



SUPPLEMENTARY MATERIAL TO
**Design, synthesis, characterization, and antimicrobial activity of
the new 2-*(E)*-[(4-aminophenyl)imino]methyl}-4,6-dichloro-
phenol and its complexes with Co(II), Ni(II), Cu(II) and
Zn(II): An experimental and DFT study**

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ANALYTICAL DATA FOR THE LIGAND AND THE PREPARED COMPLEXES

LH. Calcd. for C₁₃H₁₀Cl₂N₂O (FW: 281.14): C, 55.54; H, 3.59; N, 9.96 %.
Found: C, 55.48; H, 3.05; N, 10.06 %.

*Co(L)*₂. Calcd. for C₂₆H₁₈Cl₄CoN₄O₂ (FW: 619.19): C, 50.43; H, 2.93; N, 9.05 %.
Found: C, 49.95; H, 2.55; N, 8.45 %.

*Ni(L)*₂. Calcd. for C₂₆H₁₈Cl₄NiN₄O₂ (FW: 618.94): C, 50.45; H, 2.93; N, 9.05 %.
Found: C, 50.66; H, 2.74; N, 9.53 %.

*Cu(L)*₂. Calcd. for C₂₆H₁₈Cl₄CuN₄O₂ (FW: 623.80): C, 50.06; H, 2.91; N, 8.98 %.
Found: C, 49.67; H, 2.63; N, 9.01 %.

*Zn(L)*₂. Calcd. for C₂₆H₁₈Cl₄N₄O₂Zn (FW: 625.65): C, 49.91; H, 2.90; N, 8.96 %.
Found: C, 49.53; H, 2.41; N, 9.16 %.

TABLE S-I. Characteristic IR bands of the ligand and the complexes (cm⁻¹)

Compound	$\nu(\text{O-H})$	$\nu(\text{N-H})$	$\nu(\text{C=N})$	$\nu(\text{C-O})$
LH	3350–3200	3315–3190	1609	1290
Co(L) ₂	–	3400	1608	1294
Ni(L) ₂	–	3367	1607	1295
Cu(L) ₂	–	3446	1602	1323

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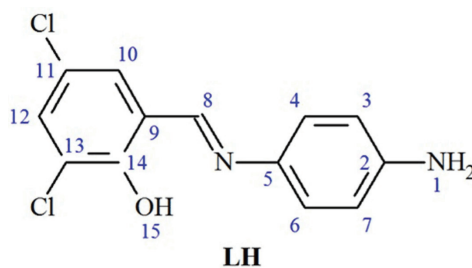


Fig. S-1. Structure of the ligand with atomic numbering.

TABLE S-II. ^1H - and ^{13}C -NMR spectral data for the ligand (δ / ppm); *s*: singlet, *d*: doubled

Compound	^1H -NMR	^{13}C -NMR
LH	15.30 (1H, <i>s</i> , H15) ^a , 8.90 (1H, <i>s</i> , H8), 7.60 (1H, <i>s</i> , H10), 7.25 (2H, <i>d</i> , H4 & H6), 6.60 (2H, <i>d</i> , H3 & H7), 5.60 (1H, <i>s</i> , H12)	156.22 (C8), 154.96 (C14), 149.61 (C5), 133.36 (C2), 122.69 (C12), 121.46 (C11), 121.26 (C4 & C6), 120.71 (C3 & C7), 119.11 (C10), 114.71 (C9), 114.08 (C13)

^aDisappears on D₂O exchange

TABLE S-III. Physical data for the ligand and the prepared complexes

Compound	Color	Yield, %	$\mu_{\text{eff}} / \mu_{\text{B}}$
LH	Orange	61	–
Co(L) ₂	Light brown	37	4.45
Ni(L) ₂	Brown	61	2.82
Cu(L) ₂	Black	52	1.77
Zn(L) ₂	Yellow	56	dia