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Accessory Publication

New Copper(II) and Nickel(II) Complexes with Bifunctional Tetrazolate-5-carboxylate Ligands: Syntheses, Crystal Structures and Magnetic Properties

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Table S1. Hydrogen bond distances and bond angles of complex **1**.

Atom involved	D-H (Å)	H···A (Å)	D···A (Å)	Angle of D-H···A (°)
O2W-H2WA···O2[a]	0.840(10)	1.837(11)	2.673(3)	174(4)
O2W-H2WB···O4W	0.844(10)	1.853(11)	2.696(3)	176(5)
O1W-H1WA···O4W[b]	0.840(10)	1.905(17)	2.714(3)	161(4)
O1W-H1WB···O1W[c]	0.841(10)	2.102(12)	2.940(5)	175(4)
O4W-H4WA··· O1[d]	0.848(10)	1.909(13)	2.736(3)	164(4)
O4W-H4WB··· N2[e]	0.853(10)	2.024(18)	2.817(3)	154(3)
O3W-H3WA···O3W[f]	0.841(10)	2.03(2)	2.803(5)	152(4)
O3W-H3WB···O1[g]	0.846(10)	2.044(16)	2.867(3)	164(4)

symmetry codes a: x, 1 - y, 0.5 + z; b: x, y - 1, z; c: -x, y, 0.5 - z; d: 0.5 - x, 1.5 - y, -z; e: 0.5 - x, 0.5 + y, 0.5 - z; f: -x, 2 - y, -z; g: x - 0.5, 0.5 + y, z.

Table S2. Hydrogen bond distances and bond angles of complex **2**.

Atom involved	D-H (Å)	H···A (Å)	D···A (Å)	Angle of D-H···A (°)
O1W-H1WA···N1^{h}	0.840(10)	2.028(15)	2.818(3)	156(3)
O1W-H1WB···O1^{i}	0.840(10)	2.043(14)	2.854(3)	162(4)
O2W-H2WA···O1^{h}	0.848(10)	2.113(18)	2.906(3)	156(3)
O2W H2WB···O2^{j}	0.850(10)	1.895(13)	2.728(3)	166(3)
O3W-H3WA···O4W	0.845(10)	1.938(12)	2.775(3)	170(3)
O3W-H3WB···O4W^{k}	0.849(10)	1.882(12)	2.723(3)	170(3)
O4W-H4WB···O1^{l}	0.838(10)	2.07(2)	2.796(3)	145(3)
O4W-H4WA···N2^{m}	0.840(10)	2.19(3)	2.859(3)	136(3) 2_445

symmetry codes h: -x - 1, -y, -z; i: x, y, z - 1; j: x - 1, y - 1, z - 1; k: -x, -y - 1, -z; l: -x, -y, 1 - z, m: -x - 1, -y - 1, -z.

Table S3. Hydrogen bond distances and bond angles of complex **3**.

Atom involved	D-H (Å)	H···A (Å)	D···A (Å)	Angle of D-H···A (°)
O1W-H1WA···O2W^{n}	0.849(10)	1.979(17)	2.799(5)	162(5)
O1W-H1WB···O4W^{n}	0.850(10)	1.955(13)	2.800(4)	173(6)
O2W-H2WA···O4W^{o}	0.844(10)	2.082(16)	2.900(4)	163(5)
O2W-H2WB···O5W^{p}	0.844(10)	2.027(14)	2.861(4)	170(5)
O3W-H3WA···O1W^{q}	0.849(10)	1.963(15)	2.791(5)	165(4)
O3W-H3WB···O5W^{n}	0.847(10)	1.981(16)	2.796(4)	161(4)
O4W-H4WA···O3W^{r}	0.846(10)	1.945(11)	2.787(4)	174(4)
O4W-H4WB···O2	0.849(10)	1.895(14)	2.731(4)	168(5)
O5W-H5WA···O1	0.844(10)	1.864(12)	2.704(4)	173(5)
O5W-H5WB···N1^{s}	0.845(10)	2.078(15)	2.906(4)	167(5)

symmetry codes n: x - 1, y, z; o: x, 0.5 - y, 0.5 + z; p: x, y, z + 1; q: x, 0.5 - y, -0.5 + z; r: x + 1,

y, z; s: 2 - x, 1 - y, 1 - z.

Table S4. Hydrogen bond distances and bond angles of complex **4**.

Atom involved	D-H (Å)	H···A (Å)	D···A (Å)	Angle of D-H···A (°)
O1W-H1WA···N2^{t}	0.850(7)	2.043(9)	2.844(3)	156.6(18)
O1W-H1WB···O1^{u}	0.845(8)	2.026(8)	2.854(3)	166(2)

symmetry codes t: -x + 1, -y - 1, -z + 1; o: -x, -1 - y, 2 - z.

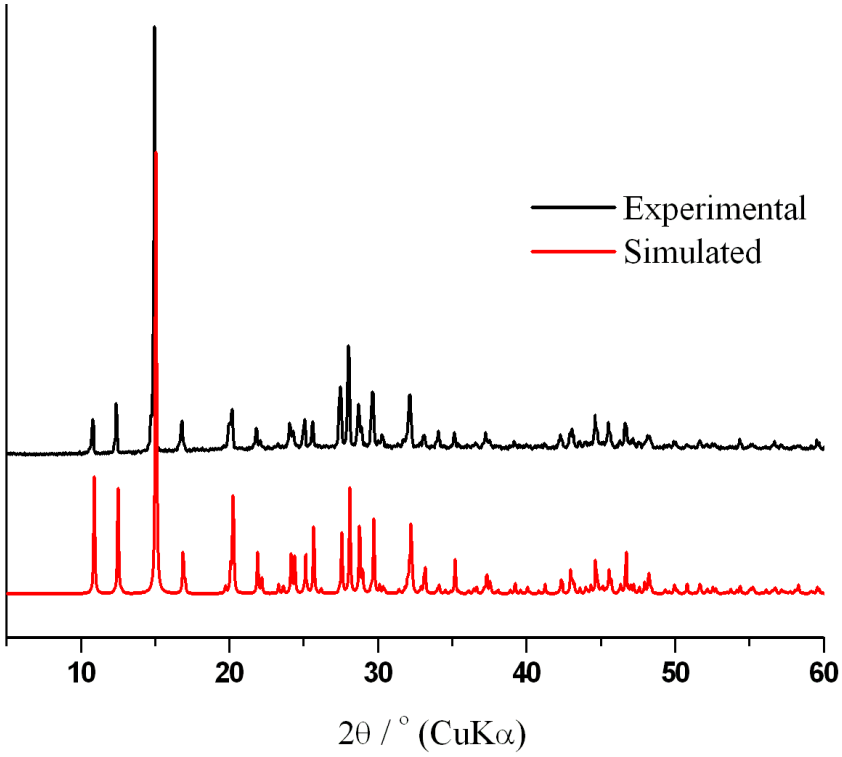

Fig. S1. The experimental and simulated PXRD diagrams of complex **1**

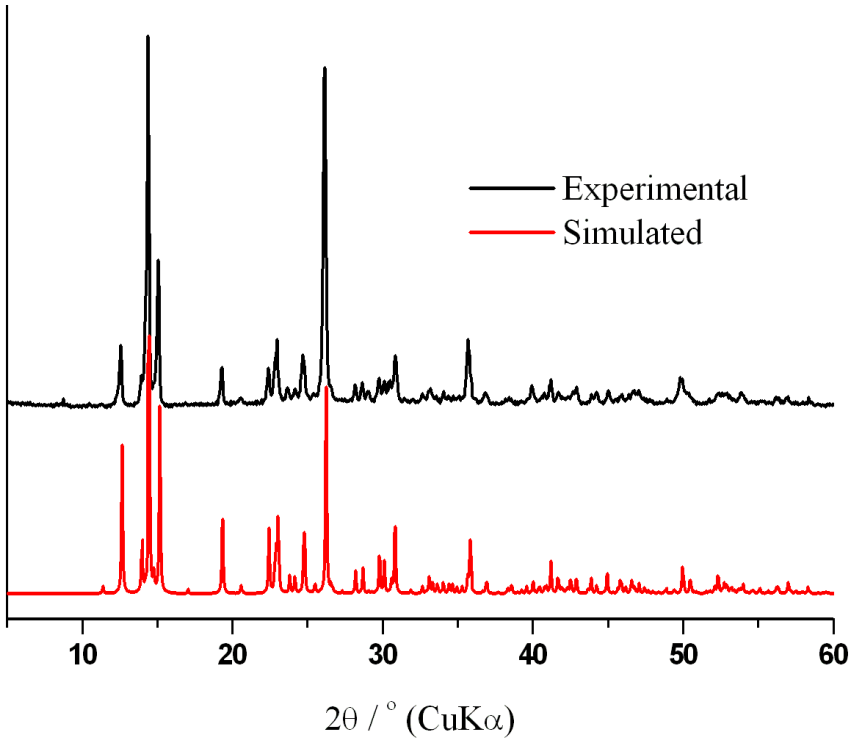

Fig. S2. The experimental and simulated PXRD diagrams of complex **2**

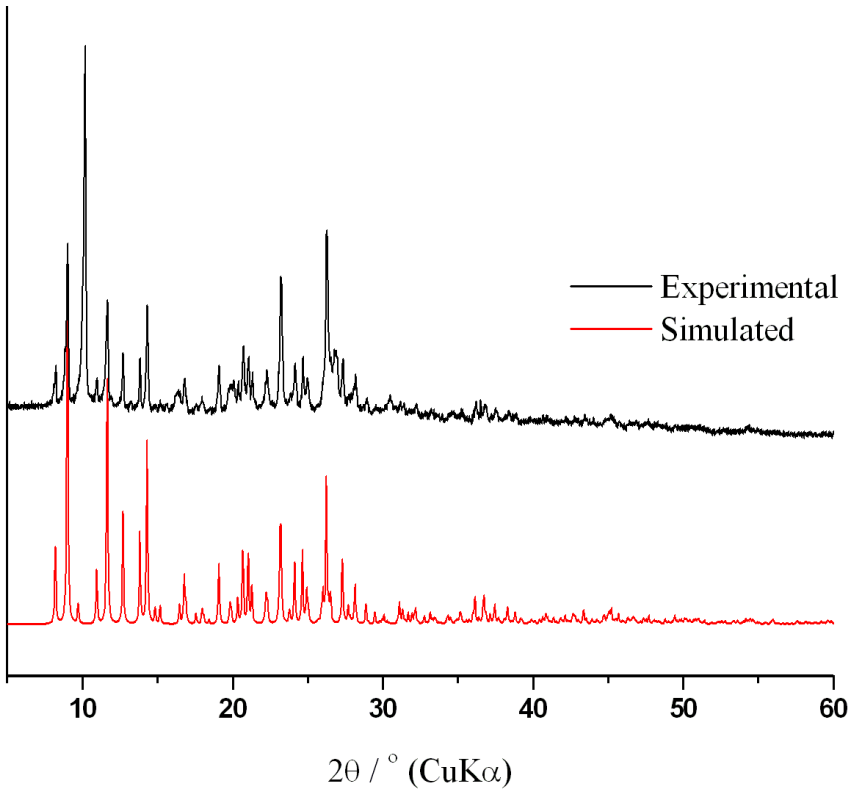

Fig. S3. The experimental and simulated PXRD diagrams of complex **3**

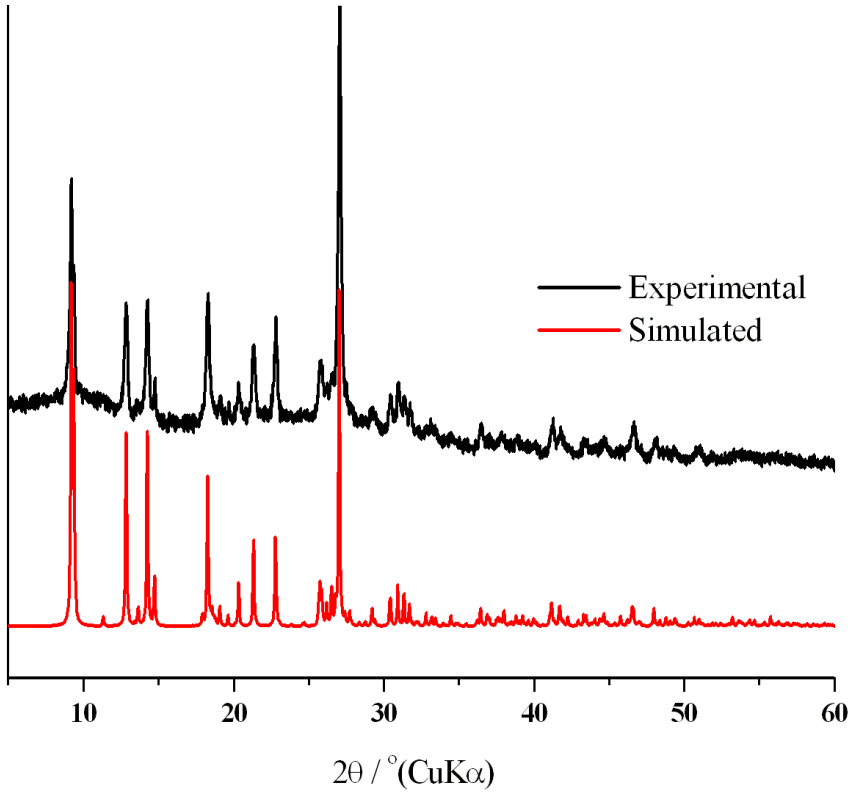

Fig. S4. The experimental and simulated PXRD diagrams of complex **4**

Notes: Powder X-ray diffraction (PXRD) patterns of complexes **1 - 4** were obtained from a Rigaku DMAX2500 powder diffractometer at 40 kV and 100 mA using Cu Kα radiation, with a scan speed of 0.375 s/step and a step size of 0.05 °. The simulated PXRD patterns were calculated using single-crystal X-ray diffraction data and processed by the free *Mercury v1.4* program provided by the Cambridge Crystallographic Data Centre.

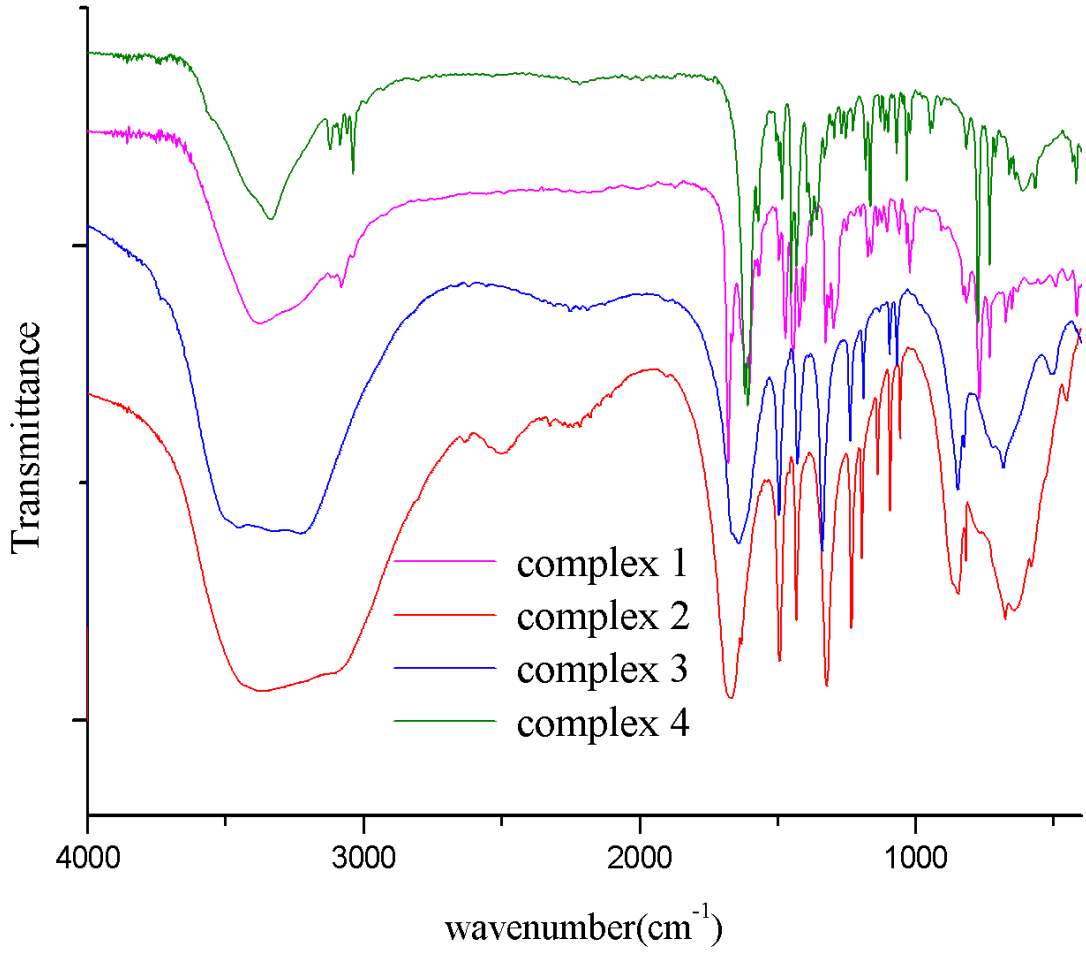

Fig. S5. The IR spectra of complexes **1**–**4**.

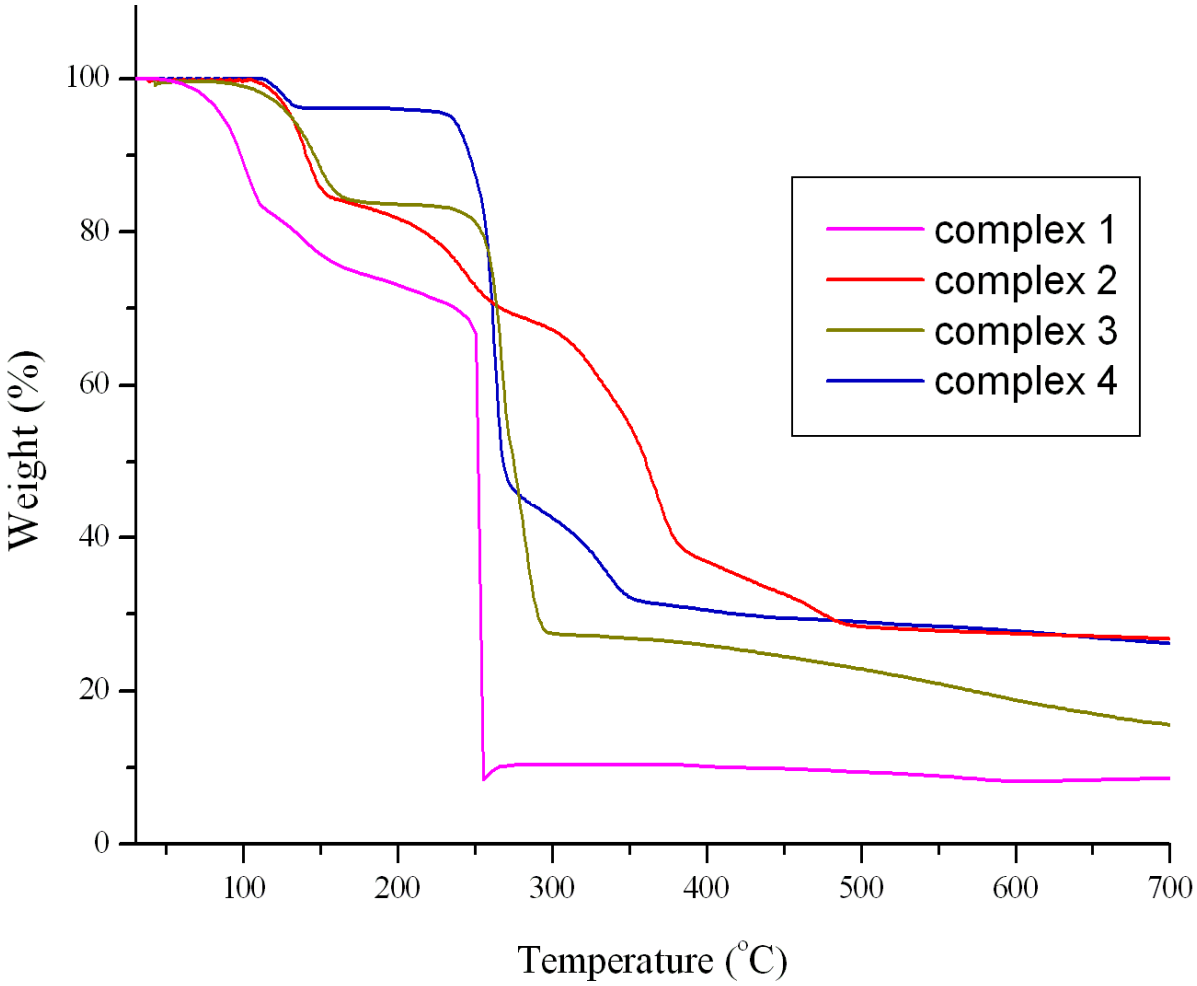

Fig. S6. The TG curves for complexes **1**–**4**.

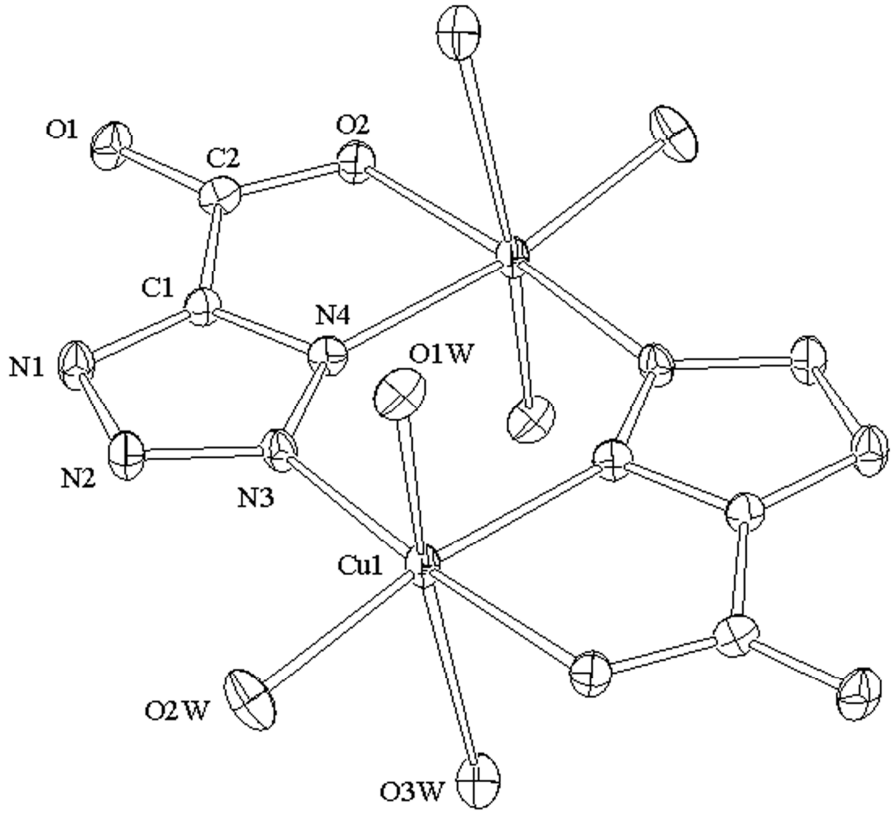

Fig. S7. ORTEP plot of complex **1** with thermal ellipse at the 30% probability level.

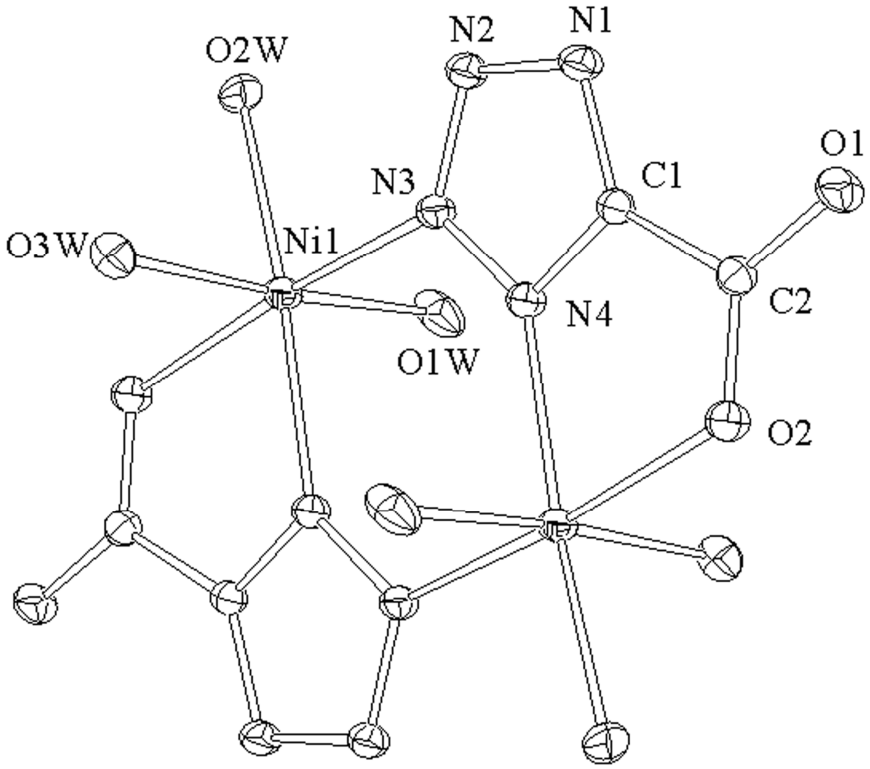

Fig. S8. ORTEP plot of complex **2** with thermal ellipse at the 30% probability level.

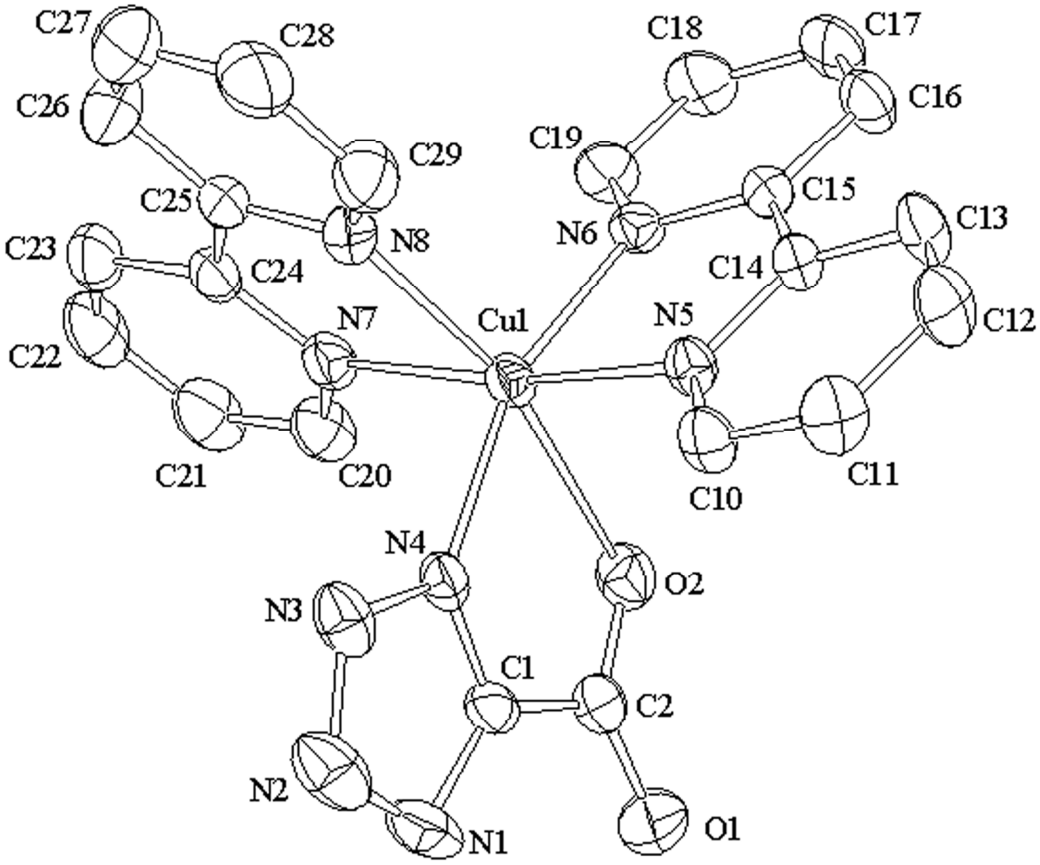

Fig. S9. ORTEP plot of complex **3** with thermal ellipse at the 25 % probability level.

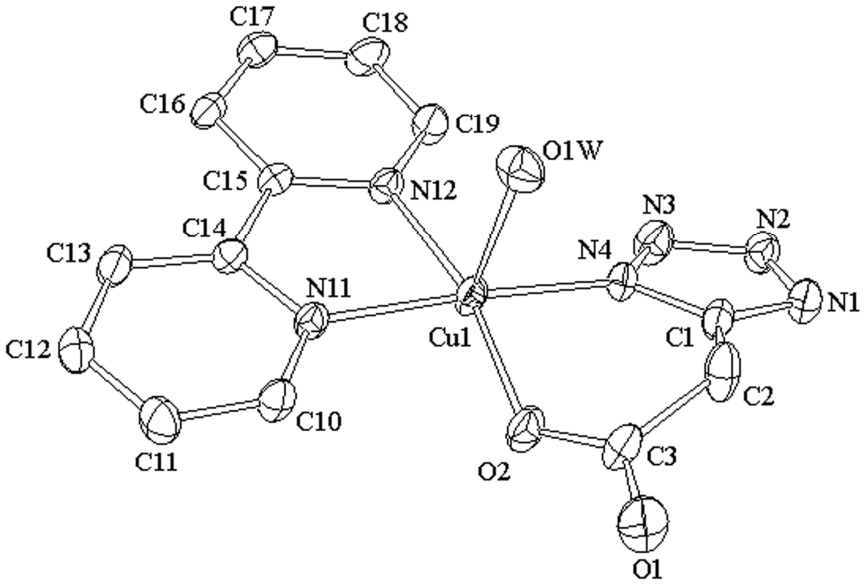

Fig. S10. ORTEP plot of complex **4** with thermal ellipse at the 30 % probability level.