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SUPPLEMENTARY MATERIAL TO

Square-pyramidal mononuclear, dinuclear and polymeric copper(II) complexes with (2-pyridinylmethyl)amino derivatives

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ANALYTICAL AND SPECTRAL DATA

4-{[2-(Pyridin-2-ylmethylamino)ethylamino]methyl}benzoic acid hydrochloride ***HL3***·*HCl*

^{1}H NMR (300 MHz, DMSO-d_6, in ppm): δ 3.35−3.41 (m, 4H, CH_2^aCH_2^b), 4.23 (s, 2H, CH_2^c), 4.33 (s, 2H, CH_2^d), 7.41 ('t', 1H, CH^f), 7.56 ('d', 1H, CH^e), 7.70 (d, $^3J_{H,H}$ = 8.0 Hz, 2H, CH^g), 7.87 ('t', 1H, CH^l), 7.95 (d, $^3J_{H,H}$ = 8.0 Hz, 2H, CH^h), 8.59 ('d', 1H, CH^m). ^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6, in ppm): δ 43.2 (s, CH_2^a), 43.4 (s, CH_2^b), 49.9 (s, CH_2^c), 50.9 (s, CH_2^d), 123.3 (s, CH^e), 123.7 (s, CH^f), 129.5 (s, CH^g), 130.1 (s, CH^h), 130.2 (s, C^j), 131.2 (s, C^k), 137.4 (s, CH^l), 149.1 (s, CH^m), 152.4 (s, C^n), 167.1 (s, CO). IR: $\tilde{\nu}$ (cm^{-1}) 3435 (s, br), 2930 (s), 2757 (s), 2696 (s), 2587 (m), 2418 (m), 1683 (s), 1615 (m), 1432 (m), 1320 (m), 1277 (m), 1232 (m), 1106(s), 809 (s), 760 (s).

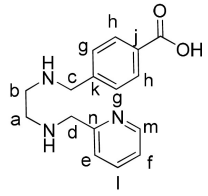

Fig. S-1. Atom numbering scheme of **HL3**.

Compound ***1***

Elemental analysis for $C_9H_{12}Cl_2CuN_2O_2$ (314.65), Calculated: C, 34.35; H, 3.84; N, 8.90 %; Found: C, 34.75, 3.91; N, 9.11 %. ESI-MS (CH_3OH), positive mode: *m*/*z* 278.2 $[M–Cl]^+$.

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IR: $\tilde{\nu}$ (cm^{-1}) 3419 (br, w), 3209 (s), 3033 (m), 2949 (m), 1751 (s), 1608 (m), 1452 (m), 1440 (m), 1419 (w), 1357 (m), 1240 (s), 1204 (m), 1159 (w), 1131 (w), 1112 (w), 1028 (m), 1008 (m), 931 (w), 772 (s).

*Compound **2***

Elemental analysis for $C_{26}H_{24}Cl_4Cu_2N_4O_4$ (725.37), Calculated: C, 43.05; H, 3.34; N, 7.72 %; Found: C, 42.83, 3.30; N, 7.72 %. ESI-MS (CH_3OH), positive mode: *m*/*z* 688.9 $[M–Cl]^+$. IR: $\tilde{\nu}$ (cm^{-1}) 3421 (br, s), 3210 (m), 2963 (m), 2360 (w), 1717 (m), 1699 (m), 1684 (w), 1608 (s), 1558 (w), 1541 (w), 1507 (w), 1261 (m), 1177 (m), 1104 (m).

*Compound **3***

ESI-MS (CH_3OH), positive mode: *m*/*z* 383.0 $[M–Cl]^+$. IR: $\tilde{\nu}$ (cm^{-1}) 3417 (br, s), 3208 (m), 3157 (m), 2925 (s), 1712 (s), 1670 (m), 1611 (m), 1452 (m), 1319 (w), 1262 (s), 1112 (s), 1023 (s), 801 (m), 769 (m).

TABLE S-I. Crystallographic parameters of copper(II) complexes **1**–**3**; †: twinned crystal needle

Name	**1**†	**2**	**3**
Formula	$C_9H_{12}Cl_2CuN_2O_2$	$C_{26}H_{24}Cl_4Cu_2N_4O_4$	$C_{16}H_{19}Cl_2CuN_3O_2$
Fw (g mol^{-1})	314.65	725.37	419.78
Temperature (K)	130(2)	130(2)	130(2)
crystal color	green	green	blue
crystal size (mm)	0.29 × 0.03 × 0.02	0.15 × 0.03 × 0.01	0.30 × 0.10 × 0.02
crystal system	monoclinic	orthorhombic	monoclinic
space group	$P2_1/c$	*Pccn*	$P2_1/c$
a (Å)	19.195(1)	8.8843(5)	13.2615(4)
b (Å)	8.7089(4)	20.018(1)	10.3590(3)
c (Å)	6.9006(4)	15.899(1)	14.5507(6)
α (°)	90	90	90
β (°)	96.350(5)	90	113.210(4)
γ (°)	90	90	90
V (nm^3)	1.1465(1)	2.8276(3)	1.8371(1)
Z	4	4	4
calcd density (g cm^{-3})	1.823	1.704	1.518
F(000)	636	1464	860
no. of collected reflns	2629	16673	15658
no. of independent reflns	2629	2501	4563
R_{int}	0.0868	0.2079	0.0563
no. of reflns observed	1602	1290	3443
restrains/parameters	0 / 150	2 / 189	0 / 293
R [$I > 2\sigma(I)$]	R_1 = 0.0629, wR_2 = 0.1359	R_1 = 0.0542, wR_2 = 0.0869	R_1 = 0.0406, wR_2 = 0.0758
R (all data)	R_1 = 0,1039, wR_2 = 0,1435	R_1 = 0,1427, wR_2 = 0,1108	R_1 = 0.0635, wR_2 = 0.0844
Goof, *S*	1.006	1.000	1.032
$\Delta\rho_{max}/\Delta\rho_{min}$ (e Å^{-3})	1.234 /−0.625	0.629/−0.497	0.478/−0.377