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SUPPLEMENTARY MATERIAL TO

Synthesis, characterization, electrochemical behavior and antibacterial/antifungal activities of $[Cd(L)X_2]$ complexes with a new Schiff base ligand

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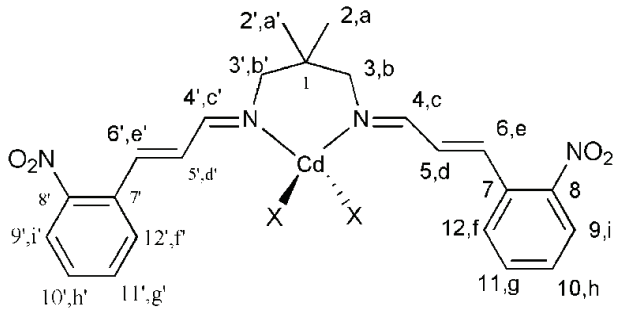

Structural formula of the $[Cd(L)X_2]$ complexes (X is Cl^-, Br^-, I^-, NCS^- and N_3^-) with atomic numbering.

PHYSICAL, ANALYTIC AND SPECTRAL DATA FOR THE LIGAND AND ITS Cd(II) COMPLEXES

Ligand. Yield: 83 %; m.p.: 85 °C; Anal. Calcd. for $C_{23}H_{24}N_4O_4$: C, 65.70; H 5.75; N, 13.33 %. Found: C, 65.5, H, 5.6, N, 13.4 %; IR (KBr, cm^{-1}): 2869*w* (iminic –CH stretching), 1636s (C=N– asym. stretching), 1614s (C=N– sym. stretching), 1529*vs* (–NO_2, asym. stretching), 1338*vs* (–NO_2, sym. stretching); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 8.09 (2H, *d*, *J* = 8.76 Hz, $H_{c,c'}$), 7.99 (2H, *dd*, *J* = 8.20 Hz, *J* = 1.12 Hz, $H_{i,i'}$), 7.74 (2H′, *dd*, *J* = 7.86 Hz, *J* = 1.0 Hz $H_{f,f'}$), 7.64 (2H, *dt*, *J* = 7.26 Hz, *J* = 7.56 Hz, *J* = 0.92 Hz, $H_{g,g'}$), 7.48 (2H, *dt*, *J* = 7.66 Hz, *J* = 7.44 Hz, *J* = 1.32 Hz, $H_{h,h}$), 7.48 (2H, *d*, *J* = 15.84 Hz. $H_{e,e'}$), 6.94 (2H, *dd*, *J* = 15.86 Hz, *J* = 8.76 Hz, $H_{d,d'}$), 3.46 (4H, *s*, $H_{b,b'}$), 1.02 (6H, *s*, $H_{a,a'}$); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 162.69 ($C_{4,4'}$), 147.96 ($C_{8,8'}$), 135.68 ($C_{6,6'}$),

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133.35 ($C_{9,9'}$), 133.04 ($C_{7,7'}$), 131.49 ($C_{5,5'}$), 129.27 ($C_{12,12'}$), 128.38 ($C_{11,11'}$), 124.87 ($C_{10,10'}$), 70.75 ($C_{3,3'}$), 36.96 (C_1), 24.59 ($C_{2,2'}$); UV–Vis ($CHCl_3$) (λ_{max} / / nm, (ε / L mol^{-1} cm^{-1})): 295 (19876), 328(*sh*) (11045); Molar conductance ($CHCl_3$) (Λ_M / S m^2 mol^{-1}): 0.011.

Cd(L)Cl$_2$. Yield: 92 %; m.p.(dec.): 243 °C; Anal. Calcd. for $C_{23}H_{24}N_4O_4CdCl_2$: C, 45.75; H 4.01; N, 9.28 %. Found: C, 45.6, H, 3.9, N, 9.1 %; IR (KBr, cm^{-1}): 2862*m* (iminic –CH stretching), 1633*s* (C=N– asym. stretching), 1613*s* (C=N– sym. stretching), 1519*vs* (–NO_2, asym. stretching), 1339*vs* (–NO_2, sym. stretching); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 8.17 (2H *d*, *J* = 8.68 Hz $H_{c,c'}$), 8.03 (2H, *d*, *J* = 8.16 Hz, $H_{i,i'}$), 7.98 (2H, *d*, *J* = 7.88 Hz, $H_{f,f'}$), 7.78 (2H, *t*, *J* = 7.64 Hz, *J* = 7.56 Hz, $H_{g,g'}$), 7.62 (2H, *t*, *J* = 7.76 Hz, *J* = = 7.72 Hz, $H_{h,h'}$), 7.43 (2H, *d*, *J* = 15.80 Hz, $H_{e,e'}$), 7.58 (2H, *dd*, *J* = 14.48Hz, *J* = 7.44 Hz, $H_{d,d'}$), 3.36 (4H, *s*, $H_{b,b'}$), 0.91 (6H, *s*, $H_{a,a'}$); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 164.30 ($C_{4,4'}$), 148.01 ($C_{8,8',6,6'}$), 136.25 ($C_{9,9'}$), 133.60 ($C_{7,7'}$), 132.11 ($C_{5,5'}$), 130.06 ($C_{12,12'}$), 128.43 ($C_{11,11'}$), 124.56 ($C_{10,10'}$), 69.82($C_{3,3'}$), 36.42 (C_1), 24.17 ($C_{2,2'}$); UV–Vis (DMF) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 269 (8946), 295 (19641), 327(*sh*) (10641); Molar conductance (DMF) (Λ_M / S m^2 mol^{-1}): 0.031.

[Cd(L)Br$_2$]. Yield: 79 %; m.p.(dec.): 235 °C; Anal. Calcd. for $C_{23}H_{24}N_4O_4CdBr_2$: C, 39.88; H 3.49; N, 8.09 %. Found: C, 39.7, H, 3.3, N, 8.3 %; IR (KBr, cm^{-1}): 2867*w* (iminic –CH stretching), 1633*s* (asym. –C=N), 1615s (–C=N sym. stretching), 1524*vs* (–NO_2, asym. stretching), 1348*vs* (–NO_2, sym. stretching); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 8.23 (2H, *d*, *J* = 9.2 Hz, $H_{c,c'}$), 8.05 (2H, *dd*, *J* = 8.10 Hz, *J* = 1.08 Hz, $H_{i,i'}$), 8.04 (2H, *d*, *J* = 7.36 Hz, $H_{f,f'}$), 7.95 (2H, *dd*, *J* = 15.44 Hz, *J* = 9.2 Hz, $H_{d,d'}$), 7.78 (2H, *d*, *J* = 15.56 Hz, $H_{e,e'}$), 7.74 (2H, *t*, *J* = 10.04 Hz, *J* = 7.88 Hz, $H_{g,g'}$), 7.59 (2H, *dt*, *J* = 7.72 Hz, *J* = 1.12 Hz, *J* = 0.96 Hz $H_{h,h'}$), 3.86(4H, *s*, $H_{b,b'}$), 1.03 (6H, *s*, $H_{a,a'}$); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 169.75 ($C_{4,4'}$), 148.21 ($C_{8,8'}$), 143.32 ($C_{6,6'}$), 133.99 ($C_{9,9'}$), 130.99($C_{5,5'}$), 129.62($C_{7,7'}$), 129.32($C_{12,12'}$), 128.82($C_{11,11'}$), 125.02 ($C_{10,10'}$), 72.38 ($C_{3,3'}$), 37.74 (C_1), 24.83 ($C_{2,2'}$); UV–Vis ($CHCl_3$) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 305 (28273), 325(*sh*) (22667); Molar conductance ($CHCl_3$) (Λ_M / S m^2 mol^{-1}): 0.009.

[Cd(L)I$_2$]. Yield: 95 %; m.p.(dec.): 237 °C; Anal. Calcd. for $C_{23}H_{24}N_4O_4CdI_2$: C, 35.12; H 3.08; N, 7.12 %. Found: C, 34.9, H, 3.2, N, 7.3 %; IR (KBr, cm^{-1}): 2861*w* (iminic –CH stretching), 1635*s* (–C=N asym. stretching), 1614*s* (–C=N sym. stretching), 1524*vs* (–NO_2, asym. stretching), 1348*vs* (–NO_2, sym. stretching); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 8.26 (2H, *d*, *J* = 9.24 Hz, $H_{c,c'}$), 8.06 (2H, *dd*, *J* = 8.16 Hz, *J* = 1.28 Hz, $H_{i,i'}$), 8.05 (2H, *dd*, *J* = 7.92 Hz, *J* = 1.08 Hz, $H_{f,f'}$), 7.99 (2H, *dd*, *J* = 15.44 Hz, *J* = 9.2 Hz, $H_{d,d'}$), 7.81 (2H, *d*, *J* = 15.52 Hz $H_{e,e'}$), 7.75 (2H, *dt*, *J* = 7.66 Hz, *J* = 7.64 Hz, *J* = 0.84 Hz, $H_{g,g'}$), 7.60 (2H, *dt*, *J* = 7.82 Hz, *J* = 7.58 Hz, *J* = 1.28Hz, $H_{h,h'}$),

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3.81(4H, *s*, $H_{b,b'}$), 1.05 (H6, *s*, $H_{a,a'}$); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 169.70 ($C_{4,4'}$), 148.15 ($C_{8,8'}$), 143.41 ($C_{6,6'}$), 133.99 ($C_{9,9'}$), 131.03 ($C_{5,5'}$), 129.71 ($C_{7,7'}$), 129.38 ($C_{12,12'}$), 128.78 ($C_{11,11'}$), 125.05 ($C_{10,10'}$), 71.47 ($C_{3,3'}$), 37.62 (C_1), 24.90 ($C_{2,2'}$); UV–Vis ($CHCl_3$) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 302 (26263), 326(*sh*) (19754); Molar conductance ($CHCl_3$) (Λ_M / S m^2 mol^{-1}): 0.011.

[Cd(L)(NCS)$_2$]. Yield: 89 %; m.p.(dec.): 210 °C; Anal. Calcd. for $C_{25}H_{24}N_6O_4CdS_2$: C, 46.26; H 3.73; N, 12.95 %. Found: C, 45.9, H, 3.6, N, 12.7 %; IR (KBr, cm^{-1}): 2860w (iminic –CH stretching), 2059*vs* (–NCS), 1633*s* (–C=N asym. stretching), 1610*s* (–C=N sym. stretching), 1521*vs* (–NO_2, asym. stretching), 1340*vs* (–NO_2 sym. stretching); ^{1}H-NMR (400 MHz, $(CD_3)_2SO$, δ / / ppm): 8.15 (2H, *d*, *J* = 8.68 Hz, $H_{c,c'}$), 8.02 (2H, *d*, *J* = 8.12 Hz, $H_{i,i'}$), 8.00 (2H, *d*, *J* = 7.8 Hz, $H_{f,f'}$), 7.75 (2H, *t*, *J* = 7.56 Hz, *J* = 7.44, $H_{g,g'}$), 7.61 (2H, *t*, *J* = = 7.52 Hz, *J* = 7.48 Hz, $H_{h,h'}$), 7.39 (2H, *d*, *J* = 15.76 Hz, $H_{e,e'}$), 7.05 (2H, *dd*, *J* = = 14.90 Hz, *J* = 8.92 Hz, *J* = 8.2 Hz. $H_{d,d'}$), 3.35 (4H, *s*, $H_{b,b'}$), 0.93 (6H, *s*, $H_{a,a'}$); ^{13}C-NMR (100 MHz, $(CD_3)_2SO$, δ / ppm): 160.57 ($C_{4,4'}$), 147.97 ($C_{8,8'}$), 143.18 ($C_{6,6'}$), 135.51 (C_{SCN}), 133.57 ($C_{9,9'}$), 132.35 ($C_{7,7'}$), 130.10 ($C_{5,5'}$), 129.89 ($C_{12,12'}$), 128.44 ($C_{11,11'}$), 124.50 ($C_{10,10'}$), 69.68 ($C_{3,3'}$), 36.53 (C_1), 24.25 ($C_{2,2'}$); UV–Vis (DMF) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 268 (12934), 297 (22549), 327(*sh*) (13751); Molar conductance (DMF) (Λ_M / S m^2 mol^{-1}): 49.20.

[Cd(L)(N$_3$)$_2$]. Yield: 29 %; m.p.(dec.): 174 °C; Anal. Calcd. for $C_{23}H_{24}N_4O_4CdBr_2$: C, 44.78; H, 3.92; N, 22.70 %. Found: C, 44.9, H, 4.1, N, 22.9 %; IR (KBr, cm^{-1}): 2865*w* (iminic –CH stretching), 2041*s* (–N_3), 1634*s* (–C=N asym. stretching), 1613*s* (–C=N sym. stretching), 1524*vs* (–NO_2, asym. stretching), 1345*vs* (–NO_2 sym. stretching); ^{1}H-NMR (400 MHz, $(CD_3)_2SO$), δ / / ppm): 8.15 (2H, *d*, *J* = 8.68 Hz, $H_{c,c'}$), 8.02 (2H, *dd*, *J* = 8.28 Hz, *J* = 0.92 Hz, $H_{i,i'}$), 7.99 (2H, *d*, *J* = 8.08 Hz, $H_{f,f'}$), 7.75 (2H, *t*, *J* = 7.56 Hz $H_{g,g'}$), 7.61 (2H, *dt*, *J* = 7.84 Hz, *J* = 7.66 Hz, *J* = 1.04 Hz, $H_{h,h'}$), 7.38 (2H, *d*, *J* = 15.84 Hz, $H_{e,e'}$), 7.04 (2H, *dd*, *J* = 15.66 Hz, *J* = 8.68 Hz, $H_{d,d'}$), 3.36 (4H, *s*, $H_{b,b'}$), 0.93 (6H, *s*, $H_{a,a'}$); ^{13}C-NMR (100 MHz, $(CD_3)_2SO$, δ / ppm): 162.96 ($C_{4,4'}$), 147.97 ($C_{8,8'}$), 135.44 ($C_{6,6'}$), 133.56 ($C_{9,9'}$), 132.37 ($C_{7,7'}$), 130.10 ($C_{5,5'}$), 129.88 ($C_{12,12'}$), 128.42 ($C_{11,11'}$), 124.50 ($C_{10,10'}$), 69.68 ($C_{3,3'}$), 36.52 (C1), 24.25 ($C_{2,2'}$); UV– –Vis (DMF) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 268 (8555), 295 (20293), 326(*sh*) (11212); Molar conductance (DMF) (Λ_m / S m^2 mol^{-1}): 74.64.

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