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SUPPLEMENTARY MATERIAL TO

Synthesis, characterization and biological study of Cu(II) complexes of aminopyridine and aminomethylpyridine Schiff bases

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TABLE S-I. Crystal data and structure refinements for [CuL^{6}Cl]

Empirical formula	$C_{14}H_{13}ClCuN_2O_2$
Formula weight	340.25
Temperature, K	266 (2)
Wavelength, nm	0.71073
Crystal system	Monoclinic
Space group	$P2_1/c$
a / nm	7.01350 (10)
b / nm	18.1484 (4)
c / nm	10.3959 (2)
V / nm^3	1282.77 (4)
Z	4
D / g cm^{-3}	1.762
μ / mm^{-1}	1.912
F (000)	692
Angle range (θ) for data collection, °	2.24 – 28.00
No. reflections/observed	3097 / 2754
$R_{int.}$	0.0208
Data/restraints/parameter	3097 / 0 / 193
Goodness-of-fit	1.034
Refinement method	Full-matrix least squares of F^2
Final R indices [$F^\circ > 4\sigma$ (F)]	$R1$ = 0.0260, $WR2$ = 0.05780
R indices (all data)	$R1$ = 0.0207, $WR2$ = 0.0558

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TABLE S-II. Physical and analytical data for the complexes; M.W: molecular weight, m.p: melting point

Complex	M.W. g mol^{-1}	M.p. °C	Colour	Yield %	Found (Calcd.), %				Λ_M / Ω^{-1} cm^2 mol^{-1}
					C	H	N	Cu	
CuL^1Cl	296.28	196–198	Brown	46	48.43 (48.65)	3.25 (3.06)	9.99 (9.42)	21.75 (21.45)	57.95[a]
$Cu(L^2)_2Cl_2·1/2H_2O$	540.03	198–200	Green	73	53.63 (53.36)	3.94 (3.92)	10.64 (10.37	10.43 (10.70)	48.55[a]
$Cu(L^3)_2Cl_2$ $1/2H_2O$	631.62	161–162	Green	56	49.16 (49.44)	3.95 (3.99)	9.84 (8.87)	9.56 (9.22)	52.90[a]
$CuL^4Cl_2·(H_2O)$	379.81	180–182	Green	55	40.79 (41.00)	3.33 (3.71)	7.51 (7.36)	16.50 (16.73)	79.75 (1:1)
$Cu(L^5)_2Cl_2·H_2O$	609.09	193–195	Green	81	51.92 (51.27)	4.14 (4.30)	9.42 (9.20)	10.87 (10.43)	50.70[a]
CuL^6Cl	682.68	172–174	Green	87	49.86 (49.26)	4.02 (4.13)	8.41 (8.21)	18.50 (18.67)	47.50[a]

[a]Neutral complexes

TABLE III. Infrared and UV–Vis spectral data for the Schiff base ligands and the complexes

Compound	ν_{OH} cm^{-1}	$\nu_{C=N}$ cm^{-1}	ν_{CO} cm^{-1}	ν_{Cu-O} cm^{-1}	ν_{Cu-N} cm^{-1}	ν_{Cu-Cl} cm^{-1}	λ_{max} / nm
L^1	3210–2071	1588	1278	–	–	–	207, 268, 304, 345
$[CuL^1Cl]$	3327	1584	1292	441	388	358, 257	210, 236, 403, 647
L^2	3109–2127	1611	1196	–	–	–	203, 217, 275, 340
$[Cu(L^2)_2Cl_2]1/2H_2O$	3119–2395	1613	1229	419	380	358, 290, 262	279, 340, 804
L^3	3058	1627	1278	–	–	–	215, 256, 316
$[Cu(L^3)_2Cl_2]1/2H_2O$	3058	1620	1274	442	372	269	268, 306, 370, 513, 685
L^4	3114–2375	1607	1275	–	–	–	270, 312, 475
$[CuL^4Cl(H_2O)]Cl$	3413, 3195–2856	1598	1299	502	424	276	233, 300, 416, 715
L^5	3109–2390	1613	1272	–	–	–	225, 286, 301
$[Cu(L^5)_2Cl_2]H_2O$	3205–2385	1606	1284	482	427	293	293, 486, 634
L^6	3104–2152	1631	1268	–	–	–	221, 262, 299, 335, 425
$[CuL^6Cl]$	–	1624	1282	501	421	314	234, 277, 388, 629

CHARACTERIZATION DATA FOR THE SCHIFF BASE LIGANDS

Ligand L^1. Yield: 1.95 g, 98 %; m.p.: 53–54 °C; Anal. Calcd. for $C_{12}H_{10}N_2O$: C, 72.71; H, 5.09; N, 14.13 %. Found: C, 72.94; H, 5.09; N, 14.17

%; IR (ATR, cm^{-1}): 3048, 1588, 1278, ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 13.50 (1H, *s*, OH), 9.50 (1H, *s*, N=CH, py), 8.60 (1H, *s*, HC=N), 7.8 (1H, *t*, J = 7.26 Hz, Ar-H), 7.50 (1H, *d*, J = 7.37 Hz, Ar-H), 7.40 (1H, *t*, J = 7.37 Hz, Ar-H), 7.36 (1H, *d*, J = 7.78 Hz, Ar-H), 7.25 (1H, *t*, J = 7.41 Hz, Ar-H), 7.10 (1H, *d*, J = 8.0 Hz, Ar-H), 7.0(1H, *t*, J = 6.92 Hz, Ar-H); ^{13}C-NMR (400 MHz, $CDCl_3$, δ / ppm): 165.20, 162.31, 158.04, 149.40, 138.92, 134.29, 133.92, 123.00, 120.89, 119.69, 119.43, 117.30.

Ligand L[2]. Yield: 1.75 g, 88 %; m.p.: 57–58 °C; Anal. Calcd. for $C_{12}H_{10}N_2O$: C, 72.71; H, 5.09; N, 14.13 %. Found: C, 72.79; H, 5.22; N, 14.13 %; IR (ATR, cm^{-1}): 3053, 1611, 1292; ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 12.80 (1H, *s*, OH), 8.67 (1H, *s*, HC=N), 8.60 (1H, *d*, J = 7.85 Hz, Ar-H), 8.57 (1H, *d*, J = 7.43 Hz, Ar-H), 7.60 (1H, *d*, J = 8.11 Hz, Ar-H), 7.45 (2H, *m*, Ar-H), 7.40 (1H, *dd*, J_1 = 7.21 Hz & J_2 = 2.1 Hz, Ar-H), 7.08 (1H, *d*, J = 7.57 Hz, Ar-H), 7.0 (1H, *t*, J = 8.21 Hz, Ar-H); ^{13}C-NMR (400 MHz, $CDCl_3$, δ / ppm): 164.97, 161.56, 148.41, 145.14, 143.49, 134.31, 133.10, 128.44, 124.30, 119.78, 119.37, 117.86.

Ligand L[3]. Yield: 1.52 g, 72 %; m.p.: 41–42 °C; Anal. Calcd. for $C_{13}H_{12}N_2O$: C, 74.00; H, 5.93; N, 13.28 %. Found: C, 73.56; H, 5.69; N, 13.20 %; IR (ATR, cm^{-1}): 3058, 1627, 1274; ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 13.0 (1H, *s*, OH), 8.60 (1H, *d*, J = 6.87 Hz, Ar-H), 8.58 (1H, *dd*, J_1 = 7.13 Hz & J_2 = 2. 31 Hz, Ar-H), 8.50 (1H, *s*, HC=N), 7.70 (1H, *d*, J = 7.81 Hz, Ar-H), 7.40 (1H, *m*, Ar-H), 7.32 (1H, *t*, J = 7.67 Hz, Ar-H), 7.0 (1H, *d*, J = 7.68 Hz, Ar-H), 6.90 (1H, *t*, J = 8.22 Hz, Ar-H), 4.85 (2H, *s*, CH_2); ^{13}C-NMR (400 MHz, $CDCl_3$, δ / ppm): 166.88, 161.33, 149.60, 149.32, 135.84, 133.15, 132.03, 124.07, 119.03, 117.51, 61.19.

Ligand L[4]. Yield: 2.05 g, 90 %; m.p.: 86–88 °C; Anal. Calcd. for $C_{13}H_{12}N_2O_2$: C, 68.40; H. 5.29; N, 12.27 %. Found: C, 68.50; H, 5.20; N, 12.30 %; IR (ATR, cm^{-1}): 3058, 1587, 1277; ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 14.0 (1H, *s*, OH), 9.40 (1H, *s*, N=CH, py), 8.40 (1H, *s*, HC=N), 7.80 (1H, *t*, J = 7.14 Hz, Ar-H), 7.30 (1H, *d*, J = 7.53 Hz, Ar-H), 7.25 (1H, *t*, J = 7.25 Hz, Ar-H), 7.16 (1H, *d*, J = 7.38 Hz, Ar-H), 7.0 (1H, *d*, J = 7.49 Hz, Ar-H), 6.90 (1H, *t*, J = 7.56 Hz, Ar-H), 3.97 (3H, *s*, OCH_3); ^{13}C-NMR (400 MHz, $CDCl_3$, δ / ppm): 165.03, 157.62, 152.92, 149.40, 148.90, 139.00, 125.30, 123.10, 121.00, 119.24, 119.05, 115.62, 56.60.

Ligand L[5]. Yield: 2.02 g, 88 %; m.p.: 109–110 °C; Anal. Calcd. for $C_{13}H_{12}N_2O_2$: C, 68.40; H, 5.29; N, 12.27 %. Found: C, 68.43; H, 5.35; N, 12.11 %; IR (ATR, cm^{-1}): 3084, 1613, 1272; ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 13.10 (1H, *s*, OH), 8.68 (1H, *s*, N=CH, py), 8.60 (1H, *s*, HC=N), 8.57 (1H, *dd*, J_1 = 6.83 Hz & J_2 = 2.27 Hz, Ar-H), 7.63 (1H, *m*, Ar-H), 7.40 (1H, *dd*, J_1 = 7.22 Hz & J_2 = 2.41 Hz, Ar-H), 7.10 (2H, *t*, J = 8.10 Hz, Ar-H), 6.90 (1H, *t*, J = 8.07 Hz, Ar-H), 3.97 (3H, *s*, OCH_3); ^{13}C-NMR (400 MHz, $CDCl_3$, δ / ppm): 165.00,

151.73, 148.94, 148.48, 144.92, 143.46, 128.49, 124.46, 124.30, 119.33, 115.84, 56.68.

Ligand L6. Yield: 2.12 g, 88 %; m.p.: 99–101 °C; Anal. Calcd. for $C_{14}H_{14}N_2O_2$: C, 69.34; H, 5.82; N, 11.56 %. Found: C, 69.65; H, 5.94; N, 11.59 %; IR (ATR, cm^{-1}): 3058, 1631, 1282; ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 13.74 (1H, *s*, OH), 8.60 (1H, *d*, *J* = 7.83 Hz, Ar-H), 8.56 (1H, *s*, HC=N), 7.70 (1H, *m*, Ar-H), 7.40 (1H, *d*, *J* = 7.84 Hz, Ar-H), 7.20 (1H, *m*, Ar-H), 7.0 (2H, *d*, *J* = 6.65 Hz, Ar-H), 6.90 (1H, *t*, *J* = 7.85 Hz, Ar-H), 4.99 (2H, *s*, CH_2), 3.94 (3H, *s*, OCH_3); ^{13}C-NMR (400 MHz, $CDCl_3$, δ / ppm): 167.25, 158.42, 152.09, 149.79, 148.93, 137.26, 123.65, 122.73, 122.24, 119.27, 118.56, 114.90, 65.16, 56.60.