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SUPPLEMENTARY MATERIAL TO

Metal complexes of *N′*-[2-hydroxy-5-(phenyldiazenyl)-benzylidene]isonicotinohydrazide. Synthesis, spectroscopic characterization and antimicrobial activity

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PHYSICAL, ANALYTICAL AND SPECTRAL DATA FOR THE LIGAND AND ITS COMPLEXES

N′-*[2-Hydroxy-5-(phenyldiazenyl)benzylidene]isonicotinohydrazide (*H_2L*)* (***1***). Yellow color; yield: 95 %; Anal. Calcd. for $C_{19}H_{15}N_5O_2$ (FW: 345.35): C, 66.08; H, 4.38; N, 20.28 %. Found: C, 65.85; H, 4.37; N, 20.22 %. IR (KBr, cm^{-1}): 3300–3550, 2540–3000 (br) (H_2O/O–H), 3174 (N–H), 1658 (C=O), 1605 (C=N), 1468 (N=N), 1289 (C–O_{ph}), 1004 (N–N); ^{1}H-NMR (270 MHz, DMSO-d_6, δ/ ppm): 12.41 (1H, *s*, OH), 11.65 (1H, *s*, NH), 8.76 (1H, *s*, H–C=N), 7.14–8.31 (12H, *m*, aromatic); MS (*m*/*z*): 345 (M^+); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 270, 320, 350, 375, 420, 455.

[VO(H_2L*)(*SO_4*)(*H_2O*)]* (***2***). Light brown color; yield: 75 %; Anal. Calcd. for $C_{19}H_{17}N_5O_8SV$ (FW: 526.37): C, 43.35; H, 3.26; N, 13.30; V, 12.72 %. Found: C, 43.29; H, 3.67; N, 13.51; V, 12.89 %. 3426 (br) (H_2O/O–H), 3239 (N–H), 1607 (C=O), 1553 (C=N), 1470 (N=N), 1290 (C–O_{ph}), 1041 (N–N), 575 (V–O), 509 (V–N); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 290, 345, 360, 395, 425, 450, 520, 575, 700; Magnetic moment (μ_{eff} / μ_B): 1.73; Molar conductivity (Ω^{-1} cm^2 mol^{-1}): 22.5.

[Cu(HL)$_2$*]·5*H_2O (***3***). Yellowish green color; yield: 55 %; Anal. Calcd. for $C_{38}H_{38}CuN_{10}O_9$ (FW: 842.33): C, 54.18; H, 4.55; N, 16.63; Cu, 7.54 %. Found: C, 54.00; H, 4.87; N, 16.32; Cu, 7.42 %; IR (KBr, cm^{-1}): 3391(br) (H_2O/O–H), 1601 (C=N), 1507 (N=C–O), 1464 (N=N), 1285 (C–O_{ph}), 1208 (C–O_{amide}),

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1026 (N–N), 593 (Cu–O), 538 (Cu←O), 466 (Cu←N); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 265, 330, 350, 380, 420, 450, 630; magnetic moment (μ_{eff} / μ_B): 1.79; molar conductivity (Ω^{-1} cm^2 mol^{-1}): 6.9.

[Cu(H$_2$L)$_2$Cl$_2$]·2H$_2$O (***4***). Olive color; yield: 70 %; Anal. Calcd. for $C_{38}H_{34}Cl_2CuN_{10}O_6$ (FW: 861.19): C, 53.00; H, 3.98; N, 16.26; Cl, 8.23, Cu, 7.38 %. Found: C, 52.56; H, 4.01; N, 16.88; Cl, 7.98; Cu, 7.04 %; 3426 (br) (H$_2$O/O–H), 3198 (N–H), 1611 (C=O), 1570 (C=N), 1476 (N=N), 1278 (C–O$_{ph}$), 1047 (N–N), 551 (Cu–O), 464 (Cu–N); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 280, 345, 365, 390, 435, 470, 675; Magnetic moment (μ_{eff} / μ_B): 1.68; Molar conductivity (Ω^{-1} cm^2 mol^{-1}): 15.4.

[Cu(H$_2$L)$_2$(NO$_3$)$_2$]·H$_2$O (***5***). Olive color; yield: 65 %; Anal. Calcd. for $C_{38}H_{32}CuN_{12}O_{11}$ (FW: 896.28): C, 50.92; H, 3.60; N, 18.75; Cu, 7.09 %. Found: C, 50.81; H, 3.78; N, 18.46; Cu, 7.10 %; IR (KBr, cm^{-1}): 3428 (br) (H$_2$O/O–H), 3187 (N–H), 1606 (C=O), 1577 (C=N), 1465 (N=N), 1290 (C–O$_{ph}$), 1031 (N–N), 534 (Cu–O), 462 (Cu–N); UV-Vis (DMSO, 10^{-3} M) (λ / nm): 265, 330, 350, 390, 405, 440, 650; magnetic moment (μ_{eff} / μ_B): 1.75; molar conductivity (Ω^{-1} cm^2 mol^{-1}): 13.1.

[Cu(H$_2$L)$_2$(SO$_4$)(H$_2$O)]·2H$_2$O (***6***). Olive color; yield: 63 %; Anal. Calcd. for $C_{38}H_{36}CuN_{10}O_{11}S$ (FW: 904.36): C, 50.47; H, 4.01; N, 15.49; Cu, 7.03 %. Found: C, 50.43; H, 4.04; N, 15.11; Cu, 6.89 %; IR (KBr, cm^{-1}): 3425 (br) (H$_2$O/O–H), 3174 (N–H), 1606 (C=O), 1546 (C=N), 1468 (N=N), 1292 (C–O$_{ph}$), 1031 (N–N), 533 (Cu–O), 457 (Cu–N); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 275, 325, 340, 355, 375, 420, 470, 660; magnetic moment (μ_{eff} / μ_B): 1.77; molar conductivity (Ω^{-1} cm^2 mol^{-1}): 19.9.

[Cu(HL)(OAc)(H$_2$O)]·1/2H$_2$O (***7***). Green color; yield: 60 %; Anal. Calcd. for $C_{21}H_{20}CuN_5O_{5.5}$ (FW: 493.96): C, 51.06; H, 4.08; N, 14.18; Cu, 12.86 %. Found: C, 51.08; H, 4.31; N, 14.01; Cu, 12.65 %. IR (KBr, cm^{-1}): 3367 (br) (H$_2$O/O–H), 1602 (C=N), 1507 (N=C–O), 1463 (N=N), 1281 (C–O$_{ph}$), 1218 (C–O$_{amide}$), 1026 (N–N), 592 (Cu–O), 538 (Cu←O), 467 (Cu←N); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 240, 266, 326, 344, 3598, 475, 650 and 740; magnetic moment (μ_{eff} / μ_B): 1.88; molar conductivity (Ω^{-1} cm^2 mol^{-1}): 12.4.

[Ni(HL)]·5H$_2$O (***8***). Beige color; yield: 61 %; Anal. Calcd. for $C_{38}H_{38}N_{10}NiO_9$ (FW: 837.49): C, 54.50; H, 4.57; N, 16.73; Ni, 7.01 %. Found: C, 54.42; H, 5.01; N, 16.58; Ni, 6.91 %; IR (KBr, cm^{-1}): 3362(br) (H$_2$O/O–H), 1600 (C=N), 1525 (N=C–O), 1465 (N=N), 1299 (C–O$_{ph}$), 1207 (C–O$_{amide}$), 1059 (N–N), 573 (Ni–O), 506 (Ni←O), 476 (Ni←N); UV-Vis (DMSO, 10^{-3} M) (λ / nm): 265, 350, 390, 405, 430, 465, 580, 660, 850; magnetic moment (μ_{eff} / μ_B): 3.01; molar conductivity (Ω^{-1} cm^2 mol^{-1}): 5.3.

[Co(HL)(OAc)(H$_2$O)]·1/2H$_2$O (***9***). Reddish brown color; yield: 58 %, Anal. Calcd. for $C_{21}H_{20}CoN_5O_{5.5}$ (FW: 489.35): C, 51.54; H, 4.12; N, 14.31; Co, 12.04 %. Found: C, 51.71; H, 4.03; N, 14.18; Co, 12.59 %; IR (KBr, cm^{-1}): 3383

(br) (H_2O/O–H), 1603 (C=N), 1512 (N=C–O), 1464 (N=N), 1293 (C–O_{ph}), 1215 (C–O_{amide}), 1026 (N–N), 595 (Co–O), 563 (Co←O), 480 (Co←N); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 270, 330, 360, 395, 435, 450, 505, 590, 650; magnetic moment (μ_{eff} / μ_B): 4.42; molar conductivity (Ω^{-1} cm^2 mol^{-1}): 13.3.

[Mn(HL)$_2$]·H$_2$O ***(10)***. Dark yellow color; yield: 55 %, Anal. Calcd. for $C_{38}H_{30}MnN_{10}O_5$ (FW: 761.66): C, 59.92; H, 3.97; N, 18.39; Mn, 7.21 %. Found: C, 60.08; H, 4.04; N, 18.27; Mn, 7.16 %; IR (KBr, cm^{-1}): 3446 (br) (H_2O/O–H), 1603 (C=N), 1546 (N=C–O), 1467 (N=N), 1312 (C–O_{ph}), 1258 (C–O_{amide}), 1019 (N–N), 594 (Mn–O), 561 (Mn←O), 473 (Mn←N); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 280, 325, 350, 380, 405, 450, 465, 540, 600, 650; magnetic moment (μ_{eff} / μ_B): 4.87; molar conductivity (Ω^{-1} cm^2 mol^{-1}): 6.8.

[Fe(HL)$_2$Cl]·4H$_2$O ***(11)***. Dark brown color; yield: 66 %; Anal. Calcd. for $C_{38}H_{36}ClFeN_{10}O_8$ (FW: 852.05): C, 53.57; H, 4.26; N, 16.44; Cl, 4.16, Fe, 6.55 %. Found: C, 53.44; H, 4.20; N, 16.45; Cl, 3.99; Fe, 6.30 %; IR (KBr, cm^{-1}): 3385 (br) (H_2O/O–H), 3211 (N–H), 1607 (C=O), 1538 (C=N), 1458 (N=N), 1244 (C–O_{ph}), 1020 (N–N), 610 (Fe–O), 566 (Fe←O), 502 (Fe←N); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 280, 330, 350, 385, 415, 460, 580, 640; magnetic moment 5.34; molar conductivity: 80.5 Ω^{-1} cm^2 mol^{-1}.

[Ru(L)Cl(H$_2$O)$_2$]·H$_2$O ***(12)***. Dark brown color; yield: 72 %; Anal. Calcd. for $C_{19}H_{19}ClN_5O_5Ru$ (FW: 533.91): C, 42.74; H, 3.59; N, 13.12; Cl, 6.64, Ru, 18.93 %. Found: C, 42.84; H, 3.96; N, 13.28; Cl, 6.54; Ru, 18.72 %; IR (KBr, cm^{-1}): 3433 (br) (H_2O/O–H), 1602 (C=N), 1489 (N=N), 1272 (C–O_{ph}), 1019 (N–N), 593 (Ru–O), 525 (Ru←O), 482 (Ru←N); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 260, 320, 345, 375, 430, 460, 560, 650; magnetic moment (μ_{eff} / μ_B): 65; molar conductivity: 21.5 Ω^{-1} cm^2 mol^{-1}.

[Zn(L)(H$_2$O)] ***(13)***. Dark yellow color; yield: 63 %; Anal. Calcd. for $C_{19}H_{15}N_5O_3Zn$ (FW: 426.73): C, 53.48; H, 3.54; N, 16.41; M, 15.32 %. Found: C, 53.90; H, 3.70; N, 16.42; M, 15.20 %; IR (KBr, cm^{-1}): 3447 (br) (H_2O/O–H), 1606 (C=N), 1515 (N=C–O), 1479 (N=N), 1228 (C–O_{ph}), 1207 (C–O_{amide}), 1035 (N–N), 586 (Zn–O), 510 (Zn←O), 469 (Zn←N); ^{1}H-NMR (270 MHz, DMSO-d_6, δ / ppm): 8.76 (1H, *s*, H–C=N), 6.70–7.96 (12H, *m*, aromatic); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 280, 320, 360, 400, 430, 475; magnetic moment (μ_{eff} / / μ_B): diamagnetic; molar conductivity (Ω^{-1} cm^2 mol^{-1}): 6.4.

[Cd(H$_2$L)$_2$(OAc)$_2$]·7H$_2$O ***(14)***. Deep yellow color; yield: 51 %; Anal. Calcd. for $C_{42}H_{50}CdN_{10}O_{15}$ (FW: 1047.32): C, 48.17; H, 4.81; N, 13.37; Cd, 10.73 %. Found: C, 48.29; H, 4.65; N, 13.55; Cd, 11.21 %; IR (KBr, cm^{-1}): 3369 (br) (H_2O/O–H), 3176 (N–H), 1607 (C=O), 1546 (C=N), 1464 (N=N), 1292 (C–O_{ph}), 1020 (N–N), 592 (Cd–O), 533 (Cd←O), 492 (Cd←N); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 280, 330, 365, 405, 425, 465; magnetic moment (μ_{eff} / μ_B): diamagnetic; molar conductivity (Ω^{-1} cm^2 mol^{-1}): 8.5.

[(UO$_2$)(L)(H$_2$O)$_2$]·H$_2$O (***15***). Orange color; yield: 77 %; Anal. Calcd. for $C_{19}H_{19}N_5O_7U$ (FW: 667.41): C, 34.19; H, 2,87; N10.49; UO_2, 40.48 %. Found: C, 34.77; H, 3.39; N, 8.54; U, 37.05 %; IR (KBr, cm^{-1}): 3401(br) (H_2O/O–H), 1603 (C=N), 1522 (C=N–O), 1472 (N=N), 1257 (C–O_{ph}), 1017 (N–N), 590 (U–O), 549 (U←O), 505 (U←N); ^{1}H-NMR (270 MHz, DMSO-d_6, δ / ppm): 7.17–8.25 (12H, *m*, aromatic), 9.01 (1H, *s*, H–C=N); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 270, 325, 360, 395, 440, 480, 530; magnetic moments (μ_{eff} / μ_B): diamagnetic; molar conductivity (Ω^{-1} cm^2 mol^{-1}): 9.5.

[Hg(HL)$_2$]·4H$_2$O (***16***). Reddish brown color; yield: 72 %; Anal. Calcd. for $C_{38}H_{36}HgN_{10}O_8$ (FW: 962.27): C, 47.48; H, 3.77; N, 14.57; Hg, 20.87 %. Found: C, 47.47; H, 3.69; N, 14.68; Hg, 20.25 %; IR (KBr, cm^{-1}): 3432 (br) (H_2O/O–H), 3207 (N–H), 1615 (C=O), 1549 (C=N), 1455 (N=N), 1227 (C–O_{ph}), 1039 (N–N), 601 (Hg–O), 536 (Hg←O), 496 (Hg←N); UV–Vis (DMSO, 10^{-3} M) (λ / nm): 270, 330, 355, 380, 420, 460; magnetic moment (μ_{eff} / μ_B): diamagnetic; molar conductivity (Ω^{-1} cm^2 mol^{-1}): 10.5.

SOME SPECTRA OF THE LIGAND AND SELECTED COMPLEXES

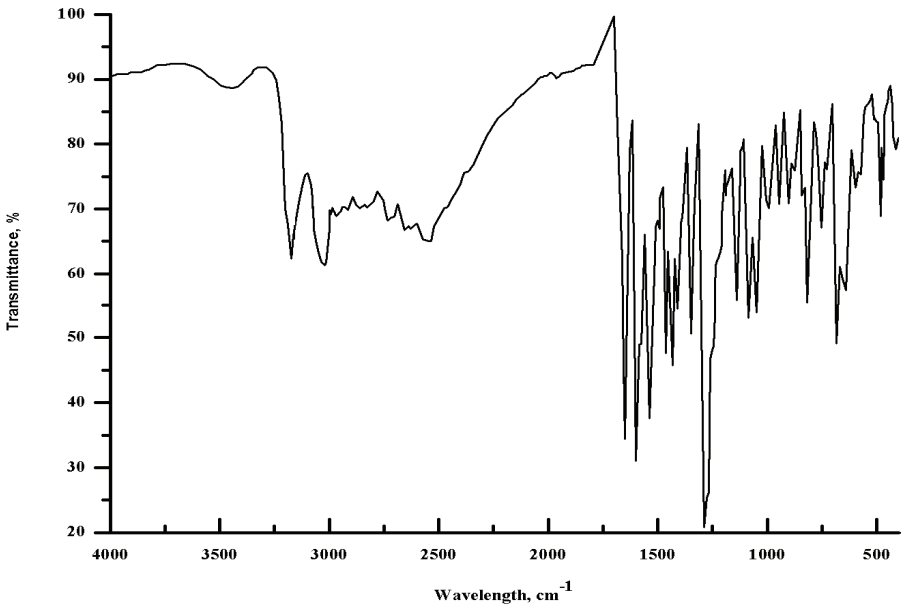

Fig. S-1. The IR spectrum of the ligand [H_2L] (**1**).

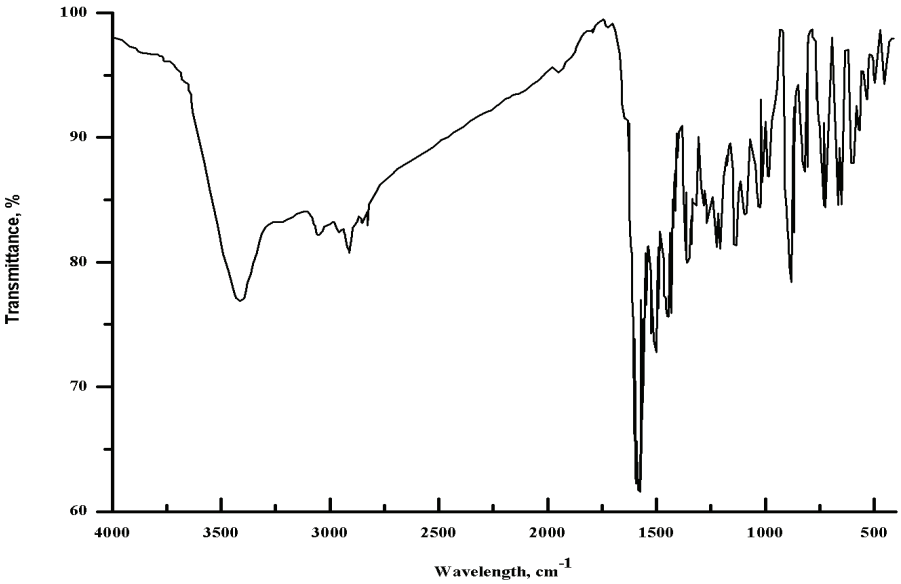

Fig. S-2. The IR spectrum of the complex $[Cu(H_2L)_2(SO_4)(H_2O)]\cdot 2H_2O$ (**6**).

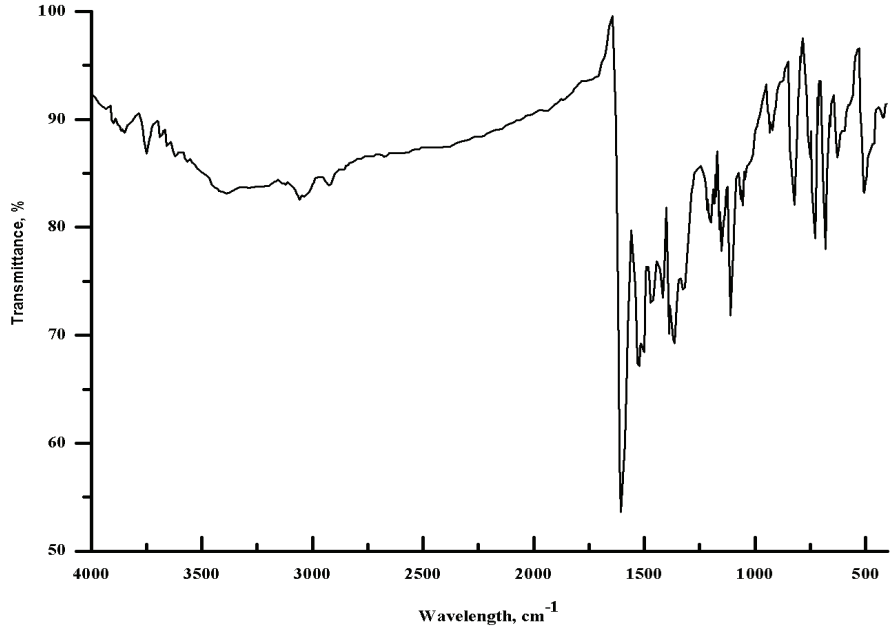

Fig. S-3.The IR spectrum of the complex $[Ni(HL)_2]\cdot 5H_2O$ (**8**).

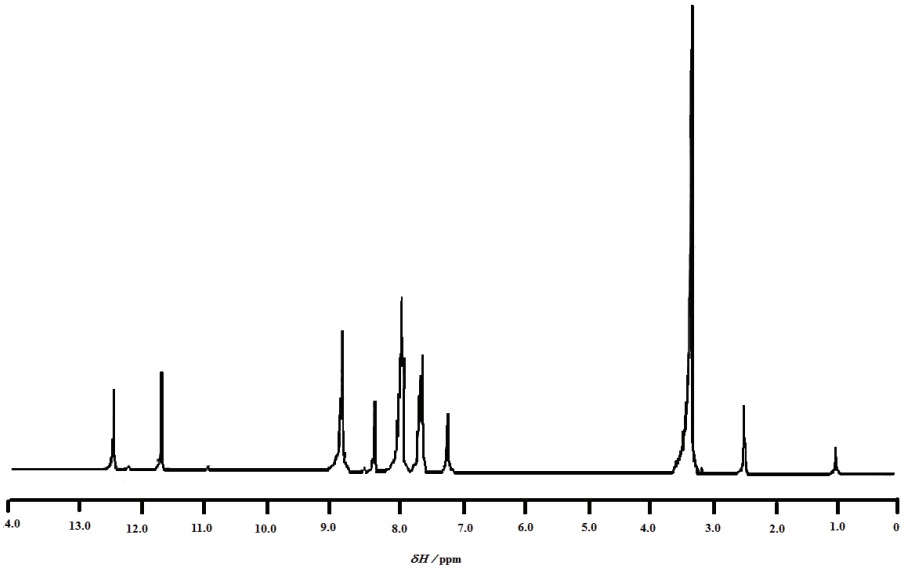

Fig. S-4. The ^{1}H-NMR spectrum of the ligand (H_2L) (**1**).

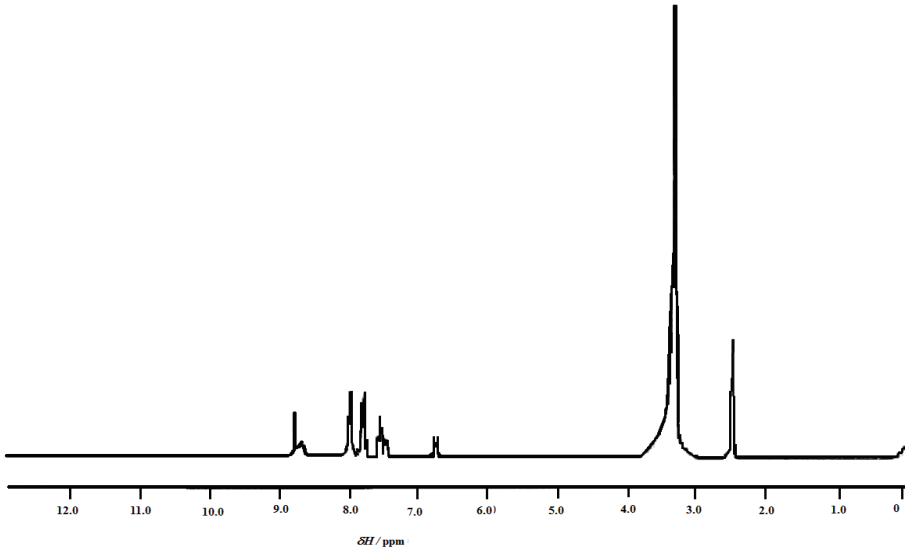

Fig. S-5. The ^{1}H-NMR spectrum of the complex [Zn(L)(H_2O)] (**13**).

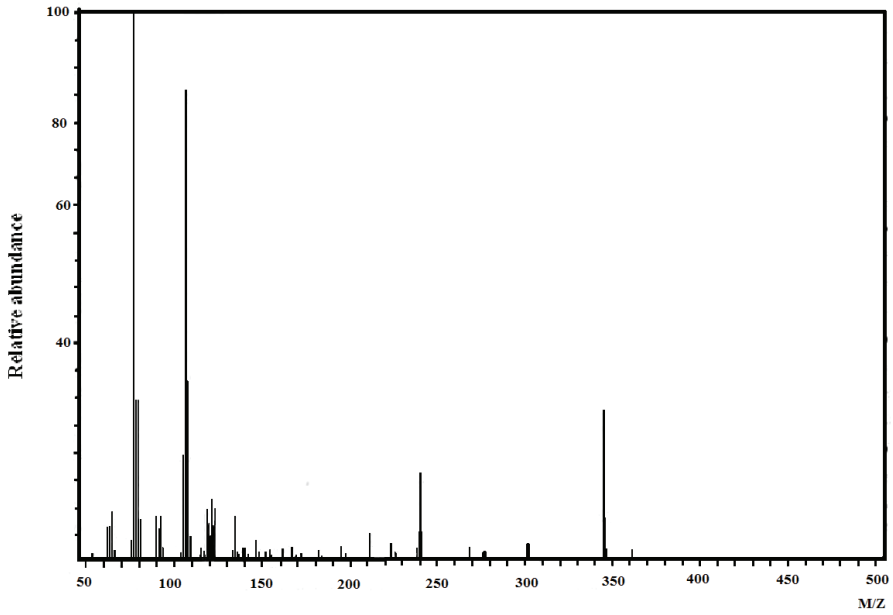

Fig. S-6. The mass spectrum of the ligand (H_2L) (**1**).

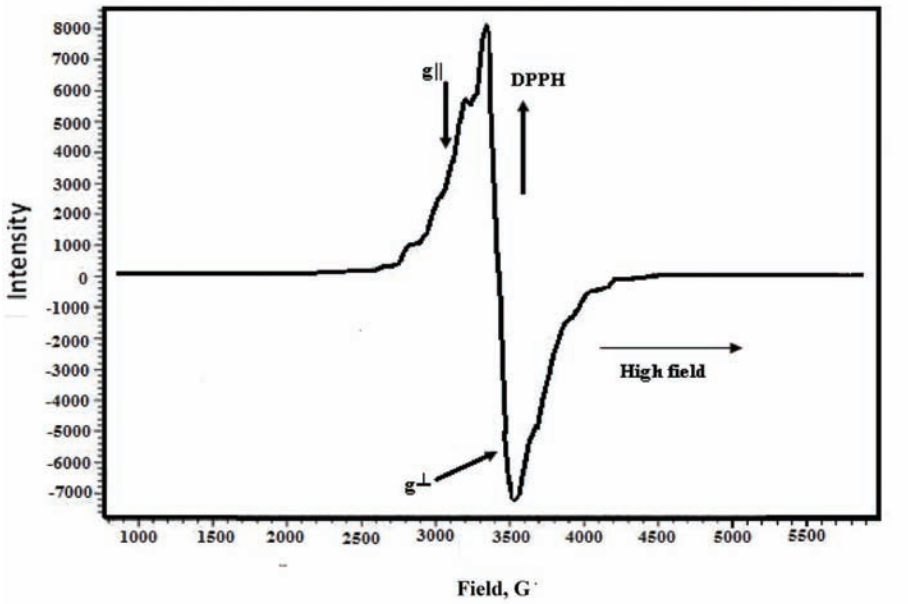

Fig. S-7. The ESR spectrum of the vanadyl(II) complex **2**.

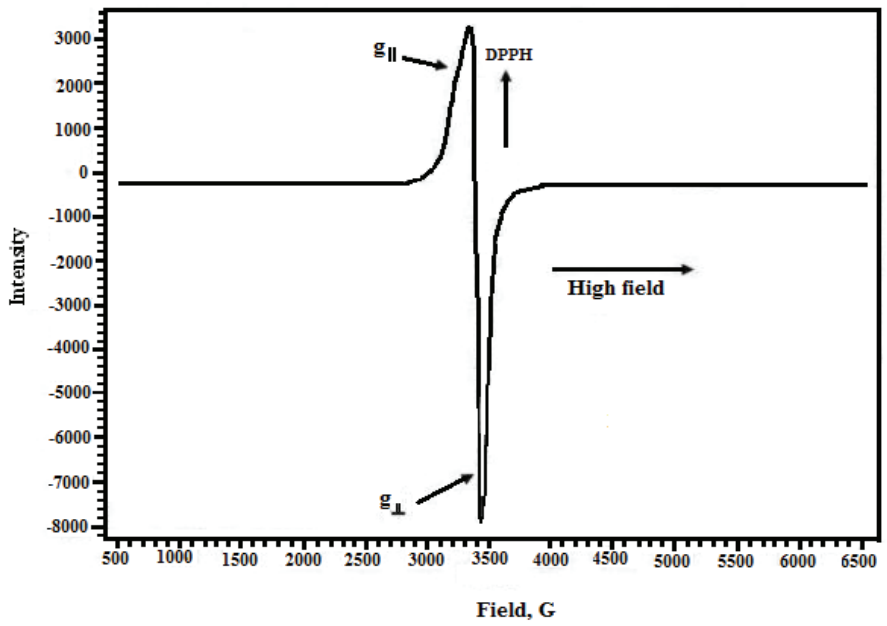

Fig. S-8. The ESR spectrum of copper(II) complex **3**.

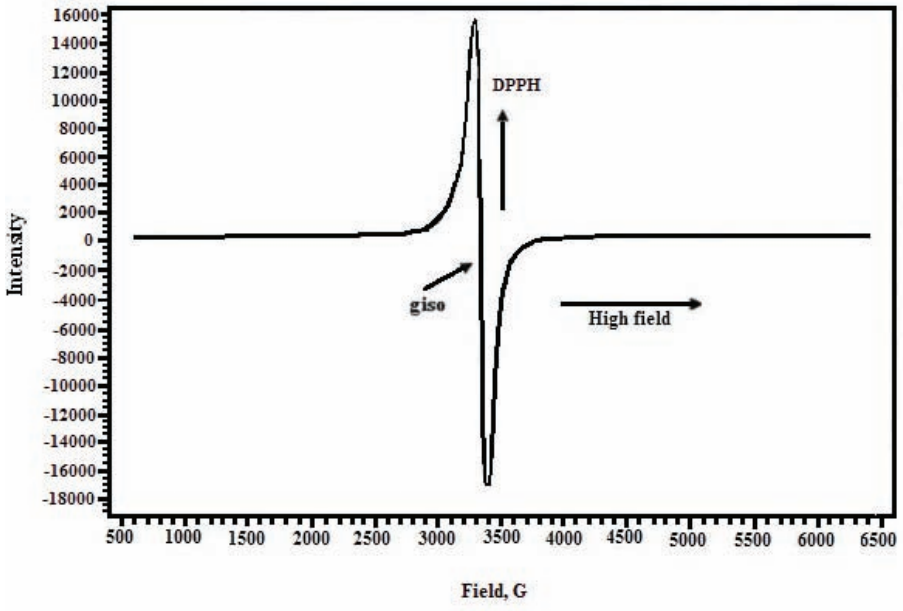

Fig. S-9. The ESR spectrum of copper(II) complex **6**.