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SUPPLEMENTARY MATERIAL TO

Synthesis, spectroscopic characterization, DFT, oxygen binding and antioxidant activity of Fe(III), Co(II) and Ni(II) complexes with a tetradentate ONNO donor Schiff base ligand

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*(7*E*)-N-benzylidene-2-styrylbenzenamine1-2-diamine-2-4-dihydroxy-phenol (**L**)*

M.p.: 285 °C; Color: Light yellow, Yield: 1.86 g (63 %); Selected infrared absorption (KBr, cm^{-1}): ν(O-H)$_{arom}$, 3204*s*; ν(C-H), 2874*m*; ν(HC=N)$_{imine}$, 1631*s*; ν(C=C), 1365*w*; ν(C-O), 1244*m*; ν(C-C), 1151*m*; γ(C-H), 754*w*; γ(O-H), 644*w*. Electronic spectra (λ_{max} / nm (ε / (mol L^{-1} cm^{-1})) in DMSO: 280(1585), 340(828). ^{1}H-NMR spectra (400 MHz, CH_3CN, δ / ppm): (O-H)$_{arom(ortho,para)}$, 13.18 (*s*, 2H), 9.91 (*s*, 2H), (HC=N)$_{imine}$, 8.81 (*s*, 2H), (Ar-H)$_{phenolic}$, 7.56 (*dd*, J_1 = 8.0, J_2 = 1.6, 2H), 7.37 (*m*, 2H), 6.36(*s*, 2H), (Ar-H)$_{phynelene}$, 6.87(*m*, 4H). ^{13}C-NMR (700 MHz, CH_3CN, δ / ppm): (C-OH), δ 173.85, (>C=N)$_{imine}$, δ 166.1, (Ar-C)$_{phenolic}$, δ 119.20, δ 116.68, δ 123.77, δ 148.14, δ 119.58, δ 117.90, δ 119.46, δ 139.44, (Ar-C)$_{benzene}$, δ 162.17, δ 158.17, δ 139.44, δ 151.95, δ 150.79, δ 128.01. ESI-Mass spectra, (*m/z*): calculated for $[C_7H_6NO_2 + H^+]^+$ = 137.0959, $[C_{13}H_{11}NO_2 + H]^+$ = 213.3582, $[C_{14}H_{11}N_2O_3 + H^+]^+$ = 240.2603, $[C_{20}H_{15}N_2O + H^+]^+$ = 332.2365, $[C_{20}H_{16}N_2O_4 + H^+]^+$ = 349.0572, observed 348.352. Combustion analysis for $C_{20}H_{16}N_2O_4$: Calculated C 68.96, H 4.63, N 8.04, O 18.37; found C 68.94, H 4.61, N 8.01, O 18.35.

*[Fe(**L**)Cl(H_2O) (**1**)*

M.p.: 340 °C; Color: light gray, Yield: 0.286 g (62 %); μ_{eff} = 5.43 B.M. Selected infrared absorption (KBr, cm^{-1}): ν(C-H), 2941*s*, ν(HC=N)$_{imine}$, 11618*s*, ν(C=C), 1351*w*, ν(C-O), 1255*m*, ν(C-C), 1190*m*, γ(C-H), 738*w*, ν(M-O), 532*s*, ν(M-N), 432*s*. Electronic spectra (λ_{max} / nm (ε / (mol^{-1} L cm^{-1})) in DMSO: Found: 340(1356); 540(389); 660(101). Molar conductance Λ_m at 25 °C (Ω^{-1} cm^2 mol^{-1}): 3 in DMSO. ESI-Mass spectra, calculated for (*m/z*): calculated for

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$[C_7H_5FeNO_2 + H^+]^+$ = 191.9625, $[C_7H_7ClFeNO_3 + H^+]^+$ = 245.4582, $[C_{13}H_{11}ClFeNO_3 + H^+]^+$ = 321.5293, $[C_{14}H_{12}ClFeN_2O_3 + H^+]^+$ = 348.5546, $[C_{20}H_{15}ClFeN_2O_4 + H^+]^+$ = 439.1125, $[C_{20}H_{16}ClFeN_2O_5 + H^+]^+$ = 456.2356, observed 455.6494. Combustion analysis for $C_{20}H_{16}ClFeN_2O_5$: Calculated. C 52.72, H 3.54, N 6.15, Cl 7.78, Fe 12.26; found C 52.62, H 3.3.46, N 6.02, Cl 7.68, Fe 12.16.

*[Co(**L**)(H$_2$O)$_2$] (**2**)*

M.p.: >350 °C; Color: light green, Yield: 0.332 g (61 %); μ_{eff} = 4.52 B.M. Selected infrared absorption (KBr, cm^{-1}): *ν*(C-H), 2871*s*, *ν*(HC=N)$_{imine}$, 1583*w*, *ν*(C=C), 1315*s*, *ν*(C-O), 1249*s*, *ν*(C-C), 1180*m*, *γ*(C-H), 750*s*, *ν*(M-O), 532*s*, *ν*(M-N), 434*m*. Electronic spectra (λ_{max} / nm (ε / (mol^{-1} L cm^{-1})) in DMSO: 350(1452); 540(324); 630(48). Molar conductance Λ_m at 25 °C (Ω^{-1} cm^2 mol^{-1}): 3 in DMSO. ESI-Mass spectra, (*m/z)*: calculated for $[C_7H_5CoNO_2 + H^+]^+$ = 195.1798, $[C_7H_9CoNO_4 + H^+]^+$ = 231.2723, $[C_{13}H_{13}CoNO_4 + H^+]^+$ = 307.1128, $[C_{14}H_{14}CoN_2O_5 + 2H^+]^+$ = 349.0572, $[C_{20}H_{17}CoN_2O_5 + H^+]^+$ = 425.0930, $[C_{20}H_{18}CoN_2O_6 + H^+]^+$ = 442.1558, observed 441.2999. Combustion analysis for $C_{20}H_{18}CoN_2O_6$: Calculated. C 54.43, H 4.11, Co 13.35; found C 54.41, H 4.09, N 6.31, Co 13.30.

*[Ni(**L**)(H$_2$O)$_2$] (**3**)*

M.p.: >350 °C; Color: dark green, Yield: 0.362 g (67 %); μ_{eff} = 3.07 B.M. Selected infrared absorption (KBr, cm^{-1}): *ν*(C-H), 2837*s*, *ν*(HC=N)$_{imine}$, 1579*s*, *ν*(C=C), 1315*w*, ν(C-O), 1232*m*, *ν*(C-C), 1132*m*, *γ*(C-H), 765*w*, *ν*(M-O), 538*m*, *ν*(M-N), 455(*m*). Electronic spectra (λ_{max} / nm (ε / (mol^{-1} L cm^{-1})) in DMSO: 370(1262); 410(1449); 550(158). Molar conductance Λ_m at 25 °C (Ω^{-1} cm^2 mol^{-1}): 2 in DMSO. ESI-Mass spectra, (*m/z)*: $[C_7H_5NiNO_2 + H^+]^+$ = 194.8135, $[C_7H_9NiNO_4 + H^+]^+$ = 228.6958, $[C_{13}H_{13}NiNO_4 + H^+]^+$ = 306.6514, $[C_{14}H_{14}NiN_2O_4 + H^+]^+$ = 333.9033, $[C_{20}H_{17}NiN_2O_5 + H^+]^+$ = 424.3259, $[C_{20}H_{18}N_2NiO_6 + H^+]^+$ = 442.2542, observed 441.0601. Combustion analysis for $C_{20}H_{18}N_2NiO_6$: Calculated. C 48.86, H, 4.59, N 7.09, Ni 14.89; found C 48.46, H 4.48, N 6.95, Ni 14.71.

TABLE S-I. FT-IR correlation data of Ligand (**L**) and Complex **2**

Peak assignment	Ligand **L**				Complex **2**			
	Wavenumber, cm^{-1}			Deviation,%	Wavenumber, cm^{-1}			Deviation,%
	Experimental	Theoretical			Experimental	Theoretical		
		Unscaled	Scaled			Unscaled	Scaled	
ν(O-H)$_{Arom}$	3207.73	3239.40	3204.52	0.1	-	-	-	-
ν(C-H)	2874.03	2881.74	2871.15	0.1	2871.39	2884.28	2865.64	0.2
ν(>C=N)	1631.83	1625.98	1630.19	0.1	1583.61	1612.12	1580.44	0.2
ν(C=C)	1365.65	1352.12	1364.28	0.1	1315.50	1345.18	1312.86	0.2
ν(C-O)	1244.13	1266.33	1242.88	0.1	1249.91	1225.41	1178.10	0.2
ν(C-C)	1151.54	1155.83	1150.38	0.1	1180.47	1153.81	1160.68	0.2
γ(C-H)	754.19	755.49	753.43	0.1	750.33	755.82	748.82	0.2
γ(O-H)	659.68	636.36	659.02	0.1	-	-	-	-
ν(M-O)	-	-	-	-	532.37	532.43	531.30	0.2
ν(M-N)	-	-	-	-	434.09	444.35	433.13	0.2

TABLE S-II. DFT ^{1}H-NMR and ^{13}C-NMR correlation data of Ligand (**L**)

Ligand L ^{1}H-NMR				Ligand L ^{13}C-NMR			
Calculated (gas phase), proton No	δ / ppm			Calculated (gas phase), carbon No	δ / ppm		
	Experimental (solid phase)	Calculated (gas phase)			Experimental (solid phase)	Calculated (gas phase)	
		TMS HF[a]	TMS B3[b]			TMS HF[a]	TMS B3[b]
H 41	13.173	12.726	9.010	C7	173.83	179.10	171.58
H 42	9.908	9.725	9.009	C4	166.15	179.09	161.57
H 39	8.806	8.985	8.125	C2	162.17	178.35	160.83
H 40	7.573	7.747	7.031	C22	158.17	177.32	160.80
H 36	7.569	7.746	6.715	C11	151.95	172.15	154.63
H 35	7.166	7.131	6.415	C12	150.79	172.15	154.63
H 38	7.162	7.130	6.415	C6	148.14	161.27	143.75
H 34	6.950	6.952	6.237	C24	134.44	161.27	143.75
H 31	6.948	6.952	6.237	C14	128.01	147.42	129.90
H 30	6.788	6.384	5.669	C15	123.77	147.38	129.86
H 33	6.361	6.384	5.669	C13	119..58	144.48	126.96
H 37	6.359	5.367	4.651	C16	119.46	144.48	126.96
H 39	6.354	5.357	4.641	C5	119.20	144.27	126.75
H 32	2.515	3.109	2.394	C19	117.90	144.24	126.75
H 27	2.506	3.007	2.291	C1	116.68	128.88	115.36
H 28	2.502	2.603	1.888	C23	116.68	128.86	111.34

[a]TMS HF/6-31G(d) GIAO; [b]TMS B3LYP/6-311+G(2d,p) GIAO

TABLE S-III. Mulliken atomic charges of ligand (**L**) and complexes

Ligand **L**		Complex **1**		Complex **2**		Complex **3**	
Atom	Charge, e	Atom	Charge, e	Atom	Charge, e	Atom	Charge, e
C1	-0.028395	C1	-0.279899	C1	-0.322932	C1	-0.306675
N2	-0.278142	N2	-0.230275	N2	-0.249254	N2	-0.218530
H3	0.142925	H3	0.221662	H3	0.221162	H3	0.220057
C4	-0.115112	C4	-0.324478	C4	-0.331823	C4	-0.338667
C5	0.081922	C5	0.325814	C5	0.292318	C5	0.299563
C6	0.081973	C6	0.327865	C6	0.271380	C6	0.276403
C7	-0.115132	C7	-0.324922	C7	-0.346469	C7	-0.346174
C8	-0.146010	C8	-0.237032	C8	-0.246337	C8	-0.243885

Ligand **L**		Complex **1**		Complex **2**		Complex **3**	
Atom	Charge, e	Atom	Charge, e	Atom	Charge, e	Atom	Charge, e
C9	-0.146009	C9	-0.237502	C9	-0.258555	C9	-0.246488
H10	0.166444	H10	0.233980	H10	0.229655	H10	0.233799
H11	0.166443	H11	0.235923	H11	0.237212	H11	0.236210
H12	0.148326	H12	0.240402	H12	0.235141	H12	0.237614
H13	0.148326	H13	0.240126	H13	0.235177	H13	0.237829
N14	-0.278212	N14	-0.294654	N14	-0.319319	N14	-0.274868
C15	-0.028300	C15	-0.294654	C15	-0.399989	C15	-0.350614
H16	0.142904	H16	0.221944	H16	0.220854	H16	0.225315
C17	0.289863	C17	0.336164	C17	0.321346	C17	0.327852
C18	-0.213903	C18	-0.537853	C18	-0.550206	C18	-0.542374
C19	0.254447	C19	0.319527	C19	0.308161	C19	0.315890
C20	-0.025395	C20	0.302496	C20	0.303553	C20	0.303514
C21	-0.124779	C21	-0.343801	C21	-0.365357	C21	-0.353685
C22	-0.178644	C22	-0.390478	C22	-0.390082	C22	-0.392229
H23	0.156160	H23	0.264406	H23	0.253554	H23	0.258561
H24	0.164082	H24	0.231393	H24	0.229525	H24	0.230108
H25	0.169641	H25	0.254307	H25	0.246727	H25	0.249797
C26	-0.212183	C26	-0.526927	C26	-0.536415	C26	-0.534553
C27	0.289440	C27	0.335216	C27	0.326542	C27	0.329656
C28	-0.178308	C28	-0.386583	C28	-0.389225	C28	-0.392594
C29	-0.125144	C29	-0.343783	C29	-0.354769	C29	-0.349727
C30	-0.024687	C30	0.274928	C30	0.280329	C30	0.285695
C31	0.253547	C31	0.293275	C31	0.288878	C31	0.295498
H32	0.155256	H32	0.266886	H32	0.259093	H32	0.259823
H33	0.169622	H33	0.256006	H33	0.251180	H33	0.251036
H34	0.164075	H34	0.234151	H34	0.232076	H34	0.230932
O35	-0.537508	O35	-0.373478	O35	-0.434564	O35	-0.419015
O36	-0.538336	O36	-0.366402	O36	-0.414691	O36	-0.400433
O37	-0.538336	O37	-0.474245	O37	-0.484140	O37	-0.480142
O38	-0.626509	O38	-0.474195	O38	-0.478871	O38	-0.478260
H39	0.366892	H39	0.361192	H39	0.354386	H39	0.358803
H40	0.332135	H40	0.363998	H40	0.357967	H40	0.359064
H41	0.332970	Fe41	0.123313	O41	-0.580976	O41	-0.631998
		O42	-0.625463	H42	0.215423	H42	0.411494
		H43	0.440434	H43	0.48896	H43	0.408144
		H44	0.441293	Co44	0.292168	O44	-0.624676
		CI45	-0.138782	O45	-0.574811	H45	0.438943
				H46	0.458307	H46	0.403533
				H47	0.433172	Ni47	0.240452

TABLE S-IV. Selected natural atomic charges and electronic configurations for the complex **2**

Atoms	Natural atomic charge	Natural electronic configuration
Co44	0.57074	[core]4s(0.26)3d(7.65)4p(0.51)4d(0.02)
N2	-0.47669	[core]2s(1.30)2p(4.15)3p(0.02)

Atoms	Natural atomic charge	Natural electronic configuration
N14	-0.54181	[core]2s(1.29)2p(4.23)3p(0.02)
O35	-0.63188	[core]2s(1.70)2p(4.93)3p(0.01)
O36	-0.61051	[core]2s(1.70)2p(4.90)3p(0.01)
O37	-0.74449	[core]2s(1.70)2p(5.04)3p(0.01)
O38	-0.73920	[core]2s(1.70)2p(5.03)3p(0.01)
C4	-0.21332	[core]2s(0.96)2p(3.24)3p(0.01)
C5	0.12347	[core]2s(0.83)2p(3.03)3p(0.02)
C15	0.04377	[core]2s(0.91)2p(3.02)3p(0.02)
C17	0.33718	[core]2s(0.86)2p(2.79)3p(0.01)
C18	-0.31043	[core]2s(0.98)2p(3.31)3p(0.01)
C26	-0.30943	[core]2s(0.98)2p(3.31)3p(0.02)
C27	0.34945	[core]2s(0.86)2p(2.78)3p(0.01)
C28	-0.28239	[core]2s(0.97)2p(3.29)3p(0.02)
H3	0.18528	1s(0.81)
H10	0.21220	1s(0.79)
H11	0.21549	1s(0.78)
H39	0.48621	1s(0.51)
H43	0.48896	1s(0.46)

TABLE S-V. The second-order perturbation energies$^{(2)}$ corresponding to the most important charge transfer interactions (donor–acceptor) of complex **2** at B3LYP/LanL2DZ//6-31^{++}G(d,p)

Donor Lewis NBO (i)	Acceptor Lewis NBO (j)	Types	$E^{(2)}$ / kcal mol^{-1}	$E_{(j)} - E_{(i)}$ / a.u.	$F_{(i,j)}$ / a.u.
C1−C30	C26−C31	π→π*	2.02	1.18	0.062
C1− C30	C28−C29	π→π*	1.81	1.18	0.059
C1−C30	C29−C30	π→π*	0.58	1.18	0.033
C1−C30	C30−C31	σ→σ*	0.66	1.19	0.035
C4−C5	N2−C5	π→π*	105.65	1.16	0.469
C4− C5	C4−C9	π→π*	1.32	1.08	0.051
C4−C5	C5−C6	π→π*	0.89	1.20	0.044
C4−C9	C4−C5	π→π*	1.80	1.23	0.059
C4−C9	C8−C9	σ→σ*	0.74	1.23	0.038
C4−C9	N2−C5	π→π*	6.98	0.40	0.075
C4−C9	N2−C5	π→π*	1.05	0.89	0.041
C4−C9	C7−C8	π→π*	11.20	0.28	0.072
C5−C6	N2−C5	π→π*	0.99	1.07	0.041
C5−C6	N2−C5	σ→σ*	0.77	0.88	0.040
C5−C6	N2−C5	π→π*	4.73	1.37	0.114
C5−C6	C4−C5	σ→σ*	0.97	1.28	0.045
C5−C6	C6−C7	π→π*	2.34	1.29	0.070
C6−C7	C5−C6	π→π*	2.49	1.38	0.074
C6 −C7	C7−C8	σ→σ*	0.99	1.25	0.045
C7−C8	C8−C9	σ→σ*	0.74	1.23	0.038
C7−C8	C4−C9	π→π*	8.68	0.28	0.064

Donor Lewis NBO (i)	Acceptor Lewis NBO (j)	Types	$E^{(2)}$ / kcal mol^{-1}	$E_{(j)} - E_{(i)}$ / a.u.	$F_{(i,j)}$ / a.u.
C8−C9	C4−C9	σ→σ*	0.77	1.24	0.039
C8−C9	C7−C8	σ→σ*	0.76	1.23	0.039
C15−C20	C18−C19	π→π*	2.02	1.17	0.062
C15−C20	C19−C20	σ→σ*	0.63	1.18	0.034
C15−C20	C20−C21	σ→σ*	0.59	1.18	0.033
C15−C20	C21−C22	π→π*	1.83	1.18	0.059
C15−C20	C21−C22	π→π*	7.17	0.29	0.058
C17−C18	C17−C22	π→π*	1.31	1.26	0.051
C17−C18	C18−C19	σ→σ*	0.92	1.25	0.043
C17−C18	C21−C22	π→π*	11.10	0.29	0.073
C17−C22	C17−C18	π→π*	1.18	1.25	0.048
C17−C22	C21−C22	σ→σ*	0.84	1.26	0.041
C18−C19	C17−C18	σ→σ*	0.96	1.24	0.044
C19−C20	C15−C20	σ→σ*	0.81	1.10	0.038
C19−C20	C18−C19	π→π*	1.29	1.26	0.051
C19−C20	C20−C 21	π→π*	1.44	1.26	0.054
C20−C21	C15−C20	σ→σ*	0.75	1.08	0.036
C20−C21	C19−C20	π→π*	1.71	1.25	0.058
C20−C21	C21−C22	π→π*	0.91	1.25	0.043
C21−C22	C15−C20	π→π*	2.41	1.08	0.064
C21−C22	C17−C22	σ→σ*	0.90	1.24	0.042
C21−C22	C20−C21	σ→σ*	1.09	1.24	0.046
C21−C22	C15−C20	π→π*	13.69	0.23	0.081
C21−C22	C17−C18	π→π*	9.16	0.28	0.067
C26−C27	C26−C31	σ→σ*	0.89	1.25	0.042
C26−C27	C28−C29	π→π*	10.04	0.29	0.069
C26−C27	C30−C31	π→π*	10.50	0.29	0.073
C26−C31	C31−C30	σ→σ*	2.75	1.08	0.069
C26−C31	C26−C27	σ→σ*	0.95	1.24	0.043
C27−C28	C26−C27	π→π*	1.16	1.25	0.048
C27− C28	C28−C29	σ→σ*	0.83	1.26	0.041
C28−C29	C27−C28	σ→σ*	0.89	1.24	0.042
C28−C29	C29−C30	σ→σ*	1.10	1.24	0.047
C28−C29	C26−C27	π→π*	10.52	0.28	0.071
C28−C29	C30−C31	π→π*	8.58	0.29	0.066
C29−C30	C1−N2	π→π*	1.22	1.24	0.049
C29−C30	C1−C30	σ→σ*	0.73	1.08	0.036
C29−C30	C28−C29	σ→σ*	0.90	1.25	0.043
C29−C30	C30−C31	π→π*	1.76	1.25	0.059
C30−C31	C1−C30	σ→σ*	0.81	1.10	0.038
C30−C31	C26−C31	π→π*	1.27	1.26	0.050
C30−C31	C29−C30	π→π*	1.49	1.27	0.055

Donor Lewis NBO (i)	Acceptor Lewis NBO (j)	Types	$E^{(2)}$ / kcal mol^{-1}	$E_{(j)} - E_{(i)}$ / a.u.	$F_{(i,j)}$ / a.u.
C30−C31	C26−C27	π→π*	9.19	0.29	0.065
C30−C31	C28−C29	π→π*	11.02	0.29	0.072
C30−C31	C30−C31	π→π*	0.29	0.29	0.012
LP(1)C1	C30−C31	π→π*	17.52	0.20	0.083
LP(1)N	O36−Co44	π→π*	28.00	0.41	0.135
LP(1)C19	C15−C20	π→π*	98.94	0.09	0.126
LP(1)C19	C17−C18	π→π*	37.97	0.15	0.110
LP*(6)Co44	N2−C5	π→π*	84.91	0.11	0.209
LP*(6)Co44	C4−C5	π→π*	16.57	0.01	0.055
N2−C5	C6	π→π*	157.60	0.04	0.200
C6−N14	C15−C20	π→π*	26.71	0.05	0.052
C15−C20	C21−C22	π→π*	44.80	0.06	0.087

TABLE S-VI. Quantum chemical parameters of compounds

Compounds	Ligand **L**	Complex **1**	Complex **2**	Complex **3**
E_{HOMO} / eV	-5.80954	-5.57444	-5.45526	-5.15538
E_{LUMO} / eV	-1.67919	-2.52899	-1.90585	-2.17551
ΔE / eV	4.13035	3.04545	3.54941	2.97987
Ionization energies, eV	5.80954	5.57444	5.45526	5.15538
Electron affinities, eV	1.67919	2.52899	1.90585	2.17551
Mullikan electronegativity, eV	3.74436	4.05171	3.68055	3.66544
Global hardness, eV	2.06517	1.52272	1.77470	1.48993
Absolute softness, eV	0.48422	0.65671	0.56347	0.67117
Chemical potential, eV	-3.74436	-4.05171	-3.68055	-3.66544
Global softness, eV	0.24211	0.32835	0.28173	0.33558
Global electrophilicity, eV	3.39445	5.39046	3.81654	4.50874
Electronic charge, eV	1.81309	2.66083	2.07389	2.46013
Varial ratio	2.0033	2.0520	2.0459	2.0485
Dipole moment, D	1.9848	10.7733	6.0253	6.9248
E (TD-HF/TD-KS*) / kcal mol^{-1}	-1181.99	-1395.63	-1478.69	-1502.84

*Time dependent Hartree-Fock / Kohn-Sham energies

TABLE S-VII. Geometrically optimized bond lengths of ligand L and complexes

Bond connectivity	Bond length, Å			
	Ligand **L**	Complex **1**	Complex **2**	Complex **3**
C=N (imine)	(C15-N14) 1.293	(C15-N14) 1.287	(C15-N14) 1.288	(C15-N14) 1.288
C=N' (imine)	(C1-N2) 1.293	(C1-N2) 1.289	(C1-N2) 1.289	(C1-N2) 1.289
$C\text{-}C_{(close\ to\ imine\ C)}$	(C21-C22) 1.543	(C21-C22) 1.398	(C21-C22) 1.398	(C21-C22) 1.398
$C\text{-}C'_{(close\ to\ imine\ C)}$	(C28-C29) 1.544	(C28-C29) 1.398	(C28-C29) 1.398	(C28-C29) 1.398
C-O	(C19-O35) 1.428	(C19-O35) 1.434	(C19-O35) 1.433	(C19-O35) 1.433
C-O'	(C31-O36) 1.430	(C31-O36) 1.432	(C31-O36) 1.431	(C31-O36) 1.431
O-H	(O35-H40) 0.960	-	-	-
O-H'	(O36-H41) 0.962	-	-	-

C-N	(C6-N14) 1.474	(C6-N14) 1.455	(C6-N14) 1.458	(C6-N14) 1.458
C-N’	(C5-N2) 1.463	(C5-N2) 1.456	(C5-N2) 1.459	(C5-N2) 1.459
M-N (imine)	-	(M41-N14) 1.888	(M44-N14) 1.879	(M47-N14) 1.879
M-N’ (imine)	-	(M41-N2) 1.889	(M44-N2) 1.884	(M47-N2) 1.884
M-Cl	-	(M41-Cl45) 2.150	-	-
$M\text{-}O_{(coordination)}$	-	(M41-O35) 1.830	(M44-O35) 1.827	(M47-O35) 1.827
$M\text{-}O'_{(coordination)}$	-	(M41-O36) 1.830	(M44-O36) 1.829	(M47-O36) 1.829
$M\text{-}O_{(water)}$	-	(M41-O42) 1.820	(M44-O41) 1.810	(M47-O41) 1.800
$M\text{-}O'_{(water)}$	-	-	(M44-O45) 1.828	(M47-O44) 1.801

TABLE S-VIII. Geometrically optimized bond angles of ligand **L** and complexes

Bond connectivity	Bond angle, °			
	Ligand **L**	Complex **1**	Complex **2**	Complex **3**
∠C-N=C	(∠C6-N14-C15) 119.99	(∠C6-N14-C15) 119.20	(∠C6-N14-C15) 119.89	(∠C6-N14-C15) 119.89
∠C=C-N	(∠C7-C6-N14) 119.99	(∠C7-C6-N14) 125.82	(∠C7-C6-N14) 125.20	(∠C7-C6-N14) 125.20
∠O-C=C	(∠O35-C19-C20) 119.99	(∠O35-C19-C20) 123.84	(∠O35-C19-C20) 123.29	(∠O35-C19-C20) 123.29
∠C-O-H	(∠C19-O35-H40) 109.47	-	-	-
∠M-N=C	-	(∠M41-C14-N15) 125.73	(∠M44-C14-N15) 125.36	(∠M47-C14-N15) 125.36
∠N-M-O	-	(∠N14-M41-O35) 98.19	(∠N14-M44-O35) 98.42	(∠N14-M47-O35) 98.42
∠Cl-M-O	-	(∠Cl45-M41-O35) 89.17	-	-
∠C-N-M	-	(∠C6-N14-M41) 115.06	(∠C6-N14-M44) 114.73	(∠C6-N14-M47) 114.73

TABLE S-IX. Values of the oxygenation constant and of the thermodynamic parameters

Temperature, K	Complex 1			Complex 2		
	K_{O2}/ atm^{-1}	$\Delta H°$ / kJ mol^{-1}	$\Delta S°$ / J mol^{-1} K^{-1}	K_{O2}/ atm^{-1}	$\Delta H°$ / kJ mol^{-1}	$\Delta S°$ / J mol^{-1} K^{-1}
273	11.5	-32.6	-81.2	13.6	-28.3	-78.4
283	5.9	-32.6	-81.2	6.6	-28.3	-78.4
293	2.9	-32.6	-81.2	3.1	-28.3	-78.4
303	1.5	-32.6	-81.2	1.5	-28.3	-78.4

TABLE S-X. DPPH free radical scavenging activity of Schiff base ligand (**L**) and complexes

Compounds	Concentrations, μM			
	0.002	0.004	0.006	0.008
	Free radical scavenging activity, %			
Ascorbic acid	76.33	84.90	87.66	91.62
Ligand (**L**)	33.33	39.00	53.66	65.33

[Fe(**L**)Cl(H_2O)]; **1**	42.66	54.66	68.33	76.00
[Co(**L**)(H_2O)$_2$]; **2**	36.66	42.33	54.66	70.66
[Ni(**L**)(H_2O)$_2$]; **3**	46.33	55.33	69.66	76.33

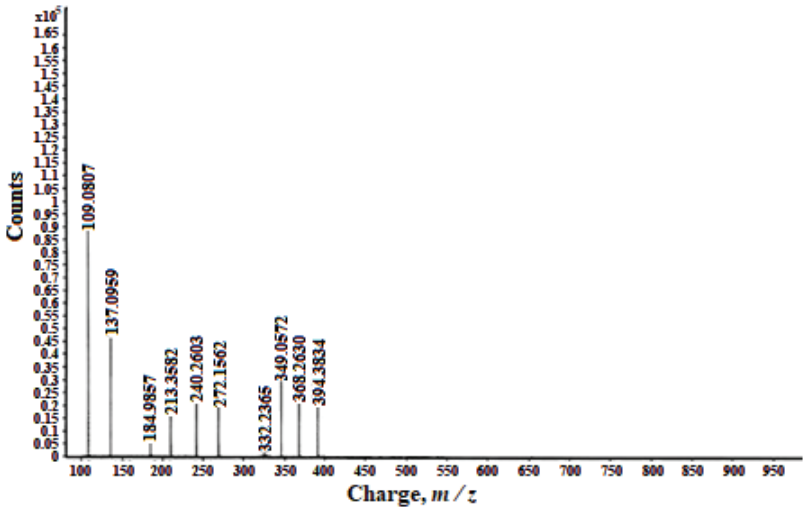

Fig. S-1. ESI-Mass spectrum of ligand **L**.

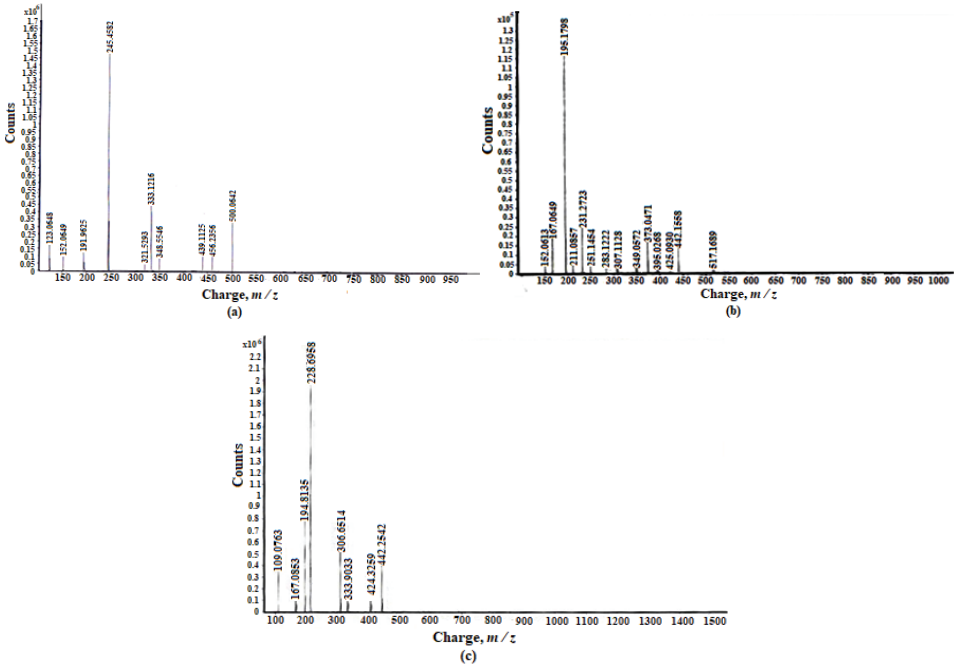

Fig. S-2. ESI-Mass spectrum of (a) complex **1**; (b) complex **2** and (c) complex **3**.

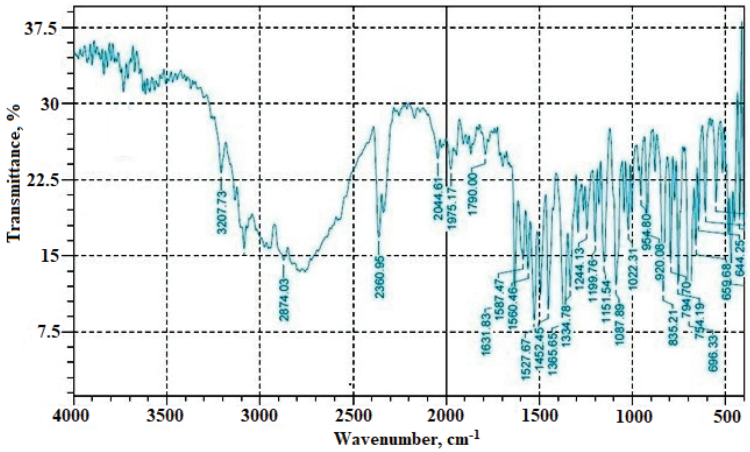

Fig. S-3. Experimental FT-IR spectrum of ligand **L**.

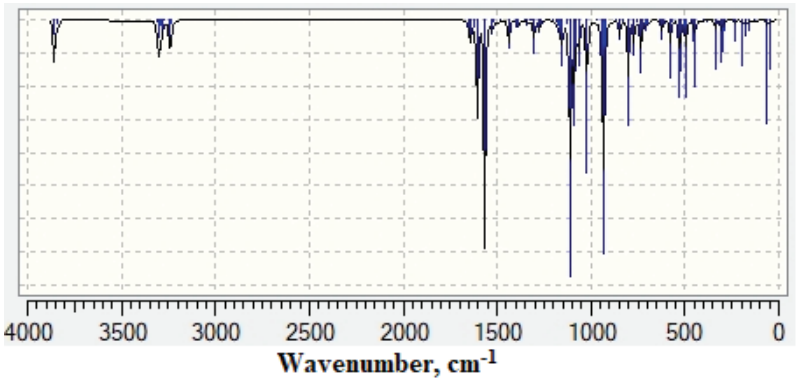

Fig. S-4. Theoretical FT-IR spectrum of ligand **L**.

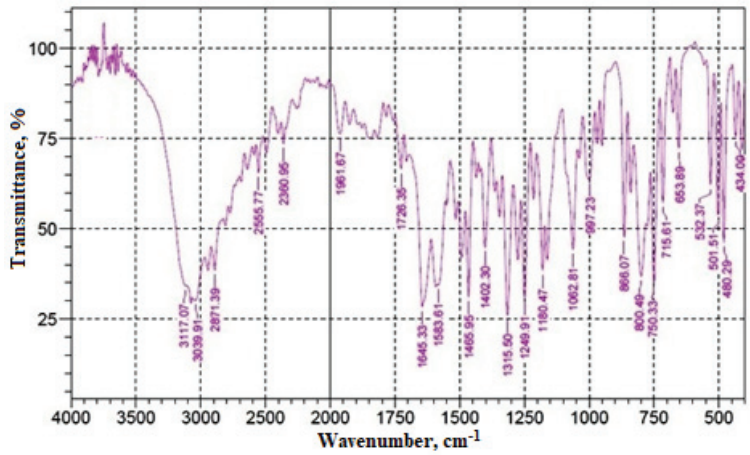

Fig. S-5. Experimental FT-IR spectrum of complex **2**.

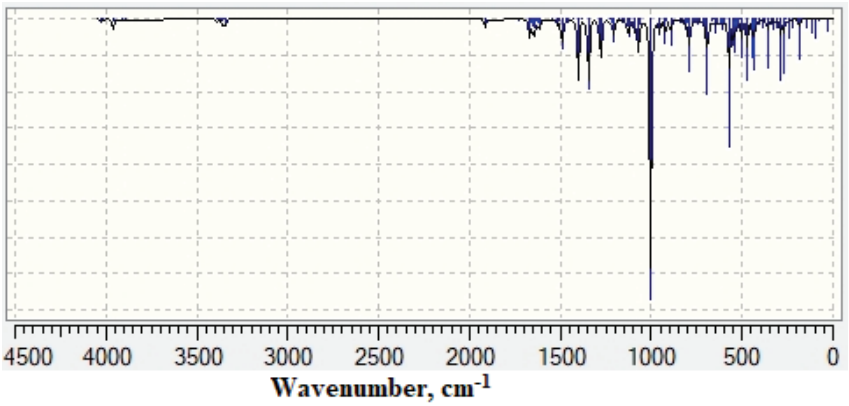

Fig. S-6. Theoretical FT-IR spectrum of complex **2**.

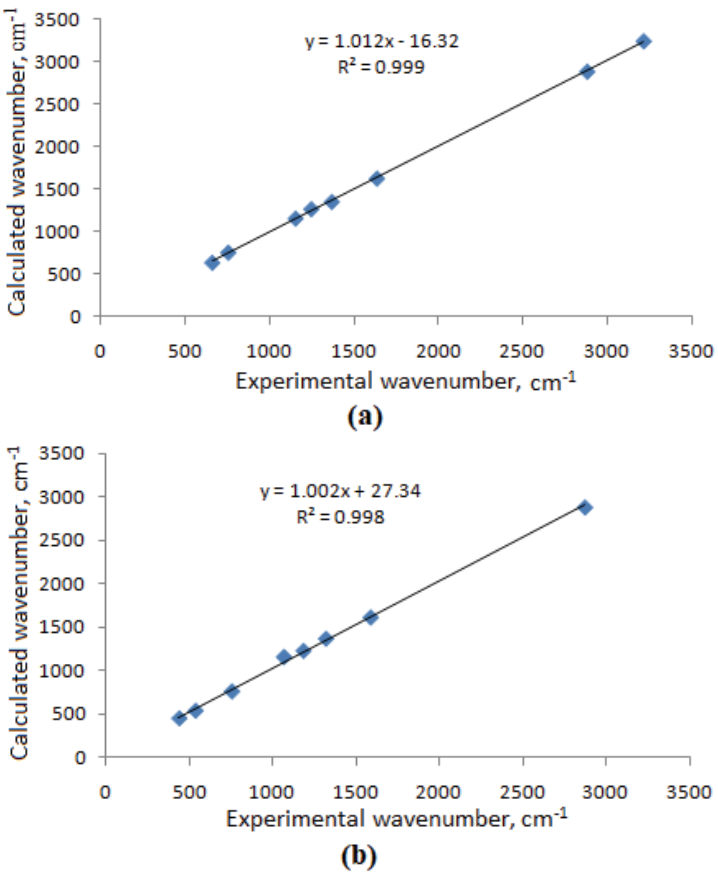

Fig. S-7. FT-IR correlation graphs of (a) ligand and (b) complex **2**.

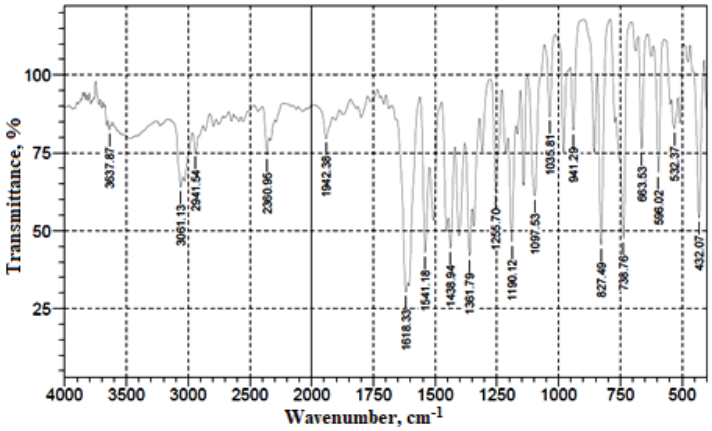

Fig. S-8. Experimental FT-IR spectrum of complex **1**.

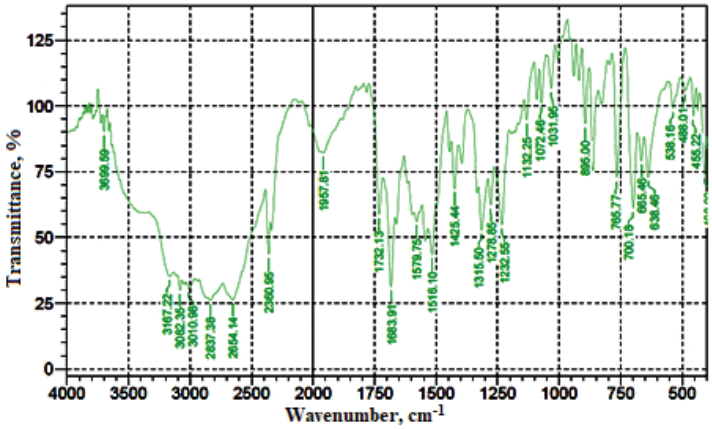

Fig. S-9. Experimental FT-IR spectrum of complex **3**.

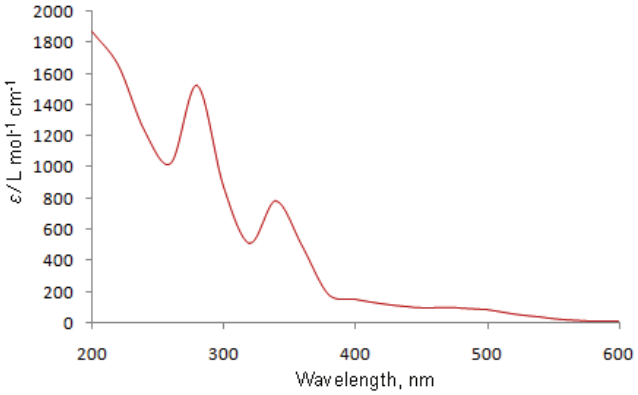

Fig. S-10. UV–Vis spectrum of Ligand **L**.

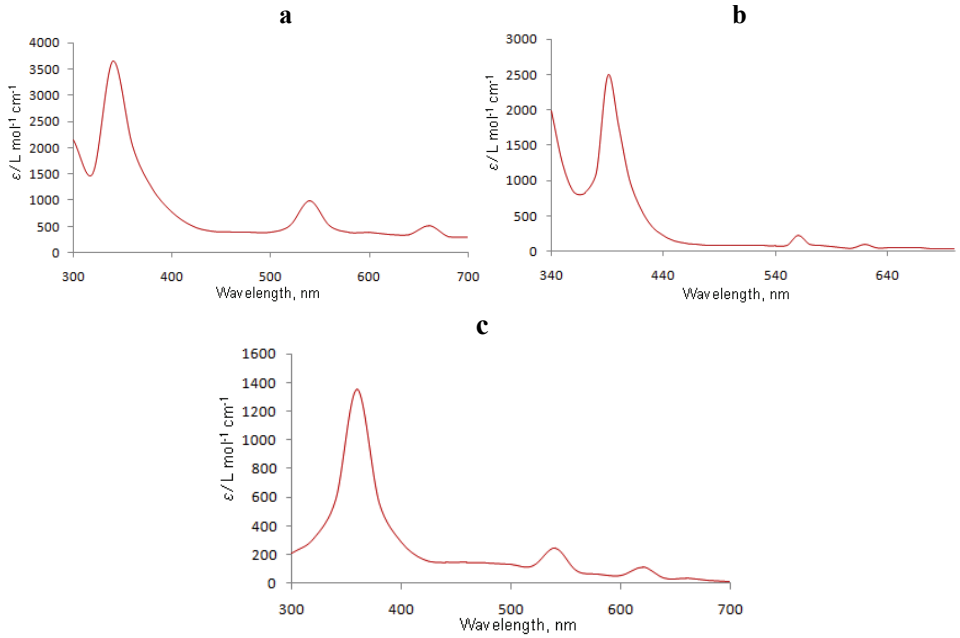

Fig. S-11. UV-Vis spectrum of: (a) complex **1**; (b) complex **2** and (c) complex **3.**

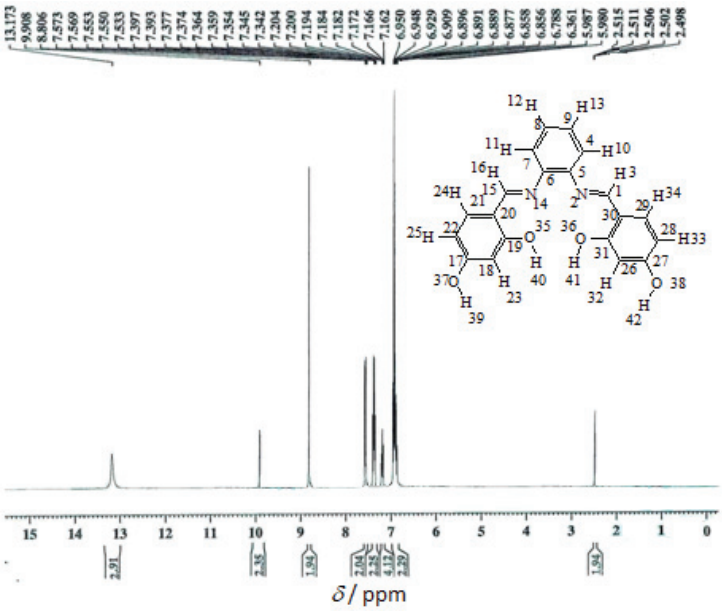

Fig. S-12. ^{1}H-NMR spectrum of Ligand **L**.

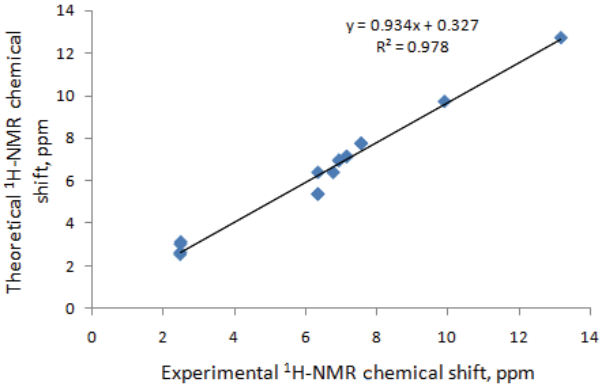

Fig. S-13. ^{1}H-NMR correlation graph of Ligand **L**.

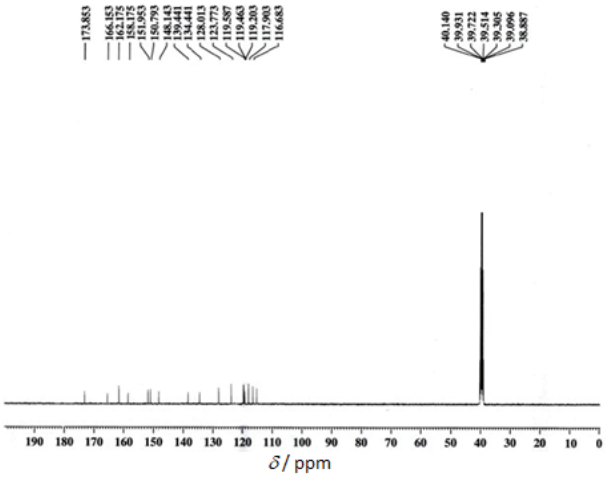

Fig. S-14. ^{13}C-NMR spectrum of Ligand **L**.

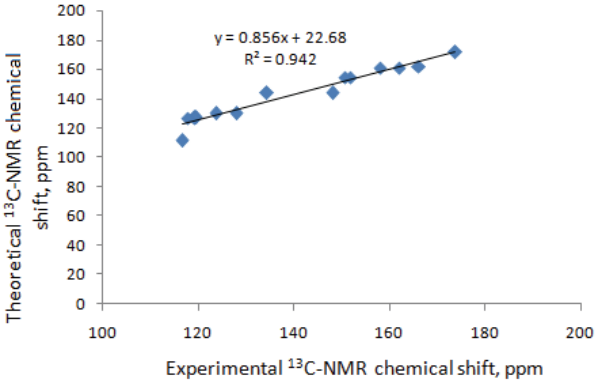

Fig. S-15. ^{13}C-NMR correlation graph of Ligand **L**.

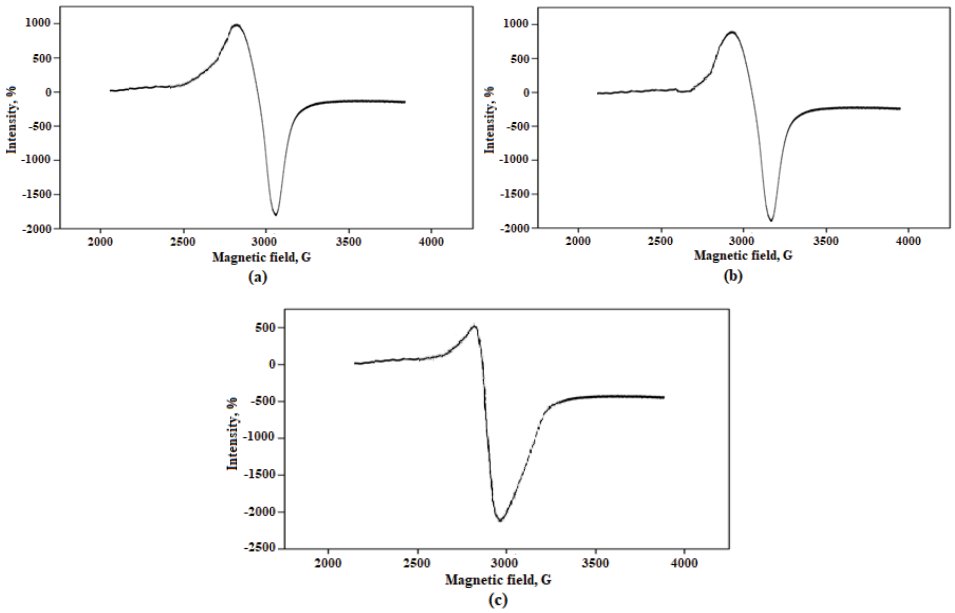

Fig. S-16. EPR spectrum of: (a) complex **1**; (b) complex **2** and (c) complex **3**.

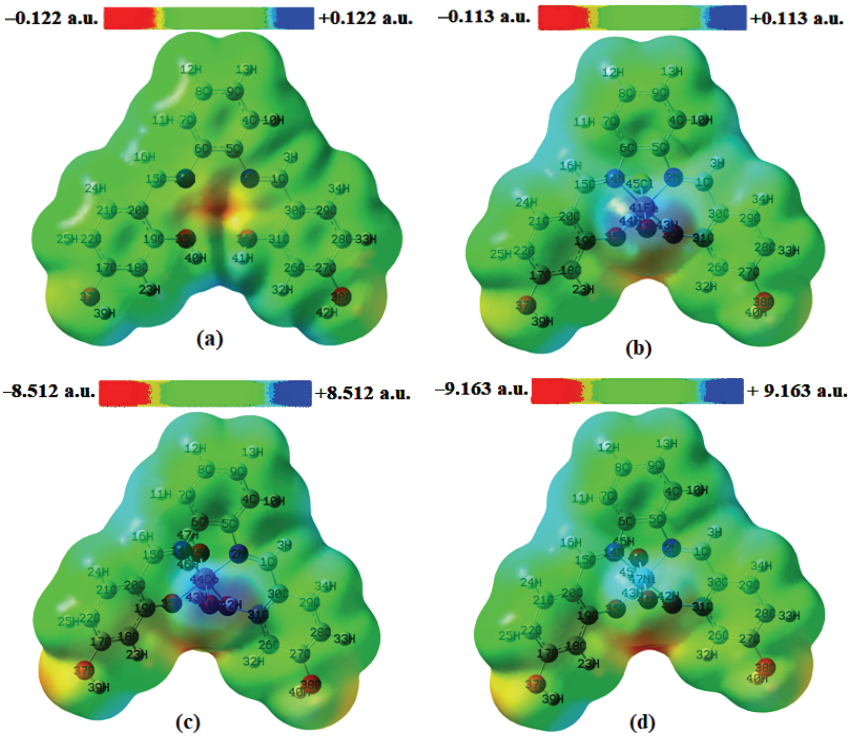

Fig. S-17. MEP of Ligand **L** (a) and complexes (b-d).

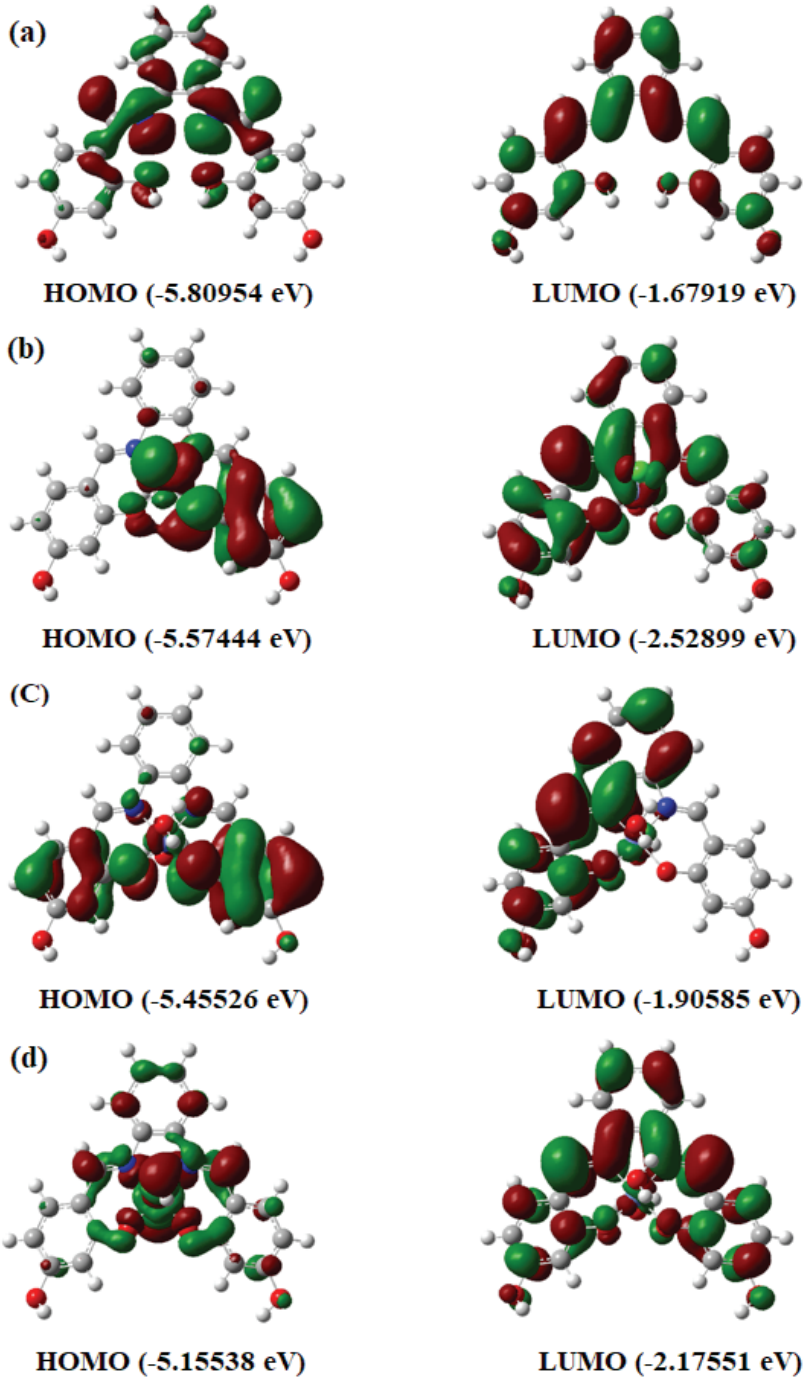

Fig. S-18. Energy level diagram of Ligand **L** (a) and Complex**es** (b-d).

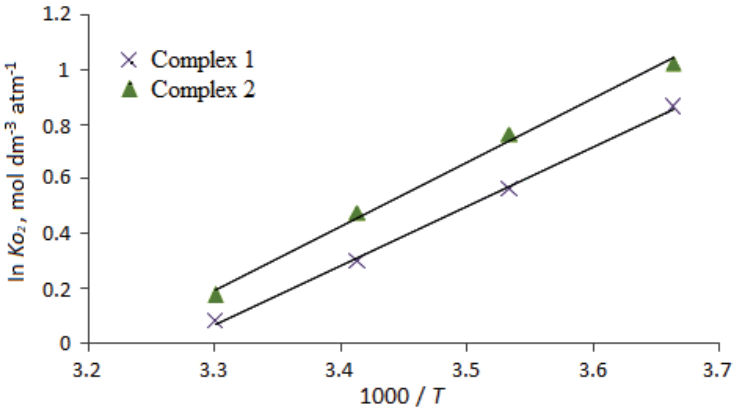

Fig. S-19. Van't Hoff diagrams for the complex **1** and **2**.