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Accessory Publication

Copper(II) Complexes with *cis*-Epoxysuccinate Ligand: Syntheses, Crystal Structures, and Magnetic Properties

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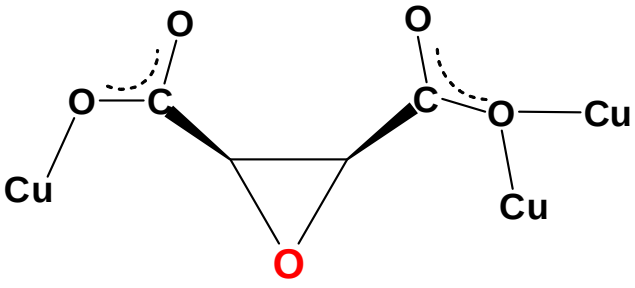
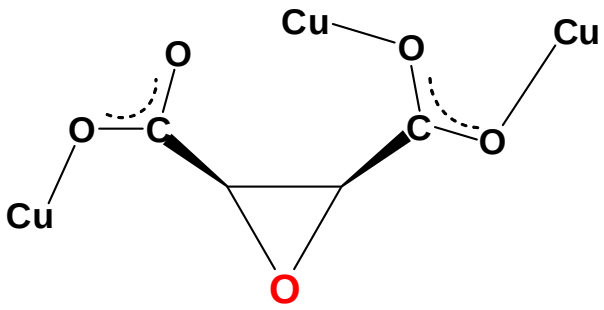


(a)



(b)

Scheme S1 Coordination modes of fully deprotonated **ces** ligand in **1**–**3**:

(a) For **1** and **2**: μ_1-η^1:η^0-monodentate mode for the carboxylate group at the left side and μ_2-η^2:η^0-bridging mode for the carboxylate group at the right side;

(b) For **3**: μ_1-η^1:η^0-monodentate mode for the carboxylate group at the left side and μ_2-η^1:η^1-*syn-anti* bridging mode for the carboxylate group at the right side.

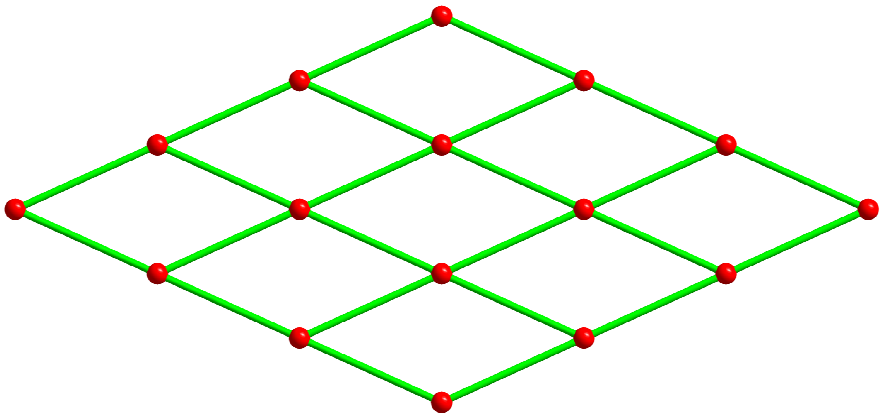


Fig. S1. Schematic representation of the (4,4) topological layer in **3**.

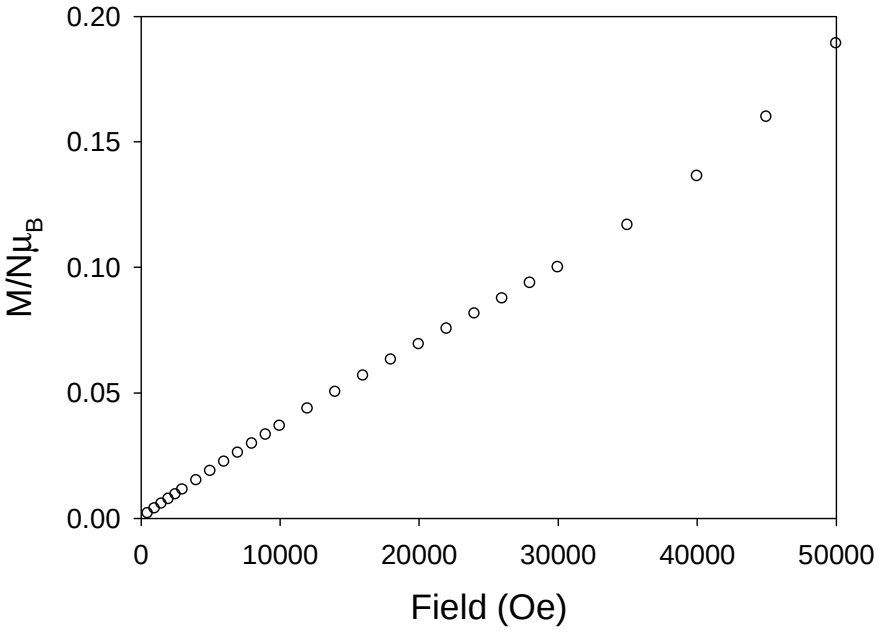
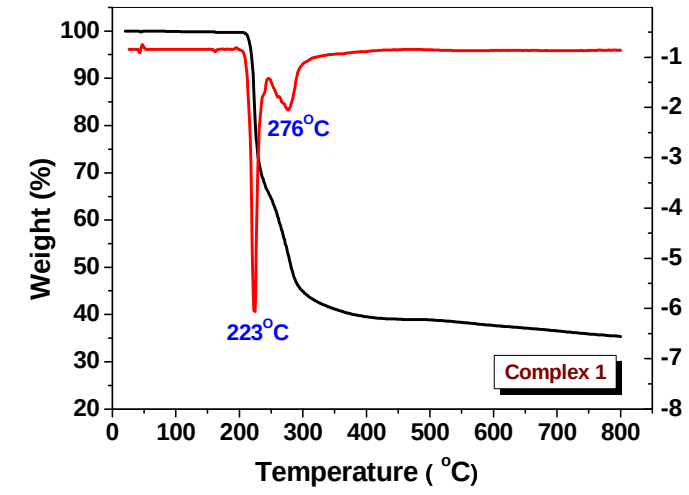
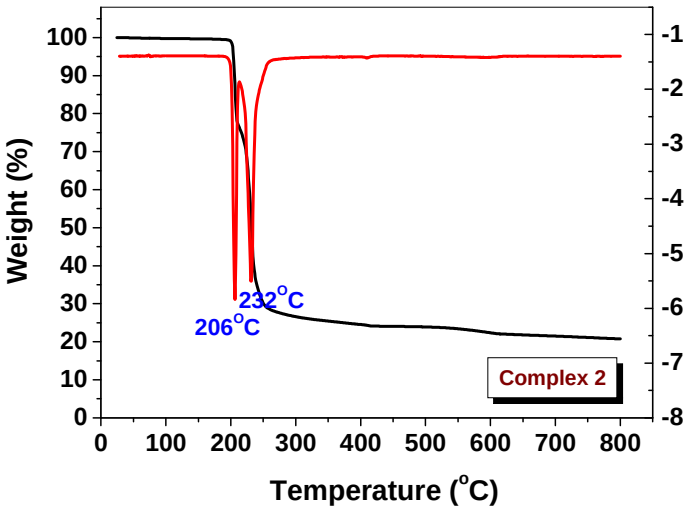


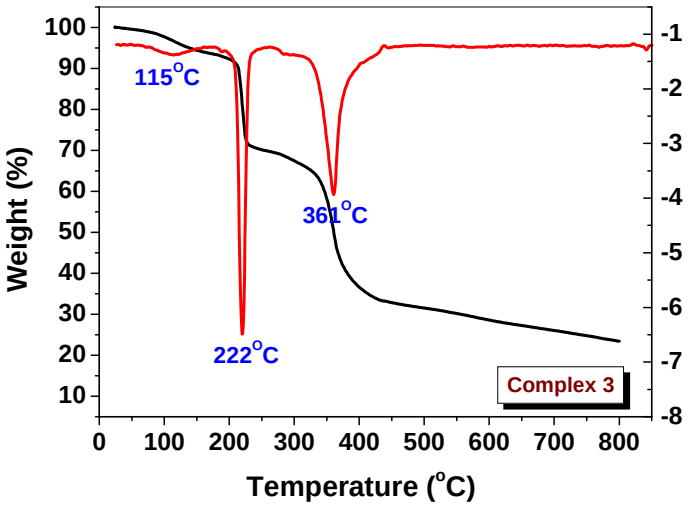
Fig. S2. Magnetization *vs.* field behavior of **3** at 2 K.



(a)

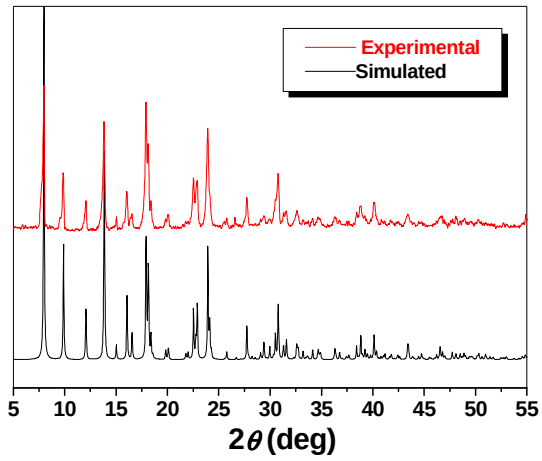


(b)

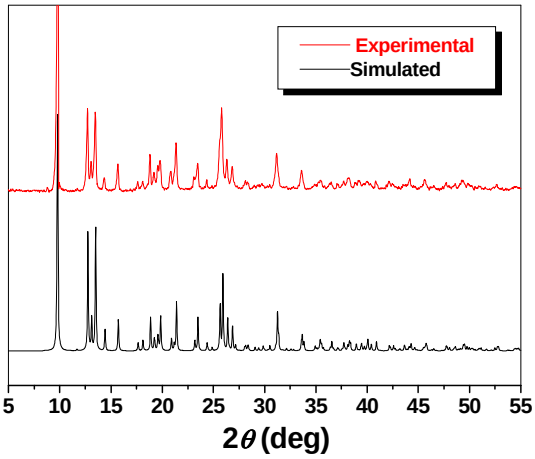


(c)

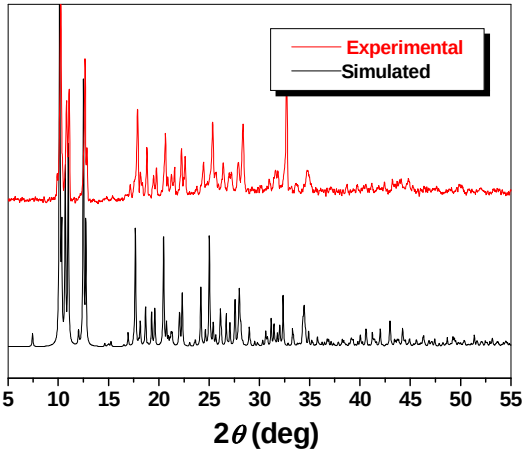
Fig. S3. Thermogravimetric analysis (TGA) plots of **1** (a), **2** (b), and **3** (c).



(a)



(b)



(c)

Fig. S4. XRPD patterns of **1** (a), **2** (b), and **3** (c).

Table S1. Selected bond distances (Å) and bond angles (°) for **1**[A]

Cu1–O4$^{\#1}$	1.9434(18)	Cu1–O1$^{\#1}$	1.9831(18)
Cu1–N1	2.008(2)	Cu1–N2	2.012(2)
Cu1–O1	2.3402(19)		
O4$^{\#1}$–Cu1–O1$^{\#1}$	92.33(8)	O4$^{\#1}$–Cu1–N1	171.17(9)
O1$^{\#1}$–Cu1–N1	95.07(8)	O4$^{\#1}$–Cu1–N2	90.51(8)
O1$^{\#1}$–Cu1–N2	176.35(8)	N1–Cu1–N2	81.91(9)
O4$^{\#1}$–Cu1–O1	93.12(7)	O1$^{\#1}$–Cu1–O1	77.01(7)
N1–Cu1–O1	93.22(8)	N2–Cu1–O1	105.14(8)
Cu1$^{\#1}$–O1–Cu1	102.99(7)		

[A] Symmetry code: #1 = $-x + 2, -y, -z$.

Table S2. Selected hydrogen–bonding geometry (Å, °) for **1**[A]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	D–H···A
C3–H3A···*Cg*1	0.98	2.82	3.636(3)	142
C7–H7A···O3[a]	0.93	2.36	3.217(3)	153
C6–H6A···O2[b]	0.93	2.37	3.049(4)	130

[A] Symmetry codes for **1**: a = $-x + 5/2$, $y + 1/2$, $-z + 1/2$; b = $x + 1$, y, z. *Cg*1 is the centroid of C11–C15/N2 pyridyl ring of phen ligand.

Table S3. Selected bond distances (Å) and bond angles (°) for **2**[A]

Cu1–O3	1.950(4)	Cu1–O1	1.984(3)
Cu1–N2	1.988(4)	Cu1–N1	1.995(4)
Cu1–O1$^{\#1}$	2.369(4)	Cu1–O5	2.478(4)
Cu1$^{\#1}$–O1	2.369(4)	Cu1–Cu1$^{\#1}$	3.4589(19)
O3–Cu1–O1	91.82(15)	O3–Cu1–N2	170.93(15)
O1–Cu1–N2	94.50(16)	O3–Cu1–N1	92.00(16)
O1–Cu1–N1	173.60(14)	N2–Cu1–N1	81.15(17)
O3–Cu1–O1$^{\#1}$	92.17(15)	O1–Cu1–O1$^{\#1}$	75.10(15)
N2–Cu1–O1$^{\#1}$	95.74(15)	N1–Cu1–O1$^{\#1}$	109.88(15)
O3–Cu1–O5	77.28(15)	O1–Cu1–O5	76.40(14)
N2–Cu1–O5	97.88(16)	N1–Cu1–O5	99.45(15)
O1$^{\#1}$–Cu1–O5	149.20(12)		

[A] Symmetry code: #1 = $-x + 1, -y + 1, -z + 1$.

Table S4. Selected hydrogen–bonding geometry (Å, °) for **2**[A]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	D–H···A
C11–H11A··· O4[a]	0.93	2.43	3.329(1)	164
C12–H12A··· O2[a]	0.93	2.42	3.341(2)	170
C15–H15A··· O2[a]	0.93	2.33	3.258(1)	179
C16–H16A··· O5[b]	0.93	2.52	3.320(2)	145

[A] Symmetry codes for **2**: a = *x*, *y*, *z* – 1/2; b = –*x*, –*y* + 1, –*z*.

Table S5. Selected bond distances (Å) and bond angles (°) for **3**[A]

Cu1–O2	1.958(3)	Cu1–N1	1.960(3)
Cu1–O4	1.964(3)	Cu1–N2	2.034(3)
Cu1–O5$^{\#1}$	2.389(3)	Cu1–O1	2.473(3)
Cu2–N6$^{\#2}$	1.973(3)	Cu2–N5	1.989(3)
Cu2–N3	1.995(3)	Cu2–N4	2.048(3)
Cu2–O6	2.449(3)	Cu2$^{\#2}$–N6	1.973(3)
Cu1$^{\#3}$–O5	2.389(3)		
O2–Cu1–N1	94.05(12)	O2–Cu1–O4	91.66(12)
N1–Cu1–O4	169.65(12)	O2–Cu1–N2	175.12(12)
N1–Cu1–N2	81.08(12)	O4–Cu1–N2	93.19(12)
O2–Cu1–O5$^{\#1}$	91.15(11)	N1–Cu1–O5$^{\#1}$	90.80(11)
O4–Cu1–O5$^{\#1}$	97.71(11)	N2–Cu1–O5$^{\#1}$	88.70(11)
O2–Cu1–O1	77.73(10)	N1–Cu1–O1	95.97(11)
O4–Cu1–O1	76.82(11)	N2–Cu1–O1	102.90(10)
O5$^{\#1}$–Cu1–O1	167.33(9)	N6$^{\#2}$–Cu2–N5	96.06(11)
N6$^{\#2}$–Cu2–N3	91.44(12)	N5–Cu2–N3	172.38(12)
N6$^{\#2}$–Cu2–N4	175.42(12)	N5–Cu2–N4	81.23(12)
N(3)–Cu2–N4	91.21(12)	N6$^{\#2}$–Cu2–O6	95.94(13)
N5–Cu2–O6	92.31(12)	N3–Cu2–O6	88.28(12)
N4–Cu2–O6	87.88(13)		

[A] Symmetry codes for **3**: #1 = $x - 1/2, -y + 3/2, z - 1/2$; #2 = $-x + 1, -y + 1, -z + 2$; #3 = $x + 1/2, -y + 3/2, z + 1/2$.

Table S6. Selected hydrogen–bonding geometry (Å, °) for **3**[A]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	D–H···A
C7–H7A···O5[a]	0.93	2.49	3.281(7)	143
C11–H11A···O3[a]	0.93	2.40	3.216(6)	146
C16–H16A···O1[b]	0.93	2.56	3.401(7)	151
C15–H15A···*Cg*1[b]	0.93	2.54	3.416(5)	156
C7–H7A···*Cg*2[c]	0.93	2.88	3.347(4)	113

[A] Symmetry codes for **3**: a = *x* – 1, *y*, *z*; b = *x*, *y*, *z* – 1; c = *x* + 1, *y* + 1, *z* + 2. *Cg*1 and *Cg*2 are the centroids of C5–C9/N2 and C13–C17/N4 pyridyl rings of phen ligands.