

# Supporting Information

## 2D Layer Structure in Two New Cu(II) Crystals: Structural Evolvment and Properties

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**Table S1.** Hydrogen-bonding parameters in **1**.

D–H···A	d(D···H)/Å	d(H···A)/Å	d(D···A)/Å	D–H···A /°	Symmetry code
O5–H5A···O1 <sup>1</sup>	0.85	1.92	2.757(2)	166.7	<sup>1</sup> -1/2+X, 3/2-Y, -1/2+Z
O5–H5B···O4 <sup>2</sup>	0.85	2.07	2.880(2)	160.1	<sup>2</sup> 5/2-X, 1/2+Y, -1/2-Z

**Table S2.** Hydrogen-bonding parameters in **2**.

D–H···A	d(D···H)/Å	d(H···A)/Å	d(D···A)/Å	D–H···A /°	Symmetry code
O1–H1···O4 <sup>1</sup>	0.82	1.78	2.5770(16)	165.4	<sup>1</sup> -1+X,+Y,+Z

**Table S3.** Selected bond lengths (Å) and angles (°) for **1**.

Cu1-N1	2.0288(15)	N2-C10	1.337(2)
Cu1-N3	2.0452(15)	C11-N3	1.354(2)
Cu1-O4 <sup>1</sup>	2.0950(13)	N3-C15	1.334(2)
Cu1-O2 <sup>2</sup>	1.9399(12)	C23-O4	1.267(2)
N1-C5	1.353(2)	C23-O3	1.236(2)
N1-C1	1.333(2)	C22-O2	1.273(2)
N1-Cu1-N3	157.18(6)	O22-Cu1-N1	99.69(6)
N1-Cu1-O4 <sup>1</sup>	97.16(6)	O22-Cu1-N3	94.26(6)
N3-Cu1-O4 <sup>1</sup>	98.64(6)	O22-Cu1-N2	146.54(6)
N2-Cu1-N1	79.43(6)	O22-Cu1-O4 <sup>1</sup>	98.17(6)
N2-Cu1-N3	78.98(6)	C5-N1-Cu1	114.83(12)
N2-Cu1-O4 <sup>1</sup>	115.20(6)	C1-N1-Cu1	125.76(13)

<sup>1</sup>-1/2+X, 3/2-Y, 1/2+Z; <sup>2</sup>-1+X, +Y, +Z

**Table S4.** Selected bond lengths (Å) and angles (°) for **2**.

Cu1-O3 <sup>1</sup>	2.2431(13)	O2-C22	1.218(2)
Cu1-O5	1.9102(11)	O5-C27	1.275(2)
Cu1-N2	1.9330(13)	N2-C10	1.335(2)
Cu1-N3	2.0217(14)	N2-C6	1.340(2)
Cu1-N1	2.0200(14)	N3-C11	1.355(2)
O3-C23	1.266(2)	N3-C15	1.337(2)
O5-Cu1-O3 <sup>1</sup>	91.43(5)	C1-N1-C5	119.32(15)
O5-Cu1-N2	168.28(6)	N2-C10-C9	120.49(14)
O5-Cu1-N3	98.81(5)	N1-C5-C6	113.64(14)
O5-Cu1-N1	99.87(5)	N1-C5-C4	121.60(15)
N2-Cu1-O3 <sup>1</sup>	100.26(5)	N3-C11-C10	113.41(14)
N2-Cu1-N3	79.90(5)	N3-C11-C12	121.55(14)

<sup>1</sup>+X, 1 +Y, +Z