

## Synthesis and Characterization of New Complexes of 2-(6-Methoxybenzo[d]thiazol-2-ylamino)-2-phenyl acetonitrile Ligand with Manganese (II), Cobalt (II), Nickel (II), Copper (II), Zinc (II) Cadmium (II) and Mercury (II) Divalent Transition Metal Ions

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**Abstract:** The synthesis and characterization of manganese (II), cobalt (II), nickel (II), copper (II), zinc (II), cadmium (II) and mercury (II) bidentate 2-(6-methoxybenzo[d]thiazol-2-ylamino)-2-phenyl acetonitrile ligand which was prepared from Benz aldehyde and 6-methoxybenzo[d]thiazol-2-amine in the presence of KCN and acidic medium. The complexes were synthesized by treating an ethanolic solution of the ligand with appropriate amount of metal salts [1:2] [M: L] ratio. The complexes were characterized by using metal and elemental chemical analysis, molar conductance, magnetic susceptibility measurements, FTIR, electronic spectral and mole ratio method. According to the obtained data the probable coordination geometries of manganese (II), cobalt (II), nickel (II), copper (II) zinc (II), cadmium (II) and mercury (II) in these complexes are octahedral. All complexes were found to be non-electrolyte in absolute ethanol, and the complexes were formulated as  $[ML_2Cl_2] \cdot XH_2O$ .

**Keywords:** 2-(6-methoxybenzo[d]thiazol-2-ylamino)-2-phenyl acetonitrile, N2-donor, transition metals.

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### I. Introduction

Strecker reaction [1], is the oldest known synthesis of  $\alpha$ -amino nitriles since 1850 when Adolph strecker interacted an aldehyde, an amine and hydrogen cyanide,  $\alpha$ -amino nitriles synthesis represents one of the simplest and most economical methods for the preparation of  $\alpha$ -amino acids [2,3] for both laboratory and industrial scales [4]. The synthesis of Nitrogen-containing heterocyclic is important such as thienopyrimidine derivatives which have antibacterial and antifungal activities higher than the corresponding antibacterial ampicillin and antifungal nystatin [5-7]. The addition of cyanide to imines provides a direct route for the synthesis of  $\alpha$ -amino nitriles. Some of the  $\alpha$ -amino nitrile derivatives like 1-amino-4-phenyl naphthalene-2-carbonitrile have been postulated to have high fungistatic activity even stronger than the activity of the commercial fungicide – Kaptan [8].  $\alpha$ -amino nitriles are useful intermediates for the synthesis of amino acids [9,10] and nitrogen-containing heterocyclic such as thienopyrimidine derivatives which have antibacterial and antifungal activities higher than the corresponding antibacterial ampicillin and antifungal nystatin [11-13]. Moreover, among many other applications, they are readily hydrolyzed to diamines, which are of interest as ligands for Platinum (II) complexes with potential antitumor properties [14, 15]. Several modifications of the Strecker reaction have been reported using a variety of cyanating agent such as  $\alpha$ -trimethylsiloxynitriles and under various reaction conditions [16, 17]. Complexes with dinitrogen N<sub>2</sub> ligand are of interest not only in theoretically but also from a practical point of view. They have found application as antitumor activity [18], antibacterial activity [19] and antiviral activity in agriculture field [20].  $\alpha$ -amino nitriles have often been used as chelating ligands through two nitrogen atoms in the field of amino coordination chemistry. This is the first study to prepare and characterize the complexes of  $\alpha$ -amino nitrile compounds with transition metal ions to reveal a new coordination field of these compounds as ligands with metal ions.

### II. Experimental

All the chemicals and solvents used for the synthesis were of reagent grade and were obtained commercially from British Drug House (BDH) with the exception of  $MnCl_2 \cdot 4H_2O$ ,  $CoCl_2 \cdot 6H_2O$ ,  $NiCl_2 \cdot 6H_2O$ ,  $CuCl_2 \cdot 2H_2O$ ,  $ZnCl_2$ ,  $CdCl_2 \cdot 2H_2O$  and  $HgCl_2$  salts were obtained from Fluka Company. The prepared ligand 2-(6-methoxybenzo[d]thiazol-2-ylamino)-2-phenyl acetonitrile was synthesized and characterized according to published work. The infrared spectra of the ligand and the complexes were recorded on a Shimadzu (8300) FTIR Spectrophotometer, as CsI disk. Electronic absorption spectra were recorded in the range ( 190 –1100 ) nm on a Shimadzu (160 A) Spectrometer in freshly prepared ( $10^{-3}M$ ) in absolute ethanol at room temperature using quartz cell (1.00) cm. Atomic Absorption technique was used to determine the metal contents of the complexes using a Shimadzu (A.A 680G) Atomic Absorption Spectrophotometer. Molar conductivity was used

to measure the conductivity of the complexes at room temperature in freshly prepared ( $10^{-3}\text{M}$ ) in absolute ethanol using (PW9526) Digital conductivity meter. Elemental analysis for carbon, hydrogen nitrogen and sulfur elements were carried out at the Euro vector-EA3000A C. H. N. Analyzer, Italy. Gallen Kamp apparatus was used to determine the melting points of the ligand and the prepared complexes. Also the chlorine content was determined gravimetrically [21].

### **2.1 Preparation method of 2-(6-methoxybenzo[d]thiazol-2-ylamino)-2-phenyl acetonitrile:**

A general method [22-24] can be adopted for [L] preparation which can be described as follows: The benzaldehyde (1 mmol) was added to (20 ml) glacial acetic acid, p-toluene sulphonic acid was added in very small portion as catalyst, followed by addition of (1 mmol) 6-methoxybenzo[d]thiazol-2-amine. The pH was adjusted to about 4 by addition of concentrated sulfuric acid drop wise to obtain Schiff base which stirred for 30 min. Potassium cyanide (2 mmol) was added to the mixture and kept under stirring for 4 days. The reaction mixture was poured into ice and then made slightly alkaline with ammonium hydroxide solution. The solid precipitate which formed was filtered, washed with water and air dried. The presence of nitrile group in the prepared  $\alpha$ -amino nitrile was indicated by treating few amount of the sample with 10% sodium hydroxide solution, the liberation of ammonia after hydrolysis of nitrile group, which was detected by wet red litmus paper, indicating the presence of nitrile group. Purity of the obtained compound was checked by TLC, using chloroform and ethyl acetate (1:1) as eluent. The product color was dark brown and the yield percentage was (89.12 %) and the melting point was (148-150  $^{\circ}\text{C}$ ). The reaction was clarified below:

### **2.2 Preparation method of metal complexes:**

The complexes  $[\text{ML}_2\text{Cl}_2] \cdot n\text{H}_2\text{O}$  have been prepared by the reaction of (0.590 gm.) (2mmole) of (L) with (1mmol) of metal chloride (0.198 gm., 0.238 gm., 0.238 gm., 0.171 gm., 0.136 gm., 0.220 gm. and 0.272 gm. for  $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ ,  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ ,  $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ ,  $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ ,  $\text{ZnCl}_2$ ,  $\text{CdCl}_2 \cdot 2\text{H}_2\text{O}$  and  $\text{HgCl}_2$ , respectively) dissolved in (20 ml) absolute ethanol and refluxed with stirring under anhydrous conditions using  $\text{Na}_2\text{SO}_4$  (anhydrous) for 24 hours. The obtained complexes were collected after evaporation of ethanol and triturated with petroleum ether (60-80  $^{\circ}\text{C}$ ) then filtered and the products were left in the desiccators to be dried under  $\text{P}_2\text{O}_5$ . The general reaction was clarified below:

### III. Results and Discussion

All the compounds reported in this work are presented in table (1) which illustrated physical properties, along with their molar conductivity at room temperature. Metal and elemental analysis of all compounds is represented in table (1) as well. The ligand 2-(6-methoxybenzo[d]thiazol-2-ylamino)-2-phenyl acetonitrile was prepared as reported in literature [17]. It was characterized by elemental analysis and infrared spectral data. The complexes have been prepared under anhydrous conditions to avoid any hydrolysis of nitrile group to amide due to the presence of water molecules and metal ion [25]. In addition to that when organic molecules are coordinated to metal cations in organo-metallic or coordination compounds, they become susceptible to nucleophilic attack like water molecules which cause hydrolysis of nitrile into amide [26]. These complexes were stable in the solid state and were characterized by the usual methods; FTIR, UV-Visible spectroscopy, metal and elemental analysis, molar conductivity, mole ratio, chloride content and magnetic susceptibility. On the basis of the characterization methods it's suggested that all complexes probably have octahedral structure with coordination number 6 that includes two atoms of coordinated chlorides. The conductivity values for the complexes of ( $10^{-3}$ M) in absolute ethanol were recorded in the range (8-16) indicating that the non-electrolytic nature of the complexes [27]. Mole ratio method was used to determine the ratio of metal ion to the ligand for the complexes at  $\lambda_{\max}$  [ $\lambda_{\max}=495$  nm for  $[\text{CoL}_2\text{Cl}_2] \cdot 5\text{H}_2\text{O}$  and  $\lambda_{\max}=486$  nm for  $[\text{CuL}_2\text{Cl}_2] \cdot 2\text{H}_2\text{O}$  in alcoholic solutions.

#### 3.1 Infrared spectroscopy:

The significant infrared bands of the ligand and its metal complexes and their assignments are given in table (4). The infrared spectral data of [L], Fig. (3) And all complexes in table (3) showed some characteristic bands related to  $\alpha$ -amino nitriles; like  $2120\text{-}2196\text{ cm}^{-1}$  which could be attributed to  $\text{C}\equiv\text{N}$  group [29]. A shift of the range  $65\text{-}117\text{ cm}^{-1}$  was observed for  $\text{C}\equiv\text{N}$  stretching vibration on coordination due to the decrease of bond order as result of metal nitrogen bond formation. The next characteristic band near  $1641\text{ cm}^{-1}$  which could be attributed to  $\delta(\text{N-H})$  group. A red shift of the range  $11\text{-}32\text{ cm}^{-1}$  was observed in N-H bending frequency on complexes indicating the coordination on nitrogen to metal ion. On the other hand the spectrum of the complexes showed new bands around  $599\text{-}617\text{ cm}^{-1}$  due to  $\nu_{\text{M-N}}$  [30, 31]. The  $\nu_{\text{M-Cl}}$ , however could not be ascertained due to non-availability of far infrared data. The presence of these bands supported the formation of complexes under investigations. The presence of lattice water molecule in all complexes table (4) was supported by the broad band in  $3500\text{-}3150\text{ cm}^{-1}$  region of infrared spectrum [30] and by its metal and elemental analysis data in table (1).

#### 3.2 Molar Conductance Data:

The molar conductance of the solid complexes ( $\Omega^{-1} \cdot \text{cm}^2 \cdot \text{mole}^{-1}$ ) was calculated. Absolute ethanol solubility of the above complexes made calculations of the molar conductivity ( $\lambda_{\max}$ )  $\text{dm}^{-3}$  of  $10^{-3}$  mol  $\text{dm}^{-3}$  solution at  $25^\circ\text{C}$  possible. The data in Table (1) showed that the molar conductance values of the manganese (II), cobalt (II), nickel (II), copper (II), zinc (II) cadmium (II) and mercury (II) complexes were relatively low, indicating the non-electrolytic nature of these complexes.

#### 3.3 Magnetic studies:

The Zn (II), Cd (II) and Hg (II) complexes are diamagnetic as expected for the  $d^{10}$  configuration [32]. Cu (II) complex shows a normal magnetic moment of 1.84 B.M. observed for the  $d^9$  system with an unpaired electron [33]. The Ni (II) complex with a magnetic moment of 3.55 B.M. reveals a spin free octahedral configuration [33]. The magnetic moment of 4.60 B.M. for the Co (II) complex suggest a high spin octahedral configuration [32, 33]. The Mn (II) complex has a magnetic moment of 5.81 B.M. as expected for high spin octahedral geometry [34].

#### 3.4 Ultra violet – visible spectroscopy:

The electronic absorption spectra are often very helpful in the evaluation of results furnished by other methods of structural investigation. The electronic spectral measurements were used to assign the stereo chemistries of the metal ions in the complexes based on the positions and number of (d-d) transition peaks. The electronic absorption spectra of the ligand and its complexes were recorded at room temperature using absolute ethanol as the solvent. The ligand showed two absorption bands in the region  $45455\text{ cm}^{-1}$  and  $37879\text{ cm}^{-1}$  corresponding to  $(\pi \rightarrow \pi^*)$  and  $(n \rightarrow \pi^*)$  transitions respectively. On complexation, these bands are shifted to higher wavelengths, suggesting coordination of the uncharged dinitrogen  $\text{N}_2$  of the ligand to the metal ion. The Mn (II), Zn (II) Cd (II) and Hg (II) complexes do not show any d-d transitions but display charge transfer bands at  $21739$ ,  $27320$ ,  $26025$  and  $29850\text{ cm}^{-1}$ , respectively. The electronic spectrum of six coordinated Cu (II) complex displays three bands at  $15120$ ,  $20565$  and  $24150\text{ cm}^{-1}$  corresponding to the following transitions:  ${}^2\text{B}_{1g} \rightarrow {}^2\text{A}_{1g}$  ( $d_{x^2-y^2} \rightarrow d_z^2$ ), ( $\nu_1$ ),  ${}^2\text{B}_{1g} \rightarrow {}^2\text{B}_{2g}$  ( $d_{x^2-y^2} \rightarrow d_{yz}$ ), ( $\nu_2$ )  ${}^2\text{B}_{1g} \rightarrow {}^2\text{E}_g$  ( $d_{x^2-y^2} \rightarrow d_{zy}d_{yz}$ ), ( $\nu_3$ ), respectively. Therefore, the Cu (II) complex may be considered to possess a tetragonal geometry around the copper ion [35,

36]. Though three transitions are expected in this case, they are very close in energy and often appear in the form of one broad band envelope [36]. The spectrum also exhibits a band at 31154 cm<sup>-1</sup>, which is assigned to a charge transfer band. The electronic spectrum of cobalt (II) complex showed two main bands are at 20200 cm<sup>-1</sup> and 16520 cm<sup>-1</sup>. These two d-d bands are attributed to the <sup>4</sup>T<sub>1g</sub>(F) → <sup>4</sup>T<sub>1g</sub>(P) (ν<sub>3</sub>) and <sup>4</sup>T<sub>1g</sub>(F) → <sup>4</sup>A<sub>2g</sub>(F) (ν<sub>2</sub>) transitions, respectively, in an octahedral geometry around the Co (II) ion [31]. The (ν<sub>1</sub>) <sup>4</sup>T<sub>1g</sub>(F) → <sup>4</sup>T<sub>2g</sub>(F) transition is expected to appear at large wavelength, therefore it could not be observed, it will be calculated theoretically through the Tanabe-Sugano diagram [38]. The Co (II) complex displays a charge transfer band at 30239 cm<sup>-1</sup> [39]. The electronic spectrum of Ni (II) complex exhibits three bands in the region 25365, 17500 and 10780 cm<sup>-1</sup> which are assigned to the <sup>3</sup>A<sub>2g</sub>(F) → <sup>3</sup>T<sub>1g</sub>(P) (ν<sub>3</sub>), <sup>3</sup>A<sub>2g</sub>(F) → <sup>3</sup>T<sub>1g</sub>(F) (ν<sub>2</sub>) and <sup>3</sup>A<sub>2g</sub>(F) → <sup>3</sup>T<sub>2g</sub>(F) (ν<sub>1</sub>) transitions, respectively, indicating an octahedral geometry around the Ni (II) ion [26]. The spectrum of Ni (II) complex also exhibits a charge transfer band at 28950 cm<sup>-1</sup>. The octahedral geometry of Co (II) and Ni (II) complexes is further supported by the value of the ν<sub>2</sub> / ν<sub>1</sub> ratio, which are 1.85 and 1.62, respectively [32]. Various ligand field parameters table (5), such as the Racah inter-electronic repulsion parameter (B'), ligand filed splitting energy (10Dq), covalency factor (β) and ligand field stabilization energy (LFSE) have been calculated for Co (II) and Ni (II) complexes [32,40].

In case of the Co (II) complex, the Racah inter-electronic repulsion parameter (B') is given by the following equation [32]:

$$B' = 1/510 \{ 7 (v_3 - 2 v_2) + 3 [81 v_3^2 - 16 v_2 (v_2 - v_3)]^{1/2} \}$$

In case of the Ni (II) complex, (B') is given by the following equation [32]:

$$B' = v_2 + v_3 - 3 v_1/15$$

The ligand field splitting energy (10Dq) is calculated as follows:

For the Co (II) complex,

$$10Dq = 1/3 (v_2 - v_3) + 15B'$$

For the Ni (II) complex, 10Dq = v<sub>1</sub>

The covalence factor (β) is obtained in the following manner:

$$\beta = B'/B \text{ (B is the free ion value)}$$

The ligand field stabilization energy (LFSE) is expressed by the equation:

$$LFSE = 12Dq$$

The (B') values for the complexes are lower than that of the free ion, which is an indication of orbital overlap and delocalization of the d-orbitals. The obtained (β) values are less than unity, suggesting the metal-ligand bonds have a considerable amount of covalent character. The (β) value for the Ni (II) complex is less than that for the Co (II) complex, indicating the greater covalent nature of the former.

**Table (1)** Analytical data and Physical properties of [L] and its metal complexes with their conductivity values

| Formula<br>M.wt. (gm./mole)                                    | Elemental Analysis Calculated<br>(Found) |                |                  |                  |                  |                | Color           | M.P. °C<br>(Dec.) | Yield<br>% | Ω <sup>-1</sup> cm <sup>2</sup><br>mol <sup>-1</sup> | Magnetic<br>moment<br>BM |
|--|--|----------------|------------------|------------------|------------------|----------------|-----------------|-------------------|------------|--|--------------------------|
|  | C%                                       | H%             | N%               | S%               | M%               | Cl%            |                 |                   |            |  |                          |
| L<br>295   | 65.08<br>(64.87)                         | 4.41<br>(4.35) | 14.24<br>(14.13) | 10.85<br>(10.67) | -----            | -----          | Dark<br>brown   | 148-<br>150       | 87.65      | -----  | -----                    |
| [MnL <sub>2</sub> Cl <sub>2</sub> ]3H <sub>2</sub> O<br>769.94 | 49.87<br>(49.33)                         | 4.16<br>(3.98) | 10.91<br>(10.73) | 8.31<br>(8.20)   | 7.14<br>(7.05)   | 9.22<br>(9.12) | brown           | 182-<br>184       | 78.32      | 11.52  | 5.81                     |
| [CoL <sub>2</sub> Cl <sub>2</sub> ]5H <sub>2</sub> O<br>809.93 | 47.41<br>(47.12)                         | 4.44<br>(4.40) | 10.37<br>(10.26) | 7.90<br>(7.82)   | 7.28<br>(7.17)   | 8.77<br>(8.65) | Dark<br>green   | 168-<br>170       | 71.89      | 16.12  | 4.60                     |
| [NiL <sub>2</sub> Cl <sub>2</sub> ]2H <sub>2</sub> O<br>755.71 | 50.81<br>(50.69)                         | 3.97<br>(3.91) | 11.16<br>(11.09) | 8.47<br>(8.33)   | 7.77<br>(7.65)   | 9.40<br>(9.29) | Green<br>yellow | 205-<br>208       | 82.68      | 10.05  | 3.55                     |
| [CuL <sub>2</sub> Cl <sub>2</sub> ]4H <sub>2</sub> O<br>796.55 | 48.21<br>(47.98)                         | 4.27<br>(4.22) | 10.55<br>(10.46) | 8.03<br>(7.98)   | 7.98<br>(7.91)   | 8.91<br>(8.85) | Light<br>brown  | 167-<br>170       | 80.33      | 14.33  | 1.84                     |
| [ZnL <sub>2</sub> Cl <sub>2</sub> ]H <sub>2</sub> O<br>744.38  | 51.59<br>(51.46)                         | 3.76<br>(3.72) | 11.28<br>(11.21) | 8.60<br>(8.54)   | 8.78<br>(8.69)   | 9.54<br>(9.43) | Pale<br>yellow  | 193-<br>195       | 85.25      | 9.87   | Dia                      |
| [CdL <sub>2</sub> Cl <sub>2</sub> ]2H <sub>2</sub> O<br>809.41 | 47.44<br>(47.29)                         | 3.71<br>(3.66) | 10.38<br>(10.68) | 7.91<br>(7.82)   | 13.89<br>(13.80) | 8.77<br>(8.68) | Light<br>green  | 173-<br>175       | 81.78      | 8.24   | Dia                      |
| [HgL <sub>2</sub> Cl <sub>2</sub> ]H <sub>2</sub> O<br>879.60  | 43.66<br>-----                           | 3.18<br>-----  | 9.55<br>-----    | 7.28<br>-----    | 22.81<br>-----   | 7.91<br>-----  | Dark<br>brown   | 225-<br>228       | 73.58      | 10.55  | Dia                      |

**Table (4)** The characteristic bands of FTIR spectra of the ligand and its metal complexes in (cm<sup>-1</sup>)

| Compound   | νO-H cm <sup>-1</sup><br>Lattice water | νN-H cm <sup>-1</sup> | νC-H cm <sup>-1</sup><br>Aromatic | νO-CH <sub>3</sub> cm <sup>-1</sup> | νC≡N<br>Nitrile | δN-H<br>cm <sup>-1</sup> | νM-N<br>cm <sup>-1</sup> |
|--|--|-----------------------|-----------------------------------|-------------------------------------|-----------------|--------------------------|--------------------------|
| L  | -----                                  | 3292                  | 3093                              | 1178                                | 2120            | 1641                     | -----                    |
| [MnL <sub>2</sub> Cl <sub>2</sub> ]5H <sub>2</sub> O | 3385                                   | 3136                  | 3005                              | 1180                                | 2160            | 1620                     | 617                      |

|  |      |      |      |      |      |      |     |
|--|------|------|------|------|------|------|-----|
| [CoL <sub>2</sub> Cl <sub>2</sub> ]5H <sub>2</sub> O | 3425 | 3130 | 3030 | 1171 | 2168 | 1611 | 605 |
| [NiL <sub>2</sub> Cl <sub>2</sub> ]H <sub>2</sub> O  | 3400 | 3117 | 3017 | 1178 | 2172 | 1618 | 599 |
| [CuL <sub>2</sub> Cl <sub>2</sub> ]2H <sub>2</sub> O | 3357 | 3118 | 3018 | 1176 | 2145 | 1622 | 608 |
| [ZnL <sub>2</sub> Cl <sub>2</sub> ]H <sub>2</sub> O  | 3422 | 3132 | 3032 | 1175 | 2196 | 1630 | 611 |
| [CdL <sub>2</sub> Cl <sub>2</sub> ]2H <sub>2</sub> O | 3375 | 3111 | 3011 | 1180 | 2136 | 1615 | 608 |
| [HgL <sub>2</sub> Cl <sub>2</sub> ]H <sub>2</sub> O  | 3410 | 3122 | 3023 | 1172 | 2148 | 1609 | 612 |

**Table (5)** Electronic spectra in absolute ethanol for the (L) and its metal complexes

| Compound  | $\lambda$ nm                             | $\nu$ cm <sup>-1</sup>                              | Transition   | B cm <sup>-1</sup> | Dq/ B | $\beta$ | 15B cm <sup>-1</sup> | Suggested structure |
|---|--|---|--|--------------------|-------|---------|----------------------|---------------------|
| L   | 220<br>264                               | 45455<br>37879                                      | $\pi \rightarrow \pi^*$<br>$n \rightarrow \pi^*$   | -----              | ----- | -----   | -----                | -----               |
| [MnL <sub>2</sub> Cl <sub>2</sub> ] 5H <sub>2</sub> O | 228<br>274<br>460                        | 43860<br>36496<br>21739                             | Ligand Field<br>Ligand Field<br>C.T  | -----              | ----- | -----   | -----                | O.h                 |
| [CoL <sub>2</sub> Cl <sub>2</sub> ] 5H <sub>2</sub> O | 255<br>288<br>410<br>-----<br>605<br>495 | 39216<br>34722<br>24390<br>8930*<br>16520<br>20200  | Ligand Field<br>Ligand Field<br>C.T<br>${}^4T_{1g}(F) \rightarrow {}^4T_{2g}(F)$<br>${}^4T_{1g}(F) \rightarrow {}^4A_{2g}(F)$<br>${}^4T_{1g}(F) \rightarrow {}^4T_{1g}(P)$     | 662                | 0.944 | 0.682   | 9930                 | O.h                 |
| [NiL <sub>2</sub> Cl <sub>2</sub> ] H <sub>2</sub> O  | 250<br>277<br>345<br>928<br>571<br>394   | 40000<br>36101<br>28950<br>10780*<br>17500<br>25365 | Ligand Field<br>Ligand Field<br>C.T<br>${}^3A_{2g}(F) \rightarrow {}^3T_{2g}(F)$<br>${}^3A_{2g}(F) \rightarrow {}^3T_{1g}(F)$<br>${}^3A_{2g}(F) \rightarrow {}^3T_{1g}(P)$     | 702                | 1.536 | 0.682   | 10530                | O.h                 |
| [CuL <sub>2</sub> Cl <sub>2</sub> ] 2H <sub>2</sub> O | 247<br>272<br>391<br>661<br>486<br>414   | 40486<br>36765<br>25533<br>15120<br>20565<br>24150  | Ligand Field<br>Ligand Field<br>C.T<br>${}^2B_{1g} \square \square \square \square \square \square$<br>${}^2B_{1g} \rightarrow {}^2B_{2g}$<br>${}^2B_{1g} \rightarrow {}^2E_g$ | -----              | ----- | -----   | -----                | O.h                 |
| [ZnL <sub>2</sub> Cl <sub>2</sub> ] H <sub>2</sub> O  | 245<br>281<br>366                        | 40816<br>35587<br>27320                             | Ligand Field<br>Ligand Field<br>C.T  | -----              | ----- | -----   | -----                | O.h                 |
| [CdL <sub>2</sub> Cl <sub>2</sub> ] 2H <sub>2</sub> O | 238<br>270<br>380                        | 42017<br>37037<br>26315                             | Ligand Field<br>Ligand Field<br>C.T  | -----              | ----- | -----   | -----                | O.h                 |
| [HgL <sub>2</sub> Cl <sub>2</sub> ] H <sub>2</sub> O  | 241<br>275<br>335                        | 41494<br>36364<br>29850                             | Ligand Field<br>Ligand Field<br>C.T  | -----              | ----- | -----   | -----                | O.h                 |

\*Calculated value

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