Electronic Supplementary Information (ESI)

Synthesis, Structural Versatility and Magnetic Properties of a Series of Copper(II) Coordination Polymers Based on Bipyrazole and Varied Dicarboxylate Ligand

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1. Table S1: Selected bond lengths (Å) and angle (°) for 1-7.

Complex 1					
Cu1-O1	1.992 (3)	Cu1-N1	2.161 (3)	Cu1-O4^{i}	1.968 (3)
Cu1-O2^{iii}	1.964 (3)	Cu1-O3^{ii}	1.970 (3)		
O1-Cu1-N1	92.29 (12)	O3^{ii}-Cu1-N1	97.33 (12)	O4^{i}-Cu1-O1	87.94 (13)
O2^{iii}-Cu1-O1	168.69 (11)	O4^{i}-Cu1-O3^{ii}	168.51 (11)	O2^{iii}-Cu1-O4^{i}	90.15 (12)
O4^{i}-Cu1-N1	94.06 (12)	O2^{iii}-Cu1-O3^{ii}	89.55 (13)	O3^{ii}-Cu1-O1	90.11 (13)
O2^{iii}-Cu1-N1	98.97 (11)				
Symmetry codes: (i) x, −y+1, z−1/2; (ii) −x+1/2, y+1/2, −z+3/2; (iii) −x+1/2, −y+3/2, −z+1.					
Complex 2					
Cu1-O2	2.220 (3)	Cu1-N3	2.024 (4)	Cu1-N5	1.988 (4)
Cu1-N9	2.011 (3)	Cu1-N7^{i}	1.999 (4)	Cu2-N12	2.029 (3)
Cu2-N13	2.020 (4)	Cu2-N2^{ii}	2.004 (3)	Cu2-N16^{iii}	1.999 (4)
Cu2-O6	2.251 (3)				
N3-Cu1-O2	101.52 (13)	N5-Cu1-O2	102.50 (14)	N5-Cu1-N3	87.63 (15)
N5-Cu1-N7^{i}	165.22 (15)	N5-Cu1-N9	88.54 (16)	N7^{i}-Cu1-O2	92.21 (14)
N7^{i}-Cu1-N3	88.03 (15)	N7^{i}-Cu1-N9	93.09 (16)	N9-Cu1-O2	89.48 (13)
N9-Cu1-N3	168.90 (14)	N2^{ii}-Cu2-O6	103.05 (13)	N2^{ii}-Cu2-N12	165.83 (14)
N2^{ii}-Cu2-N13	88.29 (15)	N12-Cu2-O6	91.12 (13)	N13-Cu2-O6	101.61 (14)
N13-Cu2-N12	88.82 (15)	N16^{iii}-Cu2-O6	89.72 (13)	N16^{iii}-Cu2-N2^{ii}	88.99 (15)
N16^{iii}-Cu2-N12	91.14 (16)	N16^{iii}-Cu2-N13	168.67 (15)		
Symmetry codes: (i) −x+1, y−1/2, −z+1; (ii) x−1, y, z−1; (iii) −x, y−1/2, −z.					
Complex 3					
Cu1-O1	1.947 (3)	Cu1-O4^{i}	1.954 (3)	Cu1-N1	2.030 (3)
Cu1-N5	2.161 (3)	Cu1-N3^{ii}	2.064 (3)		
O1-Cu1-O4^{i}	176.95 (12)	O1-Cu1-N1	89.39 (13)	O1-Cu1-N3^{ii}	93.40 (13)
O1-Cu1-N5	86.38 (12)	O4^{i}-Cu1-N1	91.27 (13)	O4^{i}-Cu1-N3^{ii}	88.02 (12)
O4^{i}-Cu1-N5	90.62 (12)	N1-Cu1-N3^{ii}	139.69 (14)	N1-Cu1-N5	113.34 (13)
N3^{ii}-Cu1-N5	106.97 (13)				
Symmetry codes: (i) x−1/2, y+1/2, −z+1/2; (ii) x, −y+2, z−1/2.					
Complex 4					
Cu1-O1	1.995 (4)	Cu1-O4^{i}	1.967 (3)	Cu1-O5	2.261 (3)
Cu1-O8^{i}	1.970 (4)	Cu1-N4	1.979 (4)	Cu2-O1W	1.987 (4)
Cu2-O2	1.928 (4)	Cu2-O4^{i}	2.425 (4)	Cu2-O5	1.983 (3)
Cu2-N1^{ii}	1.955 (4)				

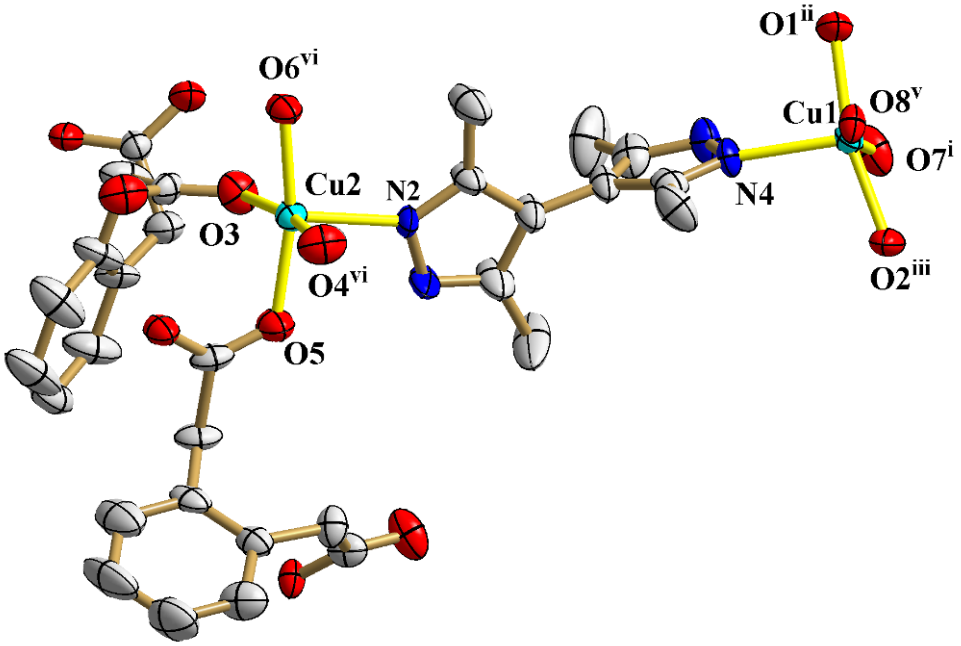
O1-Cu1-O5	91.90 (14)	O4^{i}-Cu1-O1	92.16 (15)	O4^{i}-Cu1-O5	80.32 (13)
O4^{i}-Cu1-O8^{i}	94.53 (15)	O4^{i}-Cu1-N4	173.51 (16)	O8^{i}-Cu1-O1	167.30 (15)
O8^{i}-Cu1-O5	99.85 (14)	O8^{i}-Cu1-N4	86.19 (17)	N4-Cu1-O1	85.97 (17)
N4-Cu1-O5	105.94 (15)	O1W-Cu2-O4^{i}	100.34 (15)	O2-Cu2-O1W	82.04 (16)
O2-Cu2-O4^{i}	93.80 (14)	O2-Cu2-O5	87.49 (15)	O2-Cu2-N1^{ii}	172.79 (16)
O5-Cu2-O1W	168.69 (15)	O5-Cu2-O4^{i}	76.01 (13)	N1^{ii}-Cu2-O1W	93.21 (17)
N1^{ii}-Cu2-O4^{i}	92.39 (15)	N1^{ii}-Cu2-O5	97.61 (16)		
Symmetry codes: (i) x, −y+3/2, z+1/2; (ii) x, y+1, z.					
Complex 5					
Cu1-O1	1.985 (3)	Cu1-N1	1.994 (4)		
O1^{i}-Cu1-O1	86.87 (19)	O1^{i}-Cu1-N1	165.59 (13)	O1-Cu1-N1	90.84 (14)
N1-Cu1-N1^{i}	94.8 (2)				
Symmetry code: (i) −x+3/2, −y+1, z.					
Complex 6					
Cu1-Cu1^{i}	2.6715 (19)	Cu1-O1^{ii}	1.979 (6)	Cu1-O2^{iii}	1.960 (6)
Cu1-O7^{iv}	1.996 (6)	Cu1-O8^{v}	1.949 (5)	Cu1-N4	2.146 (6)
Cu2-O3	1.966 (6)	Cu2-O4^{vi}	1.962 (7)	Cu2-O5	1.994 (6)
Cu2-O6^{vi}	1.969 (6)	Cu2-N2	2.168 (6)		
O1^{ii}-Cu1-O7^{iv}	90.9 (3)	O1^{ii}-Cu1-N4	90.5 (3)	O2^{iii}-Cu1-O1^{ii}	167.1 (3)
O2^{iii}-Cu1-O7^{iv}	87.5 (3)	O2^{iii}-Cu1-N4	102.3 (3)	O7^{iv}-Cu1-N4	92.5 (3)
O8^{v}-Cu1-O1^{ii}	89.5 (3)	O8^{v}-Cu1-O2^{iii}	89.0 (3)	O8^{v}-Cu1-O7^{iv}	165.7 (2)
O8^{v}-Cu1-N4	101.8 (2)	O3-Cu2-O5	86.5 (3)	O3-Cu2-O6^{vi}	91.2 (3)
O3-Cu2-N2	99.8 (3)	O4^{vi}-Cu2-O3	167.2 (3)	O4^{vi}-Cu2-O5	90.2 (3)
O4^{vi}-Cu2-O6^{vi}	89.4 (3)	O4^{vi}-Cu2-N2	92.6 (3)	O5-Cu2-N2	90.7 (3)
O6^{vi}-Cu2-O5	167.5 (3)	O6^{vi}-Cu2-N2	101.8 (2)		
Symmetry codes: (i) −x+2, −y+2, −z+3; (ii) −x+1, −y+2, −z+2; (iii) x+1, y, z+1; (iv) −x+2, −y+2, −z+2; (v) x, y, z+1; (vi) −x+1, −y+1, −z+1.					
Complex 7					
Cu1-N1	1.977 (3)	Cu1-O2	2.264 (3)	Cu1-O6	1.927 (3)
Cu1-O7	1.962 (3)	Cu1-O7^{i}	2.022 (3)	Cu2-N4^{ii}	1.985 (4)
Cu2-O1	1.954 (3)	Cu2-O3	1.976 (3)	Cu2-O5	2.294 (4)
Cu2-O7	1.956 (3)				
N1-Cu1-O2	87.06 (14)	N1-Cu1-O7^{i}	91.88 (13)	O6-Cu1-N1	92.02 (14)
O6-Cu1-O2	112.39 (13)	O6-Cu1-O7^{i}	161.81 (13)	O6-Cu1-O7	92.85 (12)
O7-Cu1-N1	173.59 (13)	O7-Cu1-O2	94.92 (12)	O7^{i}-Cu1-O2	85.54 (12)
O7-Cu1-O7^{i}	82.21 (12)	N4^{ii}-Cu2-O5	90.12 (14)	O1-Cu2-N4^{ii}	90.70 (15)
O1-Cu2-O3	155.03 (17)	O1-Cu2-O5	113.39 (14)	O1-Cu2-O7	88.50 (13)
O3-Cu2-N4^{ii}	85.99 (15)	O3-Cu2-O5	91.39 (16)	O7-Cu2-N4^{ii}	177.47 (14)
O7-Cu2-O3	93.73 (13)	O7-Cu2-O5	92.40 (12)		

Symmetry codes: (i) −x+2, −y+2, −z+2; (ii) x, y, z+1.

2. Table S2: Hydrogen bond parameters for 2, 3, 4, 5 and 7.

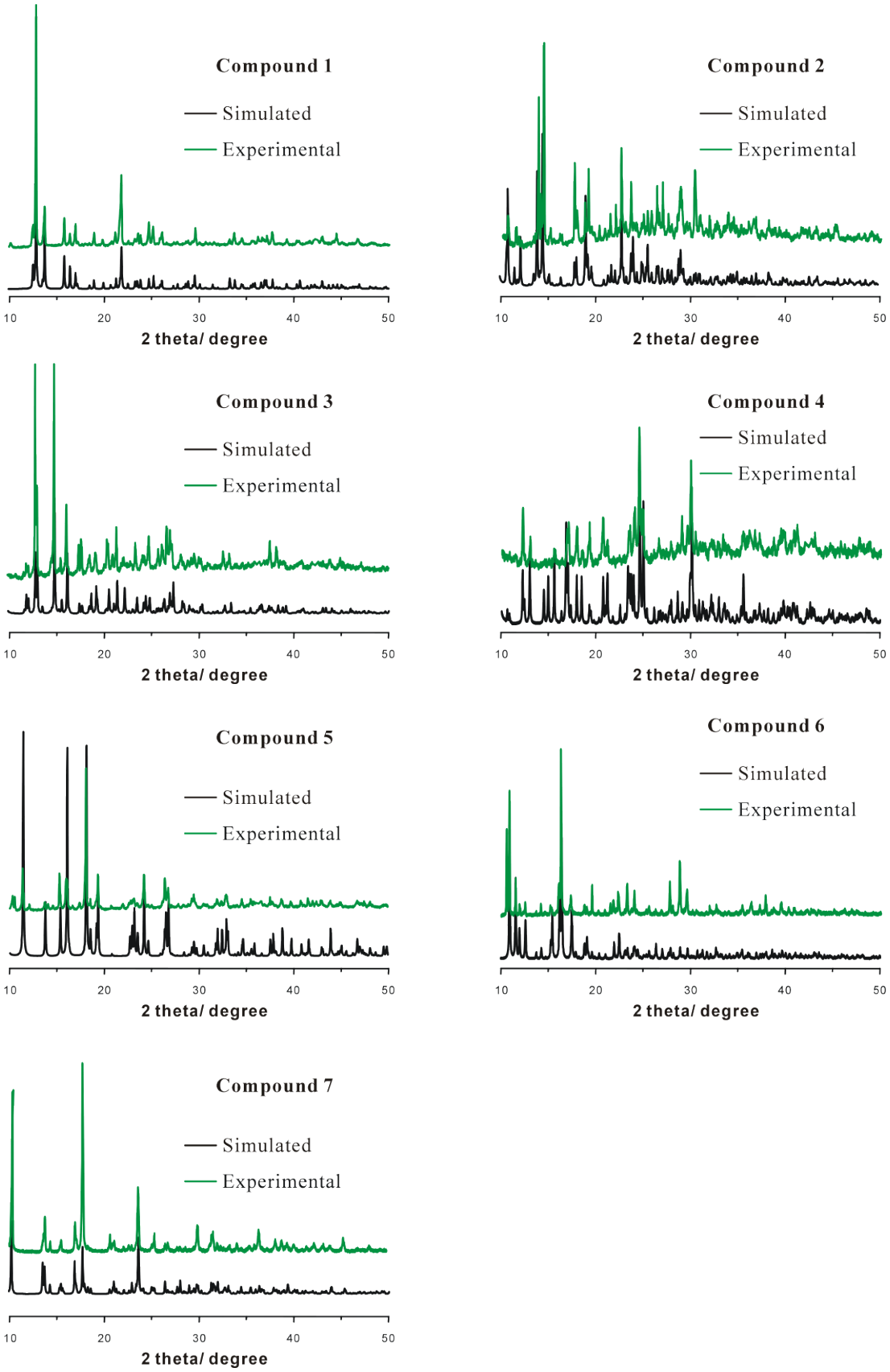
D—*H*···*A*	*D*—*H*	*H*···*A*	*D*···*A*	*D*—*H*···*A*
Complex 2				
N1—H1···O7^{i}	0.86	1.96	2.781 (5)	158.0
N4—H4···O3^{i}	0.86	1.81	2.613 (5)	153.6
N6—H6···O4^{i}	0.86	1.94	2.783 (5)	165.3
N14—H14···O8^{iii}	0.86	1.81	2.604 (5)	151.8
N8—H8···O1^{vi}	0.86	1.77	2.589 (5)	158.7
N15—H15···O7^{iv}	0.86	2.17	2.913 (5)	144.0
N15—H15···O6^{v}	0.86	2.42	2.929 (5)	118.7
Symmetry codes: (i) −x+1, y−1/2, −z+1; (iii) −x, y−1/2, −z; (iv) x−1, y, z; (v) −x, y+1/2, −z. (vi) −x+1, y+1/2, −z+1;				
Complex 3				
N2—H2···O3^{i}	0.86	1.95	2.715 (4)	147.4
N4—H4···O2^{iv}	0.86	2.02	2.736 (5)	139.6
N6—H6···O3^{iii}	0.86	2.02	2.805 (4)	151.3
O1W—H1WB···O2^{iii}	0.85	1.98	2.704 (4)	141.9
Symmetry codes: (i) x−1/2, y+1/2, −z+1/2; (iii) −x+1, y, −z+1/2; (iv) x, −y+2, z+1/2;				
Complex 4				
O1W—H1WA···O3	0.85	1.89	2.732 (5)	170.8
O1W—H1WB···O2W^{iii}	0.85	2.04	2.883 (18)	171.1
N2—H2···O7^{iv}	0.86	1.95	2.710 (6)	147.3
N3—H3···O6	0.86	1.91	2.726 (6)	158.9
Symmetry codes: (iii) −x+1, −y+2, −z; (iv) x, −y+1/2, z+1/2.				
Complex 5				
N2—H2···O2^{ii}	0.86	1.98	2.777 (4)	153.7
Symmetry code: (ii) −x+1, −y+1, −z+1.				
Complex 7				
N2—H2···O2	0.86	2.29	2.827 (5)	120.4
N2—H2···O4^{i}	0.86	2.65	3.158 (5)	119.3
N3—H3···O1W	0.86	2.07	2.882 (7)	157.1
O1W—H1WA···O2^{iii}	0.85	2.20	3.002 (7)	156.9
O1W—H1WB···O5^{iii}	0.85	2.54	3.053 (8)	120.0
N3—H3···O5^{iv}	0.86	2.47	3.000 (5)	120.5
O7—H7A···O4	0.98	1.78	2.665 (4)	148.7
Symmetry codes: (i) −x+2, −y+2, −z+2;; (iii) −x+2, −y+1, −z+1. (iv) x, y, z−1				

3. Structural graphic for compound 6



The coordination environments of Cu(II) ions in **6** with the thermal ellipsoids at 50% probability level (Symmetry codes: (i) −x+2, −y+2, −z+3; (ii) −x+1, −y+2, −z+2; (iii) x+1, y, z+1; (iv) −x+2, −y+2, −z+2; (v) x, y, z+1; (vi) −x+1, −y+1, −z+1.)

4. Fig. S2. The XRD patterns of 1 - 7.



5. Fig. S2. The IR spectra of 1 - 7.