# Supplementary information

## Synthesis, Characterization and Biological Studies of Schiff Bases and Their Complexes Derived from Aromatic Diamine Compounds with Cobalt (II).

**Abduljleel Mohammed Abduljleel[1], Jassim Mohammed Saleh Alshawi [2] and kawkab Ali Hussein [3] and Sadiq M-H. Ismael[4]**

[1] Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah, 61004 Iraq; abduljaleel.muhammad@gmail.com. ORCID; 0000-0002-4117-4053.
[2] Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah, 61004 Iraq jasim.salih@uobasrah.edu.iq.ORCID; 0000-0002-8715-4971.
[3] Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah, 61004 Iraq kawkab.ali@uobasrah.edu.iq.ORCID; 0000-0001-9796-0929.
[4] Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah, 61004 Iraq sadiq.ismael@uobasrah.edu.iq.ORCID; 0000-0002-8596-2991.
* Correspondence: kawkab.ali@uobasrah.edu.iq.

## Tables

**Table 1:** Some physical properties of prepared Schiff base ligands.

| Symbol | Molecular formula | Physical state and colour | Time of reaction (min) | Melting point (°C) | Yield (%) |
|---|---|---|---|---|---|
| **$L^1$** | $C_{22}H_{20}N_2O_4$ | Cream | 19 | 281-283 | 78 |
| **$L^2$** | $C_{23}H_{22}N2O_4$ | Yellow | 20 | 257-259 | 70 |

**Table 2:** Solubility of prepared Schiff base ligands.

| Symbol | ethanol | methanol | acetone | hexane | chloroform | Petroleum ether | $CH_2Cl_2$ | benzene | butane | acetonitrile | THF | DMF | DMSO | $H_2O$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $L^1$ | ± | ± | + | - | + | - | + | + | ± | + | + | + | + | - |
| $L^2$ | ± | ± | ± | - | + | - | + | + | + | ± | + | + | + | - |

Where : + soluble , ± partial soluble , - insoluble.

**Table 3:** Some physical properties of prepared complexes.

| Symbol | Formula | Physical state and colour | Time of reaction | Melting point (ºC) | Yield (%) |
|---|---|---|---|---|---|
| **$L^1Co$** | $[Co(L^1)(H_2O)_2]Cl_2$ | Green powder | 18 | 296-294 ºC | 68 |
| **$L^2Co$** | $[Co(L^3)(H_2O)_2]Cl_2$ | Green powder | 21 | >300ºC | 66 |

**Table 4:** Solubility of prepared complexes.

| Formula | DMSO | THF | DMF | acetone | chlorofo... | $CH_2Cl_2$ | ethyl ... | hexane | acetonit... | benzene | $H_2O$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **$[Co(L^1)(H_2O)_2]Cl_2$** | + | - | + | - | - | ± | - | - | + | - | - |
| **$[Co(L^2)(H_2O)_2]Cl_2$** | + | - | + | - | - | ± | + | - | + | - | - |

**Table 5 :** Characteristic IR bonds of the ligands and the complexes.

| Com | $\nu_{C-H}$ Alph $cm^{-1}$ | $\nu_{C-H}$ Arom $cm^{-1}$ | $\nu_{HC=N}$ $cm^{-1}$ | $\nu_{C-O}$ $cm^{-1}$ | $\nu_{C=CAr}$ $cm^{-1}$ | $\nu_{OH}$ $cm^{-1}$ | $\nu_{M-H2O}$ $cm^{-1}$ |
|---|---|---|---|---|---|---|---|
| **$L^1$** | 2900m | 3061w | 1502s | 1242s | 1448s | 3400m | ------ |
| **$L^2$** | 2897m | 3066vw | 1643s | 1224s | 1463s | 3458m | ------ |
| **$L^1Co$** | 2902w | 3044w | 1604s | 1261s | 1455s | 3150b | 819m |
| **$L^2Co$** | 2900w | 3102w | 1614s | 1267s | 1467s | 3466b | 808m |

w = (weak) , m = (medium) , s = (strong) , b = (Broad)

**Table 6:** Electronic spectral data for the ligands and their complexes.

| Com | (π—π*) phenyl Cycle (nm) | -C=N- (nm) (π—π *) | -C=N- (n—π*) (nm) | (C—T) (nm) | (d—d) (nm) |
|---|---|---|---|---|---|
| **$L^1$** | 225 | 280 | 320 | ---- | ---- |
| **$L^1Co$** | 217 | 247 | 318 | 520 | 590 |
| **$L^2$** | 225 | 275 | 326 | ---- | ---- |
| **$L^2Co$** | 240 | 287 | 334 | 520 | 590 |

**Table 7:** Chemical shift of $^{1}$H-NMR for the ligands.

| **Protons** | **δ (Chemical shift ppm)** | |
|---|---|---|
| **Symbol** | **$L^1$** | **$L^2$** |
| **$C_1$** | 8.3 | 7.75 |
| **$C_2$** | 7.3 | 7.2 |
| **$C_3$** | 7.1 | 6.75 |
| **$C_4$** | 6.75 | 6.5 |
| **$C_5$** | 5.9 | 5.9 |
| **$C_6$** | 5.34 | 5.25 |
| **$C_7$** | 3.6 | 3.75 |
| **$C_8$** | ----- | 2.4 |
| **$C_9$** | ----- | ----- |
| **$C_{10}$** | ----- | ----- |

**Table 8:** Chemical shift of $^{13}$C-NMR for the ligands.

| **Protons** | **δ (Chemical shift ppm)** | |
|---|---|---|
| **Symbol** | **$L^1$** | **$L^2$** |
| **$C_1$** | 160.08 | 160.8 |
| **$C_2$** | 149.69 | 149.69 |
| **$C_3$** | 148.23 | 148.23 |
| **$C_4$** | 131.17 | 143.88 |
| **$C_5$** | 130.57 | 138.13 |
| **$C_6$** | 124.17 | 134.17 |
| **$C_7$** | 108.37 | 132.58 |
| **$C_8$** | 106.93 | 131.17 |
| **$C_9$** | 102.12 | 128.87 |
| **$C_{10}$** | 61.27 | 127.17 |
| **$C_{11}$** | ----- | 108.37 |
| **$C_{12}$** | ----- | 106.93 |
| **$C_{13}$** | ----- | 102.12 |
| **$C_{14}$** | ----- | 61.27 |
| **$C_{15}$** | ----- | 28.78 |

**Table 9:** Molecular weight, molar conductivity, magnetic measurements and atomic absorption data of the complexes.

| Com. | Formula | M.wt Camphor Method | | Molar conductivity $Ohm^{-1}.cm^{-1}/mol$ | Metal % | | M:L ratio | Atomic magnetic susceptibility $X_A.10^{-6}$ | μeff (B.M) |
|---|---|---|---|---|---|---|---|---|---|
| | | found | Cal | | found | Cal | | | |
| $L^1Co$ | $[Co(L^1)(H_2O)_2]Cl_2$ | 482.5 | 483.07 | 219.32 | 11.17 | 11.32 | 1:1 | 2713.49 | 2.424 |
| $L^2Co$ | $[Co(L^3)(H_2O)_2]Cl_2$ | 500.02 | 498.10 | 198.18 | 12.02 | 11.98 | 1:1 | 2513.49 | 2.162 |

**Table 10:** Biological activity data of the compounds.

| Compounds | Gram positive bacteria | Gram negative bacteria |
|---|---|---|
| DMSO | - | - |
| $L^1$ | +++ | ++ |
| $L^2$ | ++++ | ++++ |
| $L^1Co$ | ++ | +++ |
| $L^2Co$ | +++ | ++++ |

**Table 11.** Ground state properties of the ligand and its metal complexes using B3LYP/6-31+G (d,p) for the ligand and B3LYP/LANL2DZ for its complexes.

| Com | HOMO eV | LUMO eV | ΔE eV | ω | Ƞ | μ | S | X | A | I |
|---|---|---|---|---|---|---|---|---|---|---|
| $L^1$ | -0.06911 | 0.02666 | 0.0957 | 0.0047 | 0.0478 | -0.0212 | 20.8833 | 0.0212 | -0.027 | 0.06911 |
| $L^2$ | -0.1414 | 0.1014 | 0.2429 | 0.00164 | 0.1214 | -0.02 | 8.2372 | 0.02 | -0.101 | 0.1414 |
| $L^1Co$ | -0.1164 | 0.09415 | 0.21061 | 0.000587 | 0.1052 | -0.01113 | 9.4989 | 0.01113 | -0.094 | 0.21055 |
| $L^2Co$ | -0.1213 | 0.0288 | 0.15020 | 0.01425 | 0.0750 | -0.04625 | 13.3244 | 0.04625 | -0.029 | 0.1213 |