Supplemental Materials

Fig. S1 Molecular structure of compound **1** [31]

Fig. S2 Molecular structure of ligand **O1** (30% probability level)

Fig. S3 Unit cell of ligand **O1** with hydrogen bonding

(1: x, y, z; 2: ½ – x, ½ + y, ½ – z; 3: – x, – y, – z; 4: ½ + x, ½ – y, ½ + z)

Table S1 Selected torsion angle (º) in ligands **O1**, **O2**, and **O3**

Torsion angle (º)	O1	O2	O3
C6-S1-N1-C1 C2-S1-N1-C13 [a]	179.94(16)	179.6(3)	179.67(17)
N1-S1-C6-N3 N1-S1-C2-N3	179.64(16)	179.1(3)	-179.08(17)
S1-N1-C5-C4 S1-N1-C1-C10	-178.98(14)	-178.9(2)	-179.23(15)
C1-N1-C5-N2 C13-N1-C1-N2	-179.79(16)	179.7(3)	179.69(17)
C5-N2-C6-N3 C1-N2-C2-N3	-179.42(17)	179.4(3)	179.14(19)
C7-N3-C6-S1 C3-N3-C2-S1	-0.3(2)	-0.9(4)	-0.9(2)
C7-N3-C6-N2 C3-N3-C2-N2	179.26(17)	178.7(3)	179.92(18)
C6-N3-C7-O1 C2-N3-C3-O1	1.7(3)	0.0(5)	-1.1(3)
C6-N3-C7-C8 C2-N3-C3-C4	-177.36(16)	179.8(3)	178.82(18)
O1-C7-C8-C9 O1-C3-C4-C9	178.75(17)	-1.1(5)	-177.3(2)
N3-C7-C8-C9 N3-C3-C4-C5	-2.1(3)	179.2(3)	-176.38(19)

[a] First molecule in **O3**

Table S2 Complete information about bond length (Å) and angle (º) in complexes **C2** and **C3**

bond length (Å)	C2	C3	bond angle (º)	C2	C3
Cu1-N2	1.988(2)	1.990(2)	N2-Cu1-N2#1/2B	180.0	168.33(9)
Cu1-N2#1/2B	1.988(2)	1.996(2)	N2-Cu1-Cl1	91.10(6)	91.92(7)
Cu1-Cl1	2.2637(14)	2.2356(10)	N2#1/2B-Cu1-Cl1	88.90(6)	91.37(7)
Cu1-Cl1#1/Cl2	2.2637(14)	2.2544(10)	N2-Cu1-Cl1#1/Cl2	88.90(6)	89.74(7)
S1-C6	1.754(2)	1.747(3)	N2#1/2B-Cu1-Cl1#1	91.10(6)	88.55(7)
S1-N1	1.795(2)	1.809(2)	Cl1-Cu1-Cl1#1/Cl2	180.0	171.94(4)
S1-O1	2.124(2)	2.076(2)	C6-S1-N1	85.53(10)	85.60(13)
N1-C5	1.361(3)	1.353(3)	C6-S1-O1	79.71(9)	80.43(12)
N1-C1	1.364(3)	1.368(3)	N1-S1-O1	165.22(7)	165.97(10)
N2-C6	1.333(3)	1.331(3)	C7-O1-S1	105.68(15)	106.36(18)
N2-C5	1.362(3)	1.363(3)	C5-N1-C1	121.4(2)	122.6(3)
N3-C6	1.328(3)	1.331(3)	C5-N1-S1	112.92(14)	112.13(19)
N3-C7	1.345(3)	1.344(3)	C1-N1-S1	125.63(15)	125.2(2)
S1B-C6B		1.754(3)	C6-N2-C5	112.73(18)	112.4(2)
S1B-N1B		1.784(2)	C6-N2-Cu1	117.29(14)	120.98(19)
S1B-O1B		2.188(2)	C5-N2-Cu1	129.87(15)	126.64(19)
N1B-C5B		1.360(3)	C6-N3-C7	111.69(19)	110.8(2)
N1B-C1B		1.368(3)	C2-C1-N1	119.4(2)	117.5(3)
N2B-C6B		1.325(3)	C6B-S1B-N1B		86.16(12)
N2B-C5B		1.359(3)	C6B-S1B-O1B		78.82(11)
N3B-C6B		1.324(3)	N1B-S1B-O1B		164.97(9)
N3B-C7B		1.354(3)	C7B-O1B-S1B		104.71(17)
			C5B-N1B-C1B		122.5(2)
			C5B-N1B-S1B		112.17(18)
			C1B-N1B-S1B		125.30(19)
			C6B-N2B-C5B		112.7(2)
			C6B-N2B-Cu1		114.82(18)
			C5B-N2B-Cu1		131.95(18)
			C6B-N3B-C7B		112.4(2)
			C2B-C1B-N1B		117.6(3)