The Investigation of Spectrum H-NMR Ligand, spectrum IR and formed Ligand complexes

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Abstract: There are many compounds in Inorganic chemistry that in this, the central atom, interact dative bond at least with a surrounding atoms (ligands). Receptors in the central atoms electron pairs, such compounds are known complex or co-ordination compounds. Central atom in these compounds is usually an electron-hole that can take unpaired electrons in a covalent ligand and can form Covalent– co-ordination (dot). In this study for confirmation the complex formation between the ligand and the tested metals, NMR and IR studies have also been performed.
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Key words: Spectrum H-NMR Ligand, Spectrum IR Ligand, Formed Ligand, Complex

1. Introduction

Solution with concentration 10th $^{-3}$ molar of ligand and cation were prepared in acetonitrile. The volumes required for the preparation of metal-ligand molar ratio 1:1 solution of both bubbles were removed by successive pat-The hour glass spills, after the mixture was placed in a location away from sunlight and other chemicals to evaporate the solvent. Then precipitated in acetonitrile solvent measuring spectrum NMR was used.

Figure of the spectrum H-NMR Ligand alone and the complexes formed by the ligands and transition metals can be seen in the below figures.

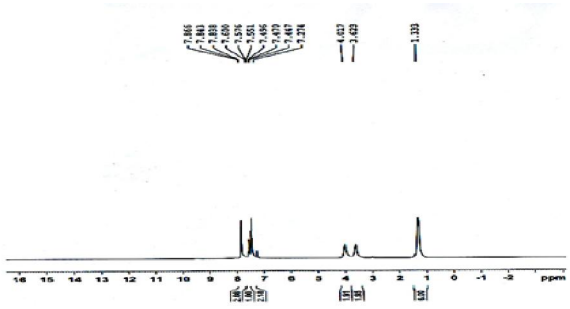

Figure 1: Spectrum H-NMR For the ligand

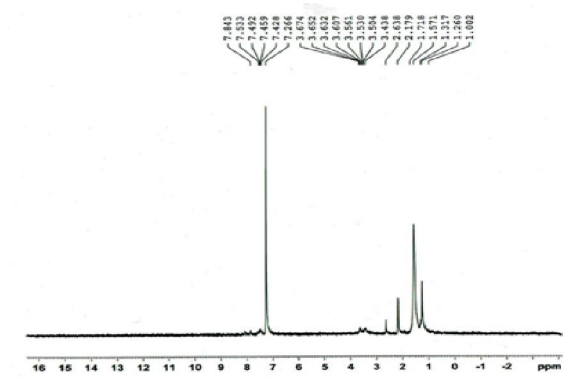

Figure 2: Spectrum H-NMR Results for L+Co $^{+2}$

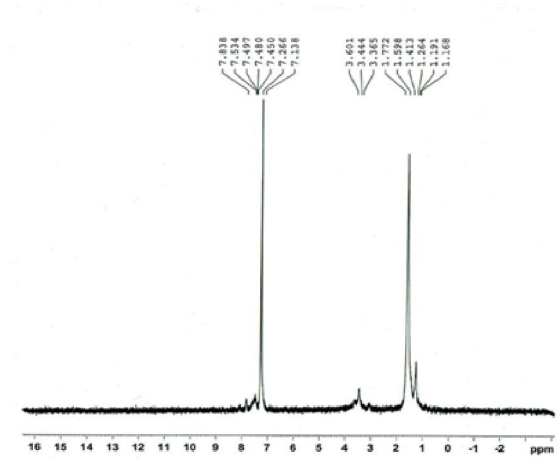

Figure 3: Spectrum H-NMR Results for L + Ni $^{+2}$

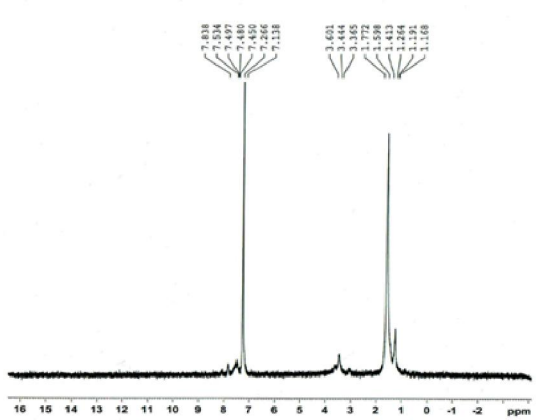

Figure 4: Spectrum H-NMR Results for L + Zn^{+2}

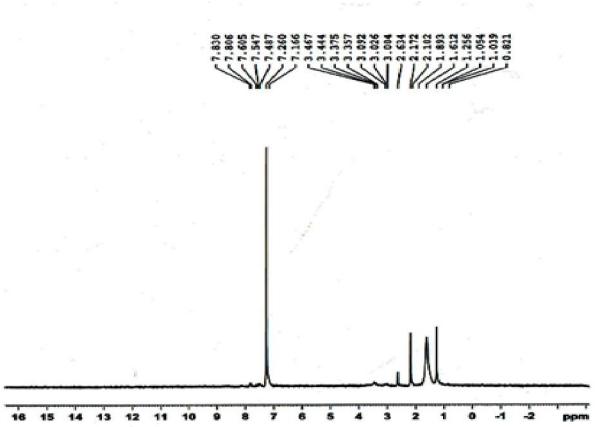

Figure 5: Spectrum H-NMR Results for L + Cu^{+2}

2. Data and Materials

Table 1: Data Spectrum H-NMR Ligand and its complexes Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}

CH_3 δ	CH_2 δ	PH δ	Speciees	[M]/[L]
1.333	3.623	7.447 - 7.838	L	0
1.612	3.357	7.260	CuL	1
1.639	3.398	7.266	ZnL	1
1.598	3.444	7.266	NiL	1
1.571	3.561	7.266	CoL	1

Chemical shifts are according to ppm.

As shown in Table. 1, this is observed that chemical shifts quantities for ligand changed after the addition of metal and this case clearly indicates that this complex formation is created or changed. Due to the Plotted spectrum H-NMR for the ligand, we see that hydrogen spectrum attached to the nitrogen spectra due to condensation of four polar flattening phenomenons cannot be identified. Nitrogen nuclear magnetic spin is I = 1 and can accept or take Spin states of +1, 0 and -1. Elements that have I ≤ ½, the core of their distribution is almost spherical. Elements that have I > 1/2 Have an elliptical load distribution around its core and thus have four polar momentums. Cores that are four magnetic poles, the magnetic field interacts with the NMR and magnetic and electrical disturbances or valence electrons are sensitive to their environment. Nitrogen has four polar average torque and seems excited states of spin speed, transfer and lifetime of the other molecule is slight. Solvent and temperature environment may also affect the speed. There are three possibilities for the nitrogen atom:

1 - Torque four small polar nitrogen: in this case the coupling occurs. A hydrogen attached (in NH) due to three possible spin of nitrogen (+1, 0 or -1) is split into three absorption peaks.

2 - Torque four major polar nitrogen: in this case there is not any coupling. Because of the rapid transitions between the three states of nitrogen spin, a proton attached (eg NH A) A spin state average (zero) for nitrogen sees. There is one single directory for nitrogen.

3 - Torque four polar medium N: This broad shrinkage of the middle peak is rather wide gap that four polar disruptions say. Attached proton is unsure of what it sees.

Spectrum H-NMR Ligand, CH_2 of the chemical shift differences were due to non-resonant electron pair bond between nitrogen and sulfur. For resonance to occur, the molecules form a page to itself and creates interference in the free spins, free spins if it is slow enough to be slower than the time required to a transfer of NMR Then the device NMR Methyl groups, which will have a different one for the team C = S and the other on the other side C = S. So they have different magnetic environments and have different chemical shift.

The spectrum of solutions for NMR After removal of the solvent was used for the studies IR was used. Spectrum Charts IR are reported in this section.

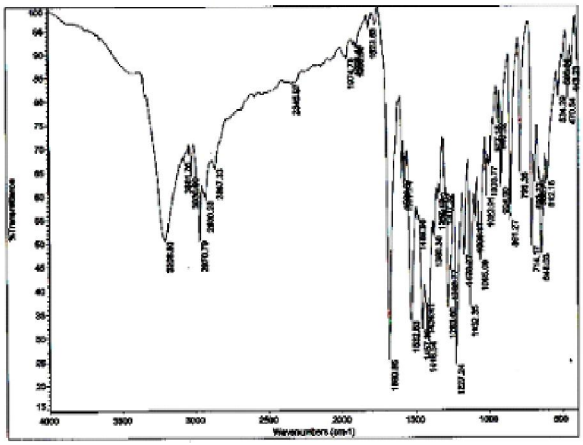

Figure 6: Spectrum IR Ligand L

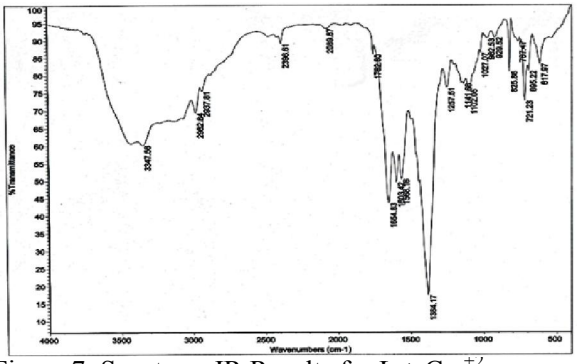

Figure 7: Spectrum IR Results for L + Co^{+2}

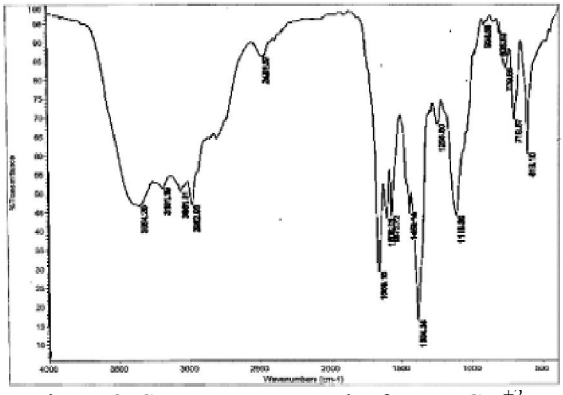

Figure 8: Spectrum IR Results for L + Cu^{+2}

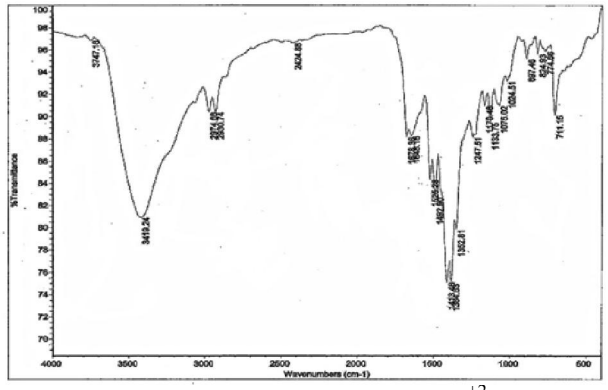

Figure 9: Spectrum IR Results for L + Zn^{+2}

3. Result and conclusion

Due to the structure of the ligand, the ligand can act as a ligand to trifid. To coordinate can get through the atoms of oxygen, nitrogen and sulfur to be done. Changes observed in the spectrum IR Is given in Table2. As you can see changes in the spectrum IR The bands C = O And C = S And NH co-ordination indicated by the three pairs of electrons from the nitrogen atom to atom, but co-ordination better because there is more of a wavelength

Table 2: Details of the variety IR Ligand L_1 And complexes formed

CN	NH	C = C	C = O	C = S	υ (cm^{-1})
1,532	3,208	1450-1600	1,680	1,344	L
1,573	3,354	1450-1600	1,663	1,384	L + Cu^{+2}
1,525	3,419	1450-1600	1,678	1,384	L + Zn^{+2}
1,568	3,347	1450-1600	1,654	1,384	L + Co^{+2}

After measuring of absorbance spectra and record the obtained spectrums, data are entered on software KIN FIT Text, and complex formation was proved.

Table 3: The values of the constants obtained from the fitting procedure for the complex L

Zn^{2+}	Ni^{2+}	Co^{2+}	Cu^{2+}	Temp = 25 °C
2.88 ± 0 0.07	3.02 ± 0 0.04	3.54 ± 0 0.03	4.18 ± 0 0.7	$\log K_f$

The fitting curves of complex formation are given below:

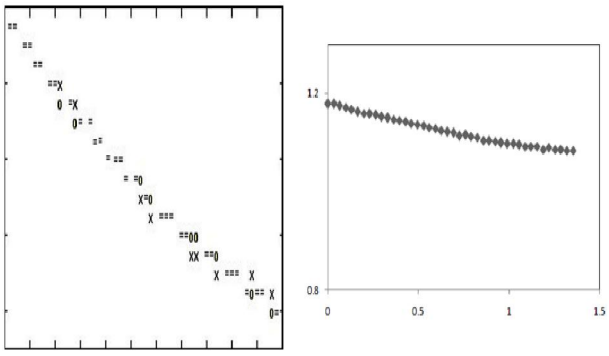

Figure 10: A Molar ratio curve for the system Co^{2+} + L Wavelength nm 240B, Computer curve fitting based on the molar absorption $[Co^{+2}] / [L]$

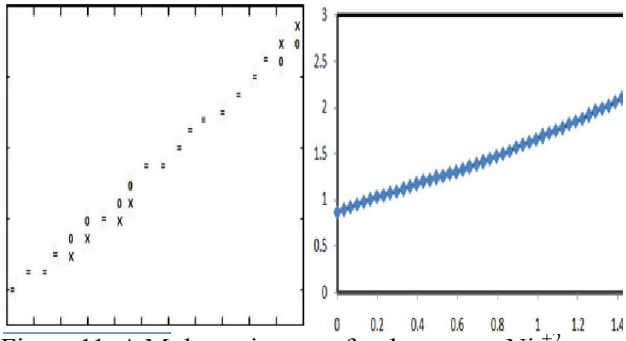

Figure 11: A Molar ratio curve for the system Ni^{+2} + L Wavelength nm 217B, Computer curve fitting based on the molar absorption $[Ni^{+2}] / [L]$

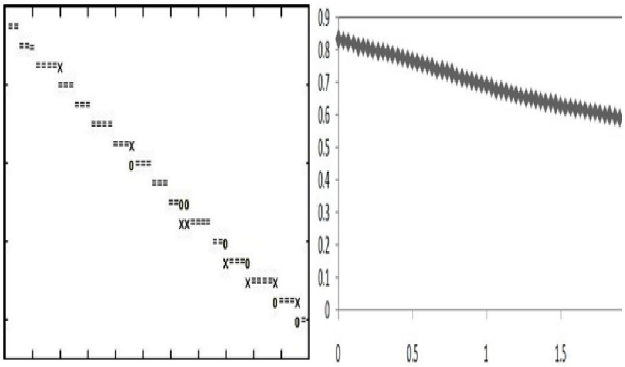

Figure 12: A Molar ratio curve for the system L + Zn^{+2} Wavelength nm 240B, Computer curve fitting based on the molar absorption $[Zn^{+2}] / [L]$

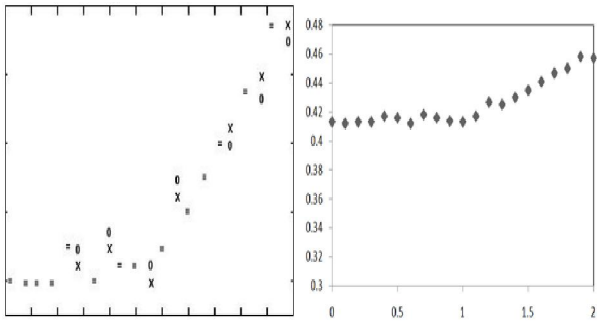

Figure 13: A Molar ratio curve for the system L + Cu^{+2} Wavelength nm 240B, Computer curve fitting based on the molar absorption $[Cu^{+2}] / [L]$

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