	161.48(13)	O5#2-Ba1-O11	123.35(11)
O7#3-Ba1-O11	80.34(11)	O4#1-Ba1-O10	71.52(12)	O5#2-Ba1-O10	126.82(11)
O7#3-Ba1-O10	70.45(11)	O11-Ba1-O10	89.97(12)	O4#1-Ba1-O9	81.29(12)
O5#2-Ba1-O9	70.08(11)	O7#3-Ba1-O9	145.19(11)	O11-Ba1-O9	113.51(12)
O10-Ba1-O9	137.35(11)	O4#1-Ba1-O3	108.82(10)	O5#2-Ba1-O3	149.62(11)
O7#3-Ba1-O3	133.51(11)	O11-Ba1-O3	65.37(10)	O10-Ba1-O3	78.76(10)
O9-Ba1-O3	79.79(11)	O4#1-Ba1-O8	135.28(11)	O5#2-Ba1-O8	69.88(10)
O7#3-Ba1-O8	97.07(11)	O11-Ba1-O8	63.17(12)	O10-Ba1-O8	152.36(11)
O9-Ba1-O8	65.55(11)	O3-Ba1-O8	94.47(10)	O4#1-Ba1-O4	65.71(12)
O5#2-Ba1-O4	120.87(11)	O7#3-Ba1-O4	142.87(11)	O11-Ba1-O4	109.16(10)
O10-Ba1-O4	73.68(11)	O9-Ba1-O4	65.28(11)	O3-Ba1-O4	44.05(9)
O8-Ba1-O4	119.49(11)				

[a]Symmetry codes, For **1**: #1 -x+1, -y+2, -z+2; #2 -x+2, -y+2, -z+1; For **2**: #1 x,-y+1/2,z+1/2; #2 -x+1,-y,-z+1; #3 x, y-1, z ; #4 -x, -y+1, -z+1; #5 x, y+1, z; #6 x, -y+1/2, z-1/2. For **3**: #1 -x+3, -y+2, -z+1; #2 x+1, y+1, z+1; #3 -x+2, -y+2, -z ;#4 -x+1, -y+1, -z; #5 x-1, y-1, z-1.

Table S2 Hydrogen bonds for compound **1, 2,** and **3** [Å and °]

D-H...A	*r* (D-H)	*r* (H...A)	*r* (D...A)	*α*(DHA)	Symmetry operation
1					
O8-H8D...O10	0.85	2.54	2.956(4)	112	
O8-H8C...O1	0.85	1.89	2.733(4)	171	
O8-H8D...O2	0.85	1.93	2.717(4)	154	*x,y-1,z*
O9-H9A...O7	0.84	1.97	2.783(4)	163	*-x+2,-y+2,-z+1*
O9-H9A...S1	0.84	2.99	3.822(3)	172	*-x+2,-y+2,-z+1*
O9-H9B...O7	0.85	1.94	2.788(4)	176	*x,y,z+1*
O10-H10C...O2	0.85	1.88	2.716(4)	170	*x,y-1,z*
O10-H10D...O5	0.85	2.11	2.947(4)	168	*-x+1,-y+1,-z+1*
O11-H11B...O9	0.85	1.96	2.792(5)	165	*-x+1,-y+2,-z+2*
O12-H12B...O1W	0.89	2.21	2.956(9)	151	*-x+1,-y+1,-z+1*
O12-H12A...O5	0.89	2.16	2.767(4)	128	*x,y,z+1*
O1W-H1W1...O1W	0.89	2.38	2.93(2)	120	*-x,-y+1,-z*
O1W-H1W2...O6	0.89	2.46	2.827(9)	105	x-1,y,z
O2W-H2W1...O1W	0.89	2.11	2.834(18)	138	
O2W-H2W2...O8	0.89	2.50	3.019(9)	118	-x+1,-y+1,-z+1
2					
O8-H8D...O4	0.85	2.58	3.085(5)	120	
O8-H8D...O5	0.85	2.56	2.965(5)	111	*x+1,y-1,z*
O8-H8E...O7	0.85	2.45	3.272(5)	162	*x+1,y-1,z*
O8-H8D...O5	0.85	2.56	2.965(5)	111	*x+1,y-1,z*
O8-H8E...S1	0.85	2.87	3.505(4)	134	*x+1,y-1,z*
3					
O11-H11A...O1	0.85	2.08	2.678(5)	127.1	
O8-H8C...O2	0.85	2.00	2.739(5)	145.4	*x,y+1,z*
O8-H8D...O6	0.85	2.18	2.927(5)	146.5	*x+1,y+1,z+1*
O8-H8D...S1	0.85	2.87	3.524(4)	135.3	*x+1,y+1,z+1*
O9-H9A...O6	0.85	2.01	2.799(5)	153.4	*x+1,y+1,z+1*
O9-H9A...S1	0.85	2.84	3.509(4)	137.1	*x+1,y+1,z+1*
O9-H9B...O8	0.85	2.09	2.793(6)	139.4	*-x+2,-y+2,-z+1*
O10-H10C...O9	0.85	2.01	2.841(5)	165.1	*-x+3,-y+2,-z+1*
O10-H10D...O2	0.85	2.25	2.910(5)	134.5	*x+1,y+1,z*
O11-H11B...O2	0.85	2.36	2.936(5)	125.9	*x,y+1,z*

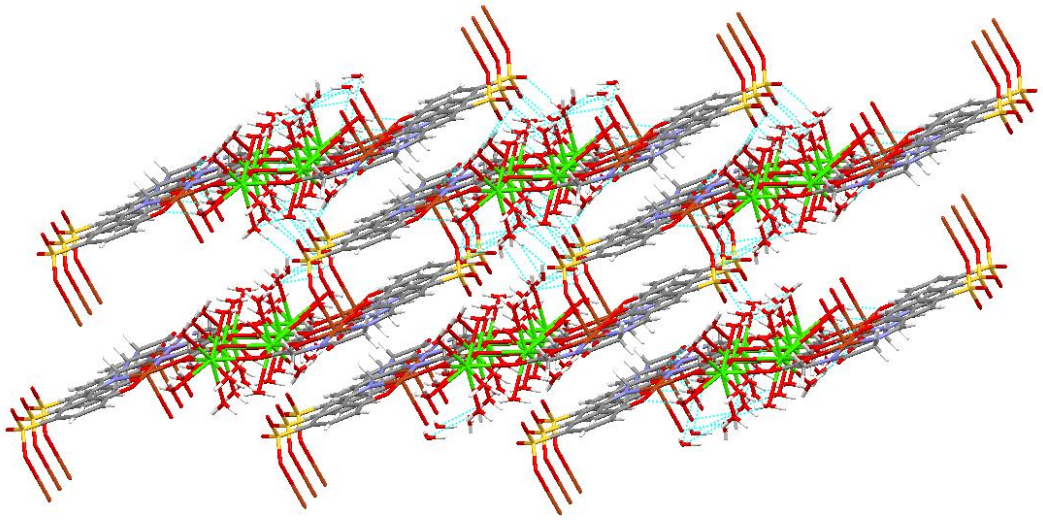


Fig. S1 View of the 3D supramolecular framework linked together by hydrogen bonding of **1**

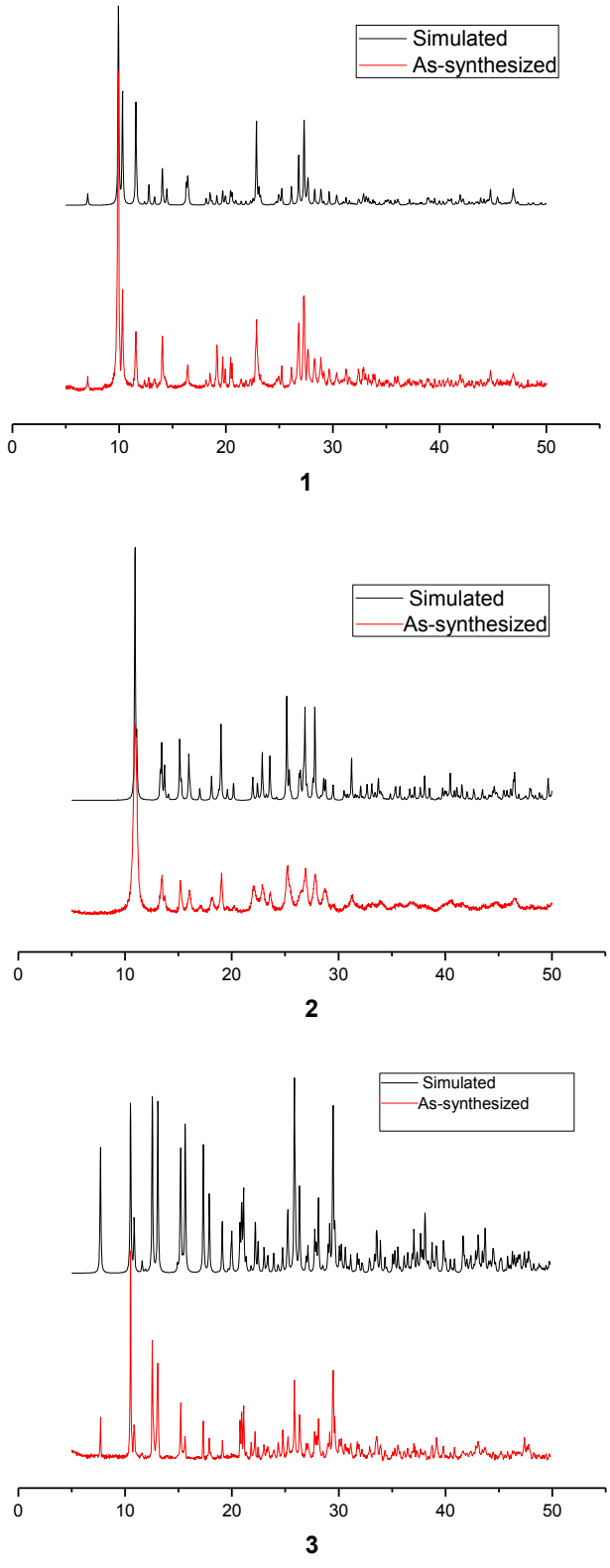
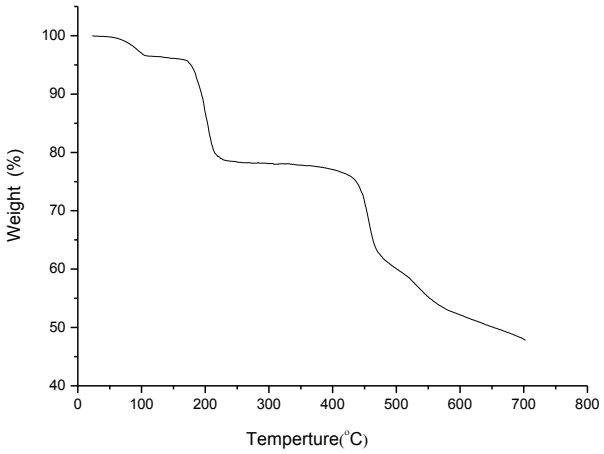
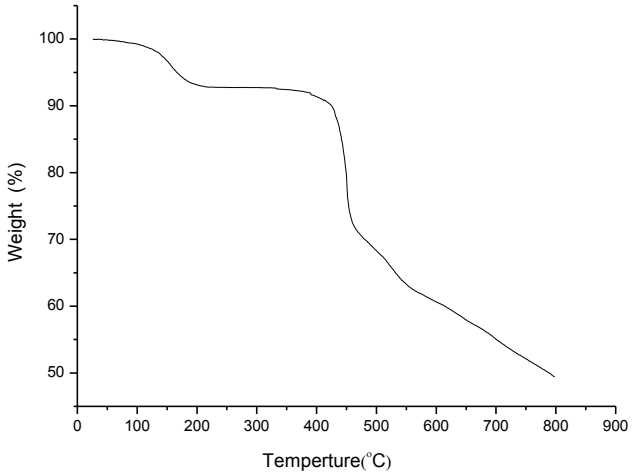


Fig.S2 Simulated(black) and as-synthesized (red) XRPD patterns of **1-3**



1



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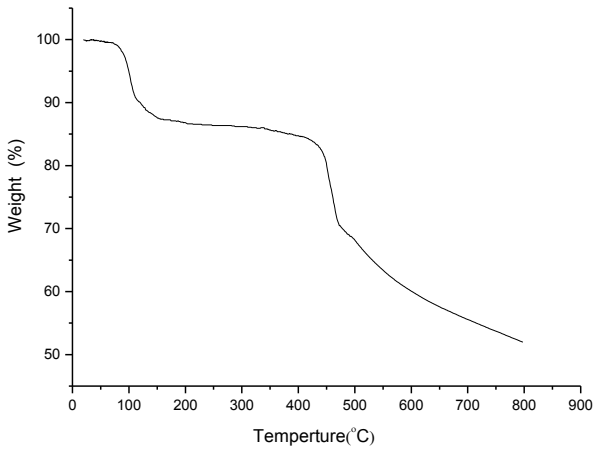

3

Fig.S3 TG curves of complexes **1- 3**.