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Supplementary material

SUPPLEMENTARY MATERIAL TO

Synthesis and characterization of bioactive binuclear transition metal complexes of a Schiff base ligand derived from 4-amino-1*H*-pyrimidin-2-one, diacetyl and glycine

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PHYSICAL AND ANALYTICAL DATA FOR COMPLEXES **1**–**4**

*[Cu$_2$(L^a)$_2$Cl$_2$] (**1**)*. Yield: 62 %; color: reddish brown; m.p. (dec.): 262 °C; Anal. Calcd. for $C_{20}H_{22}Cl_2Cu_2N_8O_6$ (FW: 668.43): C, 35.94; H, 3.32; N, 16.76; Cu, 19.01; Cl, 10.61 %. Found: C, 35.89; H, 3.30; N, 16.72; Cu, 18.98; Cl, 10.58 %; Molar conductance (Λ_M / Ω^{-1} cm^2 mol^{-1}): 8.3.

*[Ni$_2$(L^a)$_2$Cl$_2$] (**2**)*. Yield: 68 %; color: dark brown; m.p. (dec.): 280 °C; Anal. Calcd. for $C_{20}H_{22}Cl_2N_8Ni_2O_6$ (FW: 658.73): C, 36.47; H, 3.36; N, 17.01; Ni, 17.82; Cl, 10.76 %. Found: C, 36.43; H, 3.31; N, 16.96; Ni, 17.79; Cl, 10.70 %; Molar conductance (Λ_M / Ω^{-1} cm^2 mol^{-1}): 7.2.

*[Co$_2$(L^a)$_2$Cl$_2$] (**3**)*. Yield: 60 %; color: brown; m.p. (dec.): 252 °C; Anal. Calcd. for $C_{20}H_{22}Cl_2Co_2N_8O_6$ (FW: 659.21): C, 36.44; H, 3.36; N, 16.99; Co, 17.88; Cl, 10.75 %. Found: C, 36.38; H, 3.32; N, 16.94; Co, 17.85; Cl, 10.72 %; Molar conductance (Λ_M / Ω^{-1} cm^2 mol^{-1}): 5.4.

*[Zn$_2$(L^a)$_2$Cl$_2$] (**4**)*. Yield: 65 %; colorless; m.p. (dec.): 220 °C; Anal. Calcd. for $C_{20}H_{22}Cl_2N_8O_6Zn_2$ (FW: 672.17): C, 35.74; H, 3.30; N, 16.67; Zn, 19.46; Cl, 10.55 %. Found: C, 35.68; H, 3.27; N, 16.62; Zn, 19.44; Cl, 10.52 %. Molar conductance (Λ_M / Ω^{-1} cm^2 mol^{-1}): 3.4.

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TABLE S-I. Characteristic IR bands (cm^{-1}) of the Schiff base ligand (L^aH) and its binuclear metal complexes **1**–**4**; azo. = azomethine group, pym. = pyrimidine, ν_{as} = asymmetric vibration, ν_s = symmetric vibration

Compound	ν(–C=N) azo.	υ(C=N) pym.	ν_{as} (–CO_2H)	ν_s (–CO_2H)	ν_{as} (–CO_2^-)	ν_s (–CO_2^-)	ν (M–N)	ν (M–O)	ν (M–Cl)
(L^aH)	1642	1532	1748	1236	–	–	–	–	–
1	1592	1490	–	–	1604	1396	495	508	334 305
2	1588	1506	–	–	1580	1348	462	518	338 296
3	1580	1498	–	–	1574	1368	475	524	345 302
4	1584	1502	–	–	1565	1352	488	516	342 290

TABLE S-II. ^{1}H-NMR and ^{13}C-NMR spectral data for the Schiff base ligand (L^aH) and the $Zn_2[(L^a)_2Cl_2]$ complex (in DMSO-d_6) at room temperature with reference to TMS; pym. = pyrimidine

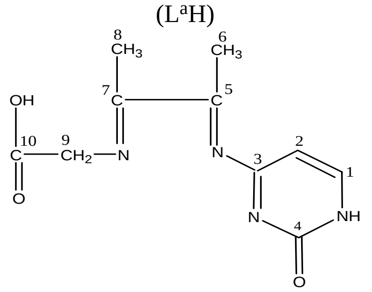
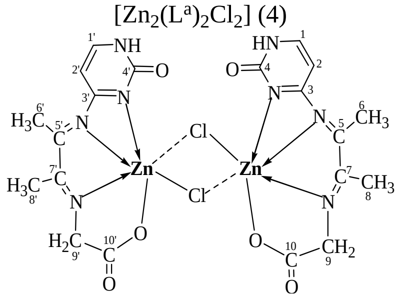
Compound	^{1}H-NMR (δ / ppm)	^{13}C-NMR (δ / ppm)
(L^aH) 	1.62 (6H, *s*, CH_3), 3.54 (2H, *s*, CH_2), 5.64 (1H, *d*, *J* = 4.2 Hz, CH=C pym.), 6.82 (1H, *d*, *J* = 1.4 Hz, =CH–N pym.), 11.10 (1H, *brs*, –NH pym.), 11.36 (1H, *s*, –OH)	20.20 (C-8), 23.50 (C-6), 46.90 (C-9), 93.90 (C-2), 148.10 (C-1), 156.10 (C-5), 161.80 (C-7), 166.90 (C-4), 169.80 (C-3), 172.60 (C-10)
$[Zn_2(L^a)_2Cl_2]$ (4) 	1.18 (12H, s, –CH_3), 3.48 (4H *s*, –CH_2), 5.68 (2H, *d*, *J* = 4.2 Hz, –CH=C pym.), 6.94 (2H, *d*, *J* = 1.4 Hz, =CH–N (pym.), 10.94 (2H, *brs*, –NH pym.)	19.90 [C-(8, 8′)], 23.10 [C-(6, 6′)], 46.34 [C-(9, 9′)], 93.74 [C-(2, 2′)], 147.92 [C-(1, 1′)], 154.60 [C-(5, 5′)], 158.40 [C-(7, 7′)], 166.70 [C-(4, 4′)], 167.22 [C-(10, 10′)], 169.18 [C-(3, 3′)]

TABLE S-III. Electronic absorption spectral data (in DMF), magnetic moment values and EPR spectral parameters of the metal complexes

Compound	λ_{max} / nm	Assignment	μ_{eff} / μ_B	EPR values		
				$g_{\parallel}$	$g_{\perp}$	g_{av}
1	762	$E_g \rightarrow {}^2T_{2g}$	1.62	2.124	2.056	2.080
2	242	INCT	2.82	–	–	–
	376	${}^3A_{2(g)} \rightarrow {}^3T_{1g}$				
	552	${}^3A_{2(g)} \rightarrow {}^3T_{2g}$				
3	462	${}^4T_{1g} \rightarrow {}^4T_{1g}$	4.56	2.314	2.014	2.112
	590	${}^4T_{1g} \rightarrow {}^4A_{2g}$				
4	328	LMCT	Diamagnetic	–	–	–
	356	LMCT				