Electronic Supplementary Information (ESI) for RSC Advances

Syntheses, crystal structures, photoluminescent/magnetic properties of four new coordination polymers based on 2,3', 4,5'-biphenyltetracarboxylic acid

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Content

Table S1 Selected bond lengths (Å) and angles (°) for 1-4.

Complex **1**							
Cu1-O1	1.935(2)	Cu1-O1^{1}	1.935(2)	Cu1-O9W^{2}	2.078(3)	Cu1-O9W^{3}	2.078(3)
Cu1-O10W	2.212(4)	Cu1-O10W^{1}	2.212(4)	Cu2-O3	1.948(2)	Cu2-O9W^{4}	1.957(3)
Cu2-O7^{5}	1.998(3)	Cu2-N1	2.031(3)	Cu2-O6^{4}	2.301(3)	Cu3-O9W	1.939(3)
Cu3-O5	1.962(3)	Cu3-N2^{6}	1.967(3)	Cu3-O4^{4}	2.005(2)	O1-Cu1-O1^{1}	180.0(2)
O1-Cu1-O9W^{2}	88.70(11)	O1^{1}-Cu1-O9W^{2}	91.30(11)	O1-Cu1-O9W^{3}	91.30(11)	O1^{1}-Cu1-O9W^{3}	88.70(11)
O9W^{2}-Cu1-O9W^{3}	180.0	O1-Cu1-O10W	97.97(13)	O1^{1}-Cu1-O10W	82.03(13)	O9W^{2}-Cu1-O10W	94.32(12)
O9W^{3}-Cu1-O10W	85.68(12)	O1-Cu1-O10W^{1}	82.03(13)	O1^{1}-Cu1-O10W^{1}	97.97(13)	O9W^{2}-Cu1-O10W^{1}	85.68(12)
O9W^{3}-Cu1-O10W^{1}	94.32(12)	O10W-Cu1-O10W^{1}	180.0(2)	O3-Cu2-O9W^{4}	96.00(10)	O3-Cu2-O7^{5}	160.43(12)
O9W^{4}-Cu2-O7^{5}	90.14(11)	O3-Cu2-N1	89.91(12)	O9W^{4}-Cu2-N1	173.93(11)	O7^{5}-Cu2-N1	83.81(12)
O3-Cu2-O6^{4}	100.86(11)	O9W^{4}-Cu2-O6^{4}	87.41(11)	O7^{5}-Cu2-O6^{4}	97.96(11)	N1-Cu2-O6^{4}	92.85(12)
O9W-Cu3-O5	92.84(11)	O9W-Cu3-N2^{6}	159.13(13)	O5-Cu3-N2^{6}	91.48(12)	O9W-Cu3-O4^{4}	95.70(11)
O5-Cu3-O4^{4}	134.77(13)	N2^{6}-Cu3-O4^{4}	95.68(12)				
Symmetry codes: ^{1}-X,-Y,1-Z; ^{2}-1+X,-1+Y,+Z; ^{3}1-X,1-Y,1-Z; ^{4}2-X,1-Y,1-Z; ^{5}+X,-1+Y,-1+Z; ^{6}1-X,-Y,-Z;							
Complex **2**							
Cu1-Cu1$^{\#1}$	2.6183(11)	Cu1-O7$^{\#1}$	1.964(3)	Cu1-O3$^{\#2}$	1.963(3)	Cu1-O8	1.961(3)
Cu1-O4$^{\#3}$	1.959(3)	Cu1-O9W	2.176(3)	Cu2-O2	1.900(3)	Cu2-O5$^{\#4}$	1.957(3)
Cu2-O12W	1.982(3)	Cu2-O10W	2.374(4)	Cu2-O11W	1.992(3)	O7^{1}-Cu1-Cu1^{1}	89.77(9)
O7^{1}-Cu1-O9W	97.13(15)	O3^{2}-Cu1-Cu1^{1}	87.55(9)	O3^{2}-Cu1-O7^{1}	87.40(13)	O3^{2}-Cu1-O9W	97.16(13)
O8-Cu1-Cu1^{1}	78.89(9)	O8-Cu1-O7^{1}	168.31(12)	O8-Cu1-O3^{2}	89.25(13)	O8-Cu1-O9W	94.40(15)
O4^{3}-Cu1-Cu1^{1}	81.12(9)	O4^{3}-Cu1-O7^{1}	89.40(15)	O4^{3}-Cu1-O3^{2}	168.24(12)	O4^{3}-Cu1-O8	91.64(15)
O4^{3}-Cu1-O9W	94.47(13)	O9W-Cu1-Cu1^{1}	171.79(12)	O2-Cu2-O5^{4}	176.20(13)	O2-Cu2-O12W	87.24(13)
O2-Cu2-O10W	88.35(16)	O2-Cu2-O11W	90.96(14)	O5^{4}-Cu2-O12W	89.16(13)	O5^{4}-Cu2-O10W	92.91(17)
O5^{4}-Cu2-O11W	92.55(14)	O12W-Cu2-O10W	90.07(15)	O12W-Cu2-O11W	175.99(14)	O11W-Cu2-O10W	93.46(15)
Symmetry codes: ^{1}-X,1-Y,2-Z; ^{2}+X,+Y,1+Z; ^{3}-X,1-Y,1-Z; ^{4}-1+X,1/2-Y,-1/2+Z;							
Complex **3**							
Co1-O12W	2.114(4)	Co1-O12W^{1}	2.114(4)	Co1-O13W	2.102(4)	Co1-O13W^{1}	2.102(4)
Co1-N1	2.147(4)	Co1-N1^{1}	2.147(4)	Co2-O1	2.046(3)	Co2-O5^{2}	2.220(4)
Co2-O6^{2}	2.154(4)	Co2-O9W	2.186(5)	Co2-O10W	2.165(5)	Co2-C15^{2}	2.505(6)
Co2-O11W	1.987(6)	O12W-Co1-O12W^{1}	180.00(16)	O12W-Co1-N1^{1}	91.10(16)	O12W-Co1-N1	88.90(16)
O12W^{1}-Co1-N1	91.10(16)	O12W^{1}-Co1-N1^{1}	88.90(16)	O13W-Co1-O12W^{1}	89.80(16)	O13W^{1}-Co1-O12W^{1}	90.20(16)
O13W^{1}-Co1-O12W	89.80(16)	O13W-Co1-O12W	90.20(16)	O13W^{1}-Co1-O13W	180.000(1)	O13W-Co1-N1	87.99(17)
O13W^{1}-Co1-N1^{1}	87.99(17)	O13W^{1}-Co1-N1	92.01(17)	O13W-Co1-N1^{1}	92.01(17)	N1-Co1-N1^{1}	180.000(1)
O1-Co2-O5^{2}	153.91(16)	O1-Co2-O6^{2}	94.18(15)	O1-Co2-O9W	92.81(16)	O1-Co2-O10W	92.81(17)
O1-Co2-C15^{2}	123.72(17)	O5^{2}-Co2-C15^{2}	30.33(17)	O6^{2}-Co2-O5^{2}	59.73(15)	O6^{2}-Co2-O9W	90.00(19)
O6^{2}-Co2-O10W	98.1(2)	O6^{2}-Co2-C15^{2}	29.75(16)	O9W-Co2-O5^{2}	87.95(17)	O9W-Co2-C15^{2}	85.44(19)
O10W-Co2-O5^{2}	90.77(18)	O10W-Co2-O9W	169.7(2)	O10W-Co2-C15^{2}	98.5(2)	O11W-Co2-O1	106.6(2)
O11W-Co2-O5^{2}	99.4(2)	O11W-Co2-O6^{2}	158.8(2)	O11W-Co2-O9W	85.3(2)	O11W-Co2-O10W	84.9(3)
O11W-Co2-C15^{2}	129.1(2)						
Symmetry codes: ^{1}2-X,1-Y,1-Z; ^{2}+X,-1+Y,+Z;							
Complex **4**							
Ni1-O2	2.019(3)	Ni1-O3^{1}	2.044(3)	Ni1-O12W	2.113(3)	Ni1-O13W	2.104(3)
Ni1-N3	2.087(4)	Ni1-N6^{2}	2.068(4)	Ni2-O6^{3}	2.059(3)	Ni2-O7	2.076(3)
Ni2-O9W	2.087(3)	Ni2-O10W	2.091(3)	Ni2-O11W	2.144(3)	Ni2-N1	2.055(4)
O2-Ni1-O3^{1}	178.91(13)	O2-Ni1-O12W	91.08(11)	O2-Ni1-O13W	88.76(12)	O2-Ni1-N3	90.16(13)
O2-Ni1-N6^{2}	89.97(13)	O3^{1}-Ni1-O12W	89.47(11)	O3^{1}-Ni1-O13W	90.71(12)	O3^{1}-Ni1-N3	90.82(13)
O3^{1}-Ni1-N6^{2}	89.06(13)	O13W-Ni1-O12W	179.13(12)	N3-Ni1-O12W	85.50(13)	N3-Ni1-O13W	93.65(13)

Table S1 Selected bond lengths (Å) and angles (º) for 1-4.

N6[2]-Ni1-O12W	93.03(13)	N6[2]-Ni1-O13W	87.82(13)	N6[2]-Ni1-N3	178.53(14)	O6[3]-Ni2-O7	85.10(12)
O6[3]-Ni2-O9W	92.31(13)	O6[3]-Ni2-O10W	91.42(12)	O6[3]-Ni2-O11W	89.07(13)	O7-Ni2-O9W	93.50(12)
O7-Ni2-O10W	175.87(12)	O7-Ni2-O11W	90.40(13)	O9W-Ni2-O10W	88.86(13)	O9W-Ni2-O11W	175.96(13)
O10W-Ni2-O11W	87.31(13)	N1-Ni2-O6[3]	175.36(14)	N1-Ni2-O7	90.68(14)	N1-Ni2-O9W	89.89(14)
N1-Ni2-O10W	92.71(14)	N1-Ni2-O11W	89.01(14)				

Symmetry codes: [1]1/2-X,1/2+Y,1/2-Z; [2]1/2+X,3/2-Y,1/2+Z; [3]-X,1-Y,1-Z;

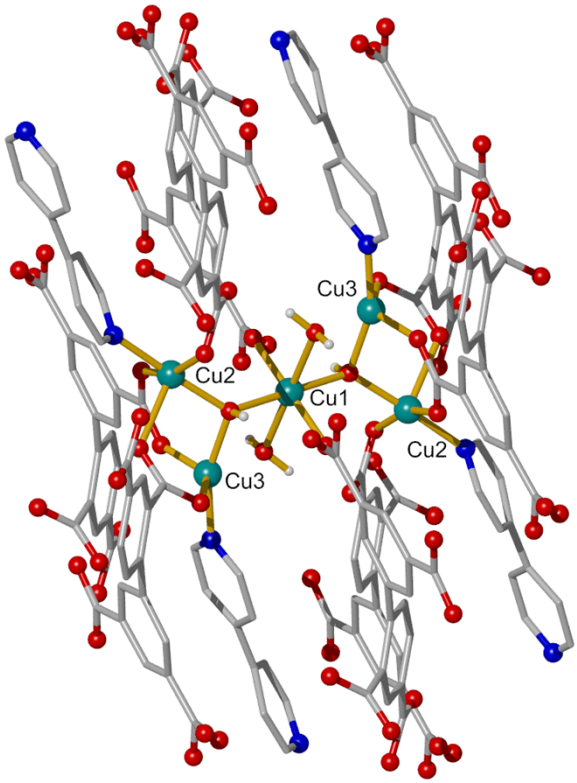

Fig.S1 The metal coordination environment of complex 1

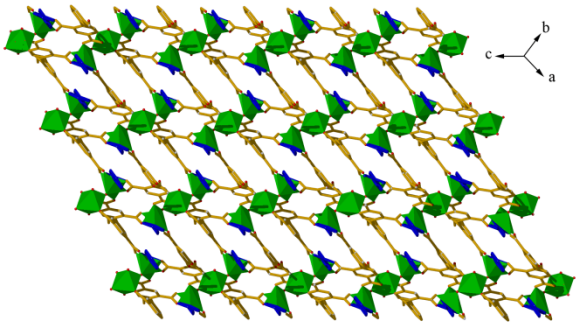

Fig. S2 View of the 3D framework of compound 1 along the [111] direction with one-dimensional channels and hydrogen atoms omitted for clarity.

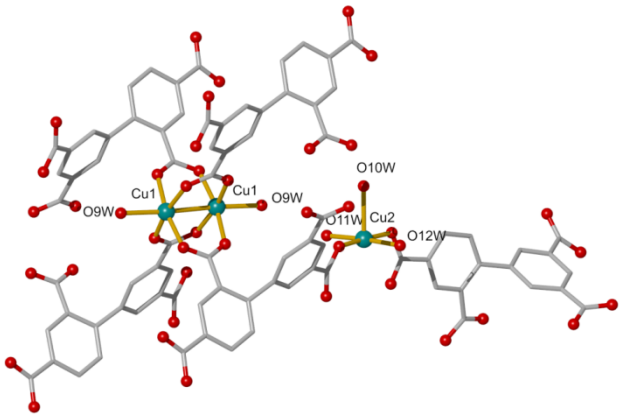

Fig.S3 The metal coordination environment of complex 2

Table S2. The hydrogen bond geometry for complex 2

Complex 2				
D-H ... A	D - H	H ... A	D ... A	∠D - H ... A
O12W - H12B ... O1	0.85	1.91	2.6735	148
O12W - H12A ... O6	0.85	1.98	2.7164	143

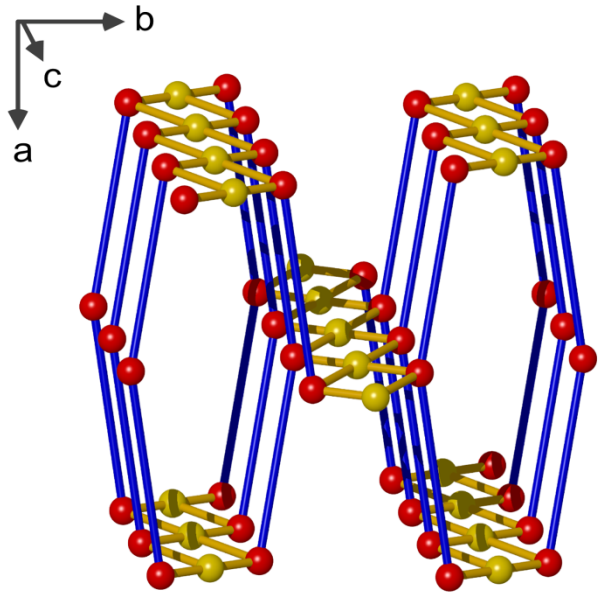

Fig.S4 Schematic view of one of the two interpenetrated nets for complex 2 (red nodes: bptc^{4-} ligands; golden nodes: binuclear Cu1 clusters; blue rods: mononuclear Cu2 ions)

Table S3. The hydrogen bond geometry for complex 3

D-H ... A	D - H	H ... A	D ... A	∠D - H ... A
O9W– H9WA ... O7[a]	0.87	1.89	2.7508	168
O10W– H10WA ... O15W[b]	0.89	2.16	2.9082	141
O11W– H11WA ... O15W[c]	0.85	1.87	2.6595	152
O8– H8 ... O4[d]	0.82	1.79	2.6050	175

Symmetry codes:a) 1-x,1-y,-z ; b) x,1+y,z;c) 2-x,1-y,1-z;d) -x,-y,-z

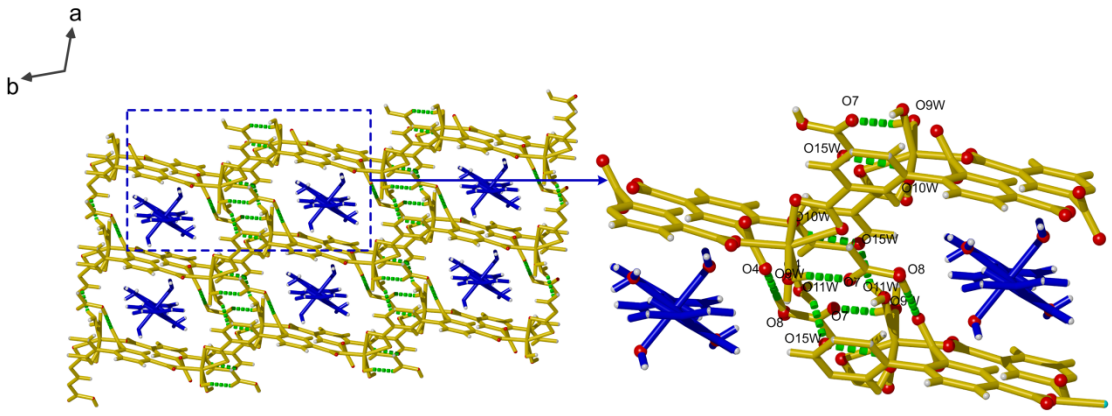

Fig. S5 The 3D supermolecular structure of complex 3 (green dashed bond: hydrogen bond; blue part: 1D cation chains).

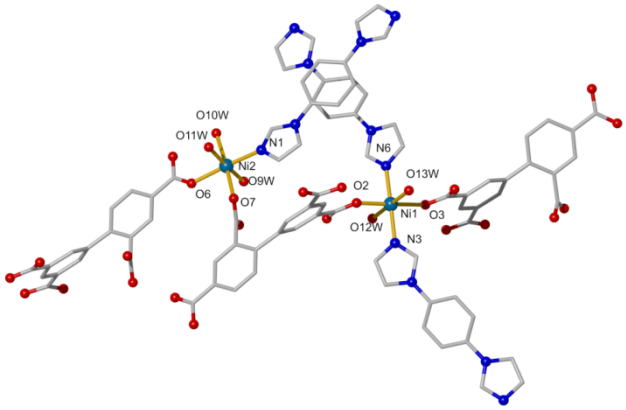

Fig.S6 The metal coordination environment of complex 4

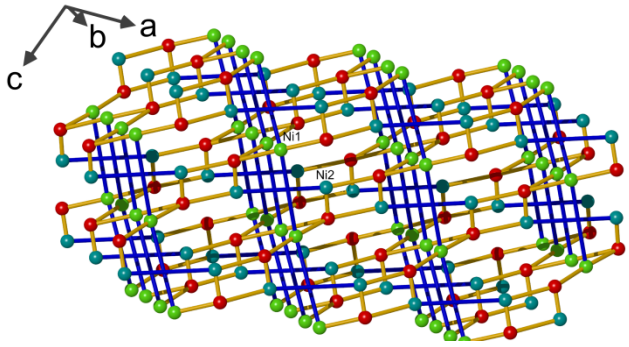

Fig.S7 Schematic view of one of the two interpenetrated nets for complex 4 (red nodes: $bptc^{4-}$ ligands; green nodes: Ni1 ions; teal nodes: Ni2 ions; blue rods: 1,4-bib ligands)

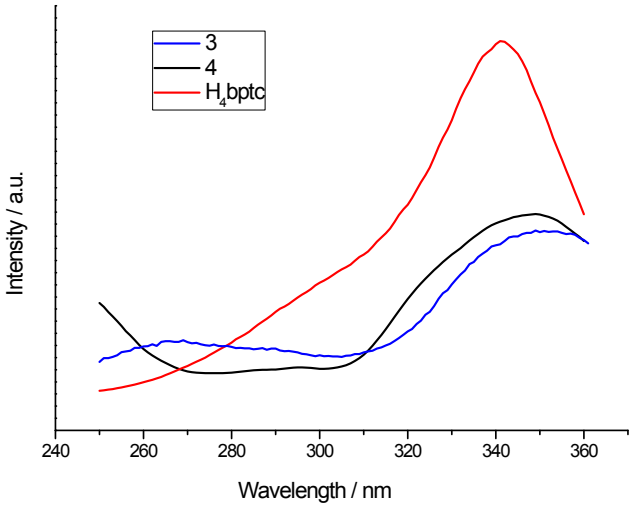

Fig. S8 The excitation spectra of complexes 3, 4 and the H4bptc ligand.