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SUPPLEMENTARY MATERIAL TO

Synthesis and crystal structure of copper(II) complexes with pyridoxal *S*-methylisothiosemicarbazone bearing a new coordination mode

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ANALYTICAL AND SPECTRAL DATA FOR **1** AND **2**

[{Cu(μ-PLITSC)NCS}$_2$](NCS)$_2$·2MeOH ***(1)***. Yield: 0.05 g (45 %); dark-green single crystals, m.p.: 149 °C, Anal. calcd. for $CuC_{13}H_{18}N_6S_3O_3$: C, 33.50; H, 3.89; N, 18.04; S, 20.64 %. Found: C, 33.38; H, 3.57; N, 17.95; S, 20.36 %. Selected IR bands (KBr, cm^{-1}): 2850(*w*), 2784(*w*), 2115(s), 2075(*vs*), 1558(*m*), 1305(*m*). Conductivity (MeOH, Λ_M / Ω^{-1} cm^2 mol^{-1}): 86.

{[Cu(μ-PLITSC)NCS]NO$_3$·MeOH}$_n$ ***(2)***. Yield: 0.04 g (38 %); dark-green single crystals, m.p.: 195 °C, Anal. calcd. for $CuC_{12}H_{18}N_6S_2O_6$: C, 30.66; H, 3.86; N, 17.88; S, 13.64 %. Found: C, 30.52; H, 3.49; N, 17.71; S, 13.51 %, Selected IR bands (KBr, cm^{-1}): 2848(*w*), 2058(*vs*), 1560(*m*), 1385(*vs*), 1329(*m*). Conductivity [MeOH, Λ_M / Ω^{-1} cm^2 mol^{-1}]: 114.

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TABLE S-I. Crystallographic and refinement details

Crystal data	**1**	**2**
Chemical formula	$C_{26}H_{36}Cu_2N_{12}O_6S_6$	$C_{12}H_{18}CuN_6O_6S_2$
M_r	466.05	469.98
Crystal system	Triclinic	Orthorhombic
Space group	$P\bar{1}$	*Pbcn*
Temperature, K	295	295
a / Å	8.7640(5)	13.4682(4)
b / Å	9.4490(6)	12.6874(3)
c / Å	12.2731(5)	22.3679(4)
α / °	82.134(4)	90
β / °	83.863(4)	90
γ / °	75.190(5)	90
V / Å^3	970.59(10)	3822.15(16)
Z	2	8
Radiation type	Mo Kα	Mo Kα
μ / mm^{-1}	1.47	1.40
Crystal size, mm	0.55 × 0.29 × 0.16	0.57 × 0.50 × 0.23
	Data collection	
Diffractometer	Gemini S (Oxford Diffraction)	
Absorption correction	Analytical	Analytical
T_{min}, T_{max}	0.578, 0.805	0.546, 0.739
Measured reflections	10369	36990
Independent reflections	3950	3909
Observed [$I > 2\sigma(I)$] reflections	3536	3442
R_{int}	0.016	0.030
$(\sin \theta/\lambda)_{max}$ / Å^{-1}	0.625	0.626
	Refinement	
$R[F^2 > 2\sigma(F^2)]$	0.029	0.034
$wR(F^2)$	0.073	0.081
S	1.05	1.15
No. of reflections	3950	3909
No. of parameters	252	253
No. of restraints	5	2
H-atom treatment	Mixed	Mixed
$\Delta\rho_{max}$, $\Delta\rho_{min}$ / e Å^{-3}	0.35, –0.22	0.31, –0.28

TABLE S-II. Selected structural parameters (Å, °) of cations in **1** and **2**

Bond	**1**	**2**
	Length, Å	
Cu1–O1	1.9163(14)	1.9106(15)
Cu1–O2^{i}	2.4706(16)	2.3707(17)
Cu1–N1	1.9595(17)	1.9728(19)
Cu1–N3	1.9760(16)	1.9926(17)
Cu1–N5	1.9331(18)	1.958(2)
C1–N1	1.281(3)	1.288(3)
C1–N2	1.357(2)	1.357(3)
N2–N3	1.378(2)	1.374(2)
C2–N3	1.285(2)	1.288(3)
C4–O1	1.293(2)	1.292(3)
	Angle, °	
O1–Cu1–N5	91.95(7)	90.77(8)
O1–Cu1–N3	89.38(6)	88.77(7)
N1–Cu1–N3	80.56(7)	79.67(8)
N1–Cu1–N5	98.08(7)	100.05(8)
O1–Cu1–O2^{i}	87.68(6)	96.31(7)
N1–Cu1–O2^{i}	98.46(7)	88.99(8)
N3–Cu1–O2^{i}	86.10(6)	102.15(6)
N5–Cu1–O2^{i}	94.25(7)	88.51(8)
O1–Cu1–N1	167.78(7)	168.09(8)
N3–Cu1–N5	178.64(7)	169.32(8)
N1–C1–N2	117.80(17)	117.1(2)
C1–N2–N3	115.13(16)	115.58(17)
N2–N3–C2	118.65(16)	117.42(17)
N3–C2–C3	121.92(17)	123.0(2)
C5–N4–C7	124.19(17)	124.80(19)