



SUPPLEMENTARY MATERIAL TO

Schiff base ligand derived from (\pm)*trans*-1,2-cyclohexanediamine and its Cu(II), Co(II), Zn(II) and Mn(II) complexes: Synthesis, characterization, styrene oxidation and a hydrolysis study of the imine bond in the Cu(II) Schiff base complex

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J. Serb. Chem. Soc. 81 (4) (2016) 369–382

PHYSICAL, ANALYTICAL AND SPECTRAL DATA FOR THE SYNTHESIZED COMPOUNDS

Ligand (H₂L). Yield: 97 %; m.p.: 180 °C; IR (KBr, cm⁻¹): 2931, 2857 (CH₂/CH stretching of cyclohexane ring), 1609 (C=N stretching of azomethine group); ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 16.6 (2H, s, OH), 6.74–7.45 (8H, m, Ar-H), 1.22–1.25 (6H, t, J = 7.7 Hz, CH₃), 1.53–1.76 (4H, m, H_c), 1.93–1.98 (4H, m, CH₂), 2.69–2.90 (4H, m, H_b), 3.91–3.93 (2H, q, J = 1.9 Hz, H_a); UV–Vis (DMSO) (λ_{max} / nm (ε / L mol⁻¹ cm⁻¹)): 260 (1058), 322 (500), 393 (b). (H_a, H_b and H_c are defined in Scheme 1).

[CuL'Cl][·]3/2CHCl₃ (**1**). Yield: 30 %; d.p. (decomposition point): 230 °C; Anal. Calcd. for C_{16.5}H_{22.5}Cl_{5.5}CuN₂O: C, 37.84; H, 4.30; N, 5.35. Found: C, 38.26; H, 4.79; N, 5.19 %. IR (KBr; cm⁻¹): 3288, 3223, 3125 (–NH stretching of primary amine), 2931, 2857 (CH₂/CH stretching of cyclohexane ring), 1603 (C=N stretching of azomethine group); UV–Vis (DMSO) (λ_{max} / nm (ε / L mol⁻¹ cm⁻¹)): 261 (12181), 314 (6171), 389 (br), 675 (br).

CuL (**2**). Yield: 40 %; d.p.: 210 °C; IR (KBr; cm⁻¹): 2936, 2863 (CH₂/CH stretching of cyclohexane ring), 1603 (C=N stretching of azomethine group); UV–Vis (DMSO) (λ_{max} / nm (ε / L mol⁻¹ cm⁻¹)): 258 (14047), 318 (7618), 400 (br), 887 (br).

[CoL][·]1/2CHCl₃[·]3/2H₂O (**3**). Yield: 70 %; d.p. > 320 °C; Anal. Calcd. for C_{24.5}H_{31.5}Cl_{1.5}CoN₂O_{3.5}: C, 56.34; H, 6.08; N, 5.36. Found: C, 56.01; H, 5.93; N, 5.48 %. IR (KBr; cm⁻¹): 2932, 2858 (CH₂/CH stretching of cyclohexane

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ring), 1604 (C=N stretching of azomethine group); UV–Vis (DMSO) (λ_{\max} / nm (ε / L mol⁻¹ cm⁻¹)): 261 (12030), 322 (5743), 396 (br), 611 (sh), 673 (112).

[ZnL][·]I/2CHCl₃·3/2H₂O (**4**). Yield: 77 %; d.p.> 320 °C; Anal. Calcd. for: C_{24.5}H_{31.5}Cl_{1.5}N₂O_{3.5}Zn: C, 55.66; H, 5.96; N, 5.30. Found: C, 54.31; H, 5.69; N, 5.69 %; IR (KBr; cm⁻¹): 2936, 2864 (CH₂/CH stretching of cyclohexane ring), 1604 (C=N stretching of azomethine group); ¹H-NMR (500 MHz, DMSO-d₆, δ / ppm): 6.72–7.53 (8H, *m*, Ar-H), 1.10–1.14 (6H, *t*, *J* = 7.5 Hz, CH₃), 1.51–1.86 (4H, *m*, H_c), 2.5–2.7 (4H, *m*, CH₂), 2.70–2.84 (4H, *m*, H_b), 3.66–3.98 (2H, *m*, H_a); UV–Vis (DMSO) (λ_{\max} / nm (ε / L mol⁻¹ cm⁻¹)): 260 (15128), 322 (5138), 387 (br).

[MnL][·]I/2CHCl₃·3/2H₂O (**5**). Yield: 56 %; d.p.: >320 °C; IR (KBr; cm⁻¹): 2936, 2862 (CH₂/CH stretching of cyclohexane ring), 1604 (C=N stretching of azomethine group); UV–Vis (DMSO) (λ_{\max} / nm (ε / L mol⁻¹ cm⁻¹)): 260 (15128), 322 (5138), 387 (br).