

## SYNTHESIS AND CHARACTERIZATION OF SULFUR DONOR LIGAND (XANTHATE) COMPLEXE WITH MANGANESE (II), IRON (II), COBALT (II), NIKEL (II), COPPER (II), AND ZINC (II) AND THIER ADDUCT WITH NITROGEN BASE LIGANDE

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### Abstract

New complexes and adducts of xanthate of the general formula  $[M(\text{cyclopentyl xant.})_2]$  and  $[M(\text{cyclopentyl xant.})_2.nL]$  Where  $M = \text{Mn(II), Fe(II), Co(II), Ni(II), Cu(II)}$  and  $\text{Zn(II)}$ , and  $(\text{cyclopentyl xant.})_2 = [\text{Cyclopentyl xanthate ligand}]$ ,  $n=2$   $L = \text{Pyridine, 3-acetyl pyridine \& Quinoline}$   $n=1$ ,  $L = \text{ethylenediamine, (1,10)-phenanthroline}$ , the prepared complexes has been evaluated based on their magnetic, electrical, and physical characteristics. And spectral methods  $^1\text{H-NMR}$  of  $(\text{cyclopentyl xant.})_2$  ligand, Based on the effective magnetic moment and electronic spectra, the structures of the kind  $[M(\text{cyclopentyl xant.})_2]$  indicate a tetrahedral geometry whereas structures of the kind  $[M(\text{cyclopentyl xant.})_2.nL]$  has an octahedral geometry. The density functional theory (DFT) calculations of ligands and their complexes were performed by the DFT/B3LYP/6-311++G(d,p) method to obtain the optimized molecular geometry, the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), and electronic properties, thermodynamic parameters are done for four coordinates.

**Keyword:** Xanthate complexes, Complexes of [Manganese (II), Iron (II), Cobalt (II), Nickel (II), Copper (II) & Zinc (II)], Four-coordinate, sex-coordinate complexes, characterizations DFT of four coordinates.

### 1. INTRODUCTION

Xanthates" derives from xanthic acid, and organic molecules with a  $-\text{OCS}_2$  functional group. [1] Sulfur and oxygen-containing ligands called xanthates produce an array of different and plentiful coordination complexes with metals from the transition and main group. [2]. Due to the important roles that several xanthate reactions play, the chemistry of xanthates holds a unique place among sulfur-containing reagents. [3]. as well as the different radical chemistry of xanthates. [4]. Modern industrial operations like metal plating, mining, metallurgy, alloys, machine production, chemical industry, electronics, and instrumentation have developed. [5]. Chemistry professionals have been drawn to the significant class of organic compounds known as xanthates because of their wide range of potential uses. [6]. When sulphide ores are processed for minerals, xanthate salts are frequently used. [7]. Recent investigations have shown that Xanthate ligands can exhibit a variety of bonding modes in their complexes, including

symmetric and asymmetric chelating, bridging, chelating-bridging, and monodentate. [8]. However, the study of metal complexes with sulfur as the donor atom received greater attention in recent years, and this topic has been studied. [9]. Extensive research has been done on metal-organic sulfur ligand complexes as catalysts for various processes. [10]. As the computed parameters depend on the final geometry, molecular geometry optimization is the most crucial phase in a computational chemistry study. The initial geometry predictions for the molecules of both the collector ions and metal-collector complexes used various forms and configurations.[11]. The DFT approach was recently established for vibrational analysis. [12]. This article explains how several transitions and non-transition metal complexes with cyclopentyl xanthate ligands are prepared, characterized, and added to nitrogenous bases. In addition, a DFT-based theoretical calculation has been performed in this study (the Gaussian 09W).

## 2. EXPERIMENTAL

### 2.1 Materials and instrumentation

The solvents and chemical reagents were of analytical grade. Almost all of the used materials were accessible at the university of duhok. like  $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ ,  $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ ,  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ ,  $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ ,  $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ ,  $\text{ZnCl}_2$ , cyclopentanol, potassium hydroxide, (1,10)-Phenanthroline, Ethylenediamine, diethyl ether, And Pyridine, quinoline from the university of Zakho, and 3-acetyl pyridine from the university Mosul. And carbon disulfide ( $\text{CS}_2$ ) was purchased from Romi company (Indian). ethanol was purchased from shareable a company (Spanish). Dimethyl formamide (DMF) was purchased from Thomas baker (Spanish). NMR Ultrashield was used for analyzing  $^1\text{H-NMR}$  spectra of synthesized ligands in Iran, the sample was dissolved in deuterated Dimethylsulfoxide (DMSO) at room temperature (298 K). FT-IR spectra were recorded on Perkin-Elmer 1710 spectrophotometer in the range ( $400 - 4000 \text{ cm}^{-1}$ ) using a KBr disc, which was done at the university of Salahuddin. At  $25^\circ\text{C}$ , magnetic measurements were made. using the Gouy method in the solid-state using Sherwood scientific magnetic susceptibility balance, at Zakho University. UV spectrophotometer instrument (janway 6800 double beams) used for recoding electronic spectra in DMF solvent with  $10^{-3} \text{ M}$  at  $25^\circ \text{C}$  using 1cm quartz cells. The melting point or decomposition temperature for ligands and their complexes was measured using the Thermal Electro-Melting point. Conductivity measurements for complexes were carried out at  $10^{-3} \text{ M}$  concentration in DMF solvent at  $25^\circ$  using (a 430 PH conductivity meter). Metals content was measured using AA500G atomic absorption, the last four were done at the university of Duhok.

### 2.2 Synthesis of [Cyclopentyl xanthate ligand]

(2.80g, 0.05mol) potassium hydroxide was added to (4.30g, 0.05mol) of cyclopentanol during one-hour reflux. In an ice bath, the solution was cooled. and then carbon disulfide (3.80gm, 0.05mol) was added to it while being continuously stirred for 30 minutes in the ice bath. The reaction was tracked till completion using TLC. The formation of the yellow precipitate was followed by two washes with (50ml) diethyl

ether, recrystallized with ethanol, and vacuum-assisted drying.

### 2.3 Synthesis of complexes [M (cyclopentyl xant.)<sub>2</sub>]

M = Mn(II), Fe(II), Co(II), Ni(II), Cu(II) & Zn(II) in an ethanolic solution of  $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$  (0.49g, 0.0025mol), or  $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$  (0.69g, 0.0025mol), or  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  (0.59g, 0.0025mol), or  $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$  (0.59g, 0.0025mol) or  $\text{CuCl}_2 \cdot 2 \text{H}_2\text{O}$  (0.42g, 0.0025 mol) or  $\text{ZnCl}_2$  (0.34g, 0.0025mol) potassium cyclopentyl xanthate (1g, 0.005mol) was dropwise added to an ethanolic solution with agitation for 30 minutes to cause total precipitation. The precipitate was removed by filtration, rinsed with ethanol, dried in a vacuum, and then washed again with diethyl ether.

### 2.4 Synthesis of complexes [M (cyclopentyl xant.)<sub>2</sub>(L)]

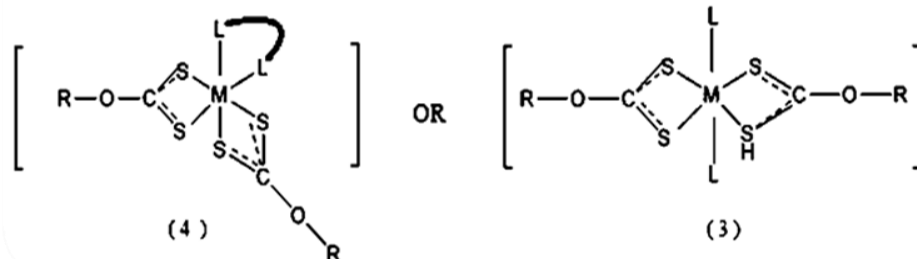
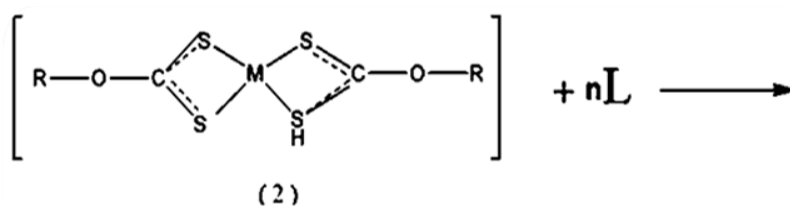
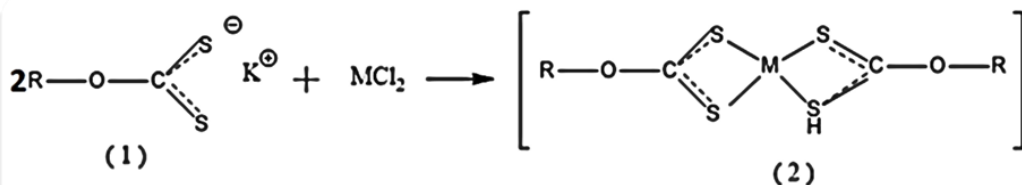
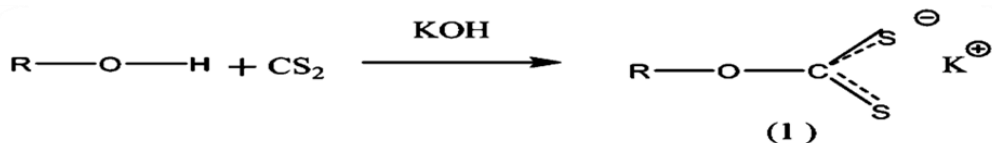
L = 1,10-Phenanthroline, Ethylenediamine Prepared similarly as in 2.3, Precipitate produced was given treatment with (0.0025mol) of (1,10-phenanthroline & ethylenediamine) dropwise for 30 minutes while stirring continuously. The resultant precipitate was filtered off, then dried after being washed with ethanol

### 2.5 Synthesis of complexes [M (cyclopentyl xant.)<sub>2</sub>(L)<sub>2</sub>]

L<sub>2</sub> = Pyridine, 3-acetyl pyridine & Quinoline Prepared similarly as in 2.3, Precipitate produced was given treatment with (0.005mol) of pyridine, 3-acetyl pyridine, quinoline,) dropwise for 30 minutes while stirring continuously. The resultant precipitate was filtered off, then dried after being washed with ethanol.

## 3. RESULT & DISCUSSION

Cyclopentanol and carbon disulfide were reacted with potassium hydroxide and carbon disulfide in a basic media to produce the Xanthate ligand. Direct interaction between metal chloride and sulfide salts was used to make the complexes, the salts,  $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$   $\text{Fe SO}_4 \cdot 7\text{H}_2\text{O}$  or  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  or  $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$  or  $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$  and  $\text{ZnCl}_2$ .unhydrous with the ligand in (1:2) molar ratio. The base adducts complexes were prepared by adding the base (Pyridine, 3-acetyl pyridine, Quinoline, 1, 10-Phenanthroline & Ethylenediamine) to the prepared bis-complexes in (1:2) or (1:1) molar ratios as shown.



The reaction of the Synthesis of Potassium Cyclopentyl xanthate Ligands and their Complexes,

Where  $\text{M} = \text{Mn(II), Fe(II), Co(II), Ni(II), Cu(II) \& Zn(II)}$ ,  $\text{L} = 1,10\text{-Phenanthroline}$ , Ethylenediamine,  $\text{L}_2 = \text{Pyridine, 3-acetyl pyridine \& Quinoline}$ .

### 3.1 Magnetic susceptibility measurements

The effective magnetic moment ( $\mu_{eff}$ ) of Complexes was calculated. at (25 °C) as shown in (Table 1). The magnetic moments for

$\text{Mn(II), Fe(II), Co(II), Ni(II) \& Cu(II)}$  complexes from **1, 2, 3, 4, 5 and 6** are in the range in (1.58 – 4.65) suggesting a tetrahedral geometry [13]. The low values of the effective magnetic moments compared to the spin-only magnetic moment for complexes **4 and 5** are due to antiferromagnetic interaction. The magnetic moment's values of the other complexes **7-36** were in the range (2.00-6.18B.M.) suggesting an octahedral geometry [14]. All Zn (II) complexes are diamagnetic.

**Table(1):** The formula, the compounds' physical characteristics, molar conductivity, and effective magnetic moment.

No	Formula of complexes	couleure	M.P C <sup>0</sup>	Molar conductivity $\Omega^{-1}.\text{cm}^2.\text{mol}^{-2}$	$\mu_{eff}$ B.M	M% (Practical) theoretical	% Yield
L	[Cyclopentyl xanthate ligand]	Pale yellow	250	-----	-----	-----	-----
1	Mn (cyclopentyl xant.) <sub>2</sub>	Dark brown	230 D	18.98	4.65	(15.93 %) 15.64 %	60
2	Fe (cyclopentyl xant.) <sub>2</sub>	brown	177 D	4.99	4.28	(14.50 %) 14.32 %	94
3	Co (cyclopentyl xant.) <sub>2</sub>	Dark green	167 D	7.90	3.09	(15.90 %) 15.50 %	98
4	Ni (cyclopentyl xant.) <sub>2</sub>	Dark yellow	173 D	8.50	2.15	(15.99 %) 15.44 %	99
5	Cu (cyclopentyl xant.) <sub>2</sub>	yellow	162 D	16.79	1.58	(17.80 %)	97

						17.55 %	
6	Zn (cyclopentyl xant.) <sub>2</sub>	Off white	176 D	14.44	Di	(16.63 %)	93
						16.41 %	
7	Mn (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	brown	231 D	15.10	6.18	(8.93 %)	50
						8.44 %	
8	Fe (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	Reddish brown	170 D	4.71	5.00	(7.92 %)	57
						7.61 %	
9	Co (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	Dark green	184 D	4.10	3.80	(9.81 %)	56
						9.23 %	
10	Ni (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	Light brown	155 D	22.10	3.00	(9.23 %)	60
						9.19 %	
11	Cu (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	Dark yellow	161 D	35.01	2.19	(9.61 %)	50
						9.38 %	
12	Zn (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	Off white	148	10.38	Di	(10.58 %)	80
						10.14 %	
13	Mn (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	Light yellow	220 D	19.23	5.91	(11.91 %)	53
						11.66%	
14	Fe (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	brown	250 D	7.81	4.91	(10.88 %)	60
						10.44 %	
15	Co (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	Dark green	240 D	5.77	3.41	(11.70 %)	81
						11.11 %	
16	Ni (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	green	160 D	8.79	2.90	(10.80 %)	89
						10.60 %	
17	Cu (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	green	161	7.11	1.89	(12.41 %)	67
						12.01 %	
18	Zn (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	Off white	185	27.61	Di	(12.63 %)	70
						12.01 %	
19	Mn(cyclopentylxant.) <sub>2</sub> (3Acet. P) <sub>2</sub>	brown	260 D	26.61	5.94	(8.51 %)	58
						8.26 %	
20	Fe (cyclopentyl xant.) <sub>2</sub> (3Acet.P) <sub>2</sub>	Reddish brown	110	13.66	4.91	(9.58 %)	58
						9.02 %	
21	Co (cyclopentyl xant.) <sub>2</sub> (3acet.P) <sub>2</sub>	Dark green	167 D	8.51	3.89	(10.84 %)	71
						10.45 %	
22	Ni (cyclopentyl xant.) <sub>2</sub> (3acet.P) <sub>2</sub>	green	180	8.33	2.87	(9.91 %)	60
						9.42 %	
23	Cu (cyclopentyl xant.) <sub>2</sub> (3acet.P) <sub>2</sub>	Yellow	147	16.84	2.00	(10.91 %)	84
						10.12 %	
24	Zn (cyclopentyl xant.) <sub>2</sub> (3acet.P) <sub>2</sub>	Off white	145	19.91	Di	(11.60 %)	63
						11.39 %	
25	Mn(cyclopentylxant.) <sub>2</sub> (1,10,phen)	Light brown	170	25.46	5.93	(9.51 %)	64
						9.16 %	
26	Fe (cyclopentyl xant.) <sub>2</sub> (1,10,phen)	Reddish	160 D	29.44	4.99	(7.50 %)	57
						7.08 %	
27	Co(cyclopentyl xant.) <sub>2</sub> (1,10,phen)	green	140 D	8.92	3.95	(10.92 %)	89
						10.25 %	
28	Ni (cyclopentyl xant.) <sub>2</sub> (1,10,phen)	Light brown	150	6.75	2.84	(6.91 %)	53
						6.45 %	
29	Cu(cyclopentyl xant.) <sub>2</sub> (1,10,phen)	brown	150	8.36	2.04	(11.9 %)	64
						11.51 %	
30	Zn (cyclopentylxant.) <sub>2</sub> (1,10,phen)	Light yellow	180	10.44	Di	(12.85 %)	56
						12.53 %	
31	Mn (cyclopentyl xant.) <sub>2</sub> (en)	Dark yellow	144	39.22	5.92	(14.92 %)	92
						14.51 %	
32	Fe (cyclopentyl xant.) <sub>2</sub> (en)	Reddish-Brown	130	19.14	5.12	(11.79 %)	98
						11.24 %	

33	Co (cyclopentyl xant.) <sub>2</sub> (en)	Dark green	145	6.40	4.23	(11.92 %) 11.42 %	54
34	Ni (cyclopentyl xant.) <sub>2</sub> (en)	Light brown	220 D	28.21	2.98	(13.91 %) 13.54 %	97
35	Cu (cyclopentyl xant.) <sub>2</sub> (en)	dark brown	166 D	15.82	1.89	(14.91 %) 14.52 %	72
36	Zn (cyclopentyl xant.) <sub>2</sub> (en)	Yellow	143	34.77	Di	(13.51 %) 13.10 %	96

D=decomposition.

### 3.2 Electronic spectra studies

The UV-Visible spectra of the ligand and its complexes of  $10^{-3}$  M solution in DMF were recorded; the results are illustrated in (Table 2). for ligand, the high-intensity absorption peak that appears in the range (44523-49734 $\text{cm}^{-1}$ ) were referred to ( $\pi \rightarrow \pi^*$ ,  $n \rightarrow \pi^*$ ) intra ligand transition [15].

The UV-Visible spectrum of Mn(II) complex give absorption bands at the (30687-36235 $\text{cm}^{-1}$ ) range corresponding to charge transfer transition. In the high spin  $d^5$  manganese (II) configuration, the (d-d) electronic transitions are spin forbidden and Laporte forbidden, due to the presence of five unpaired electrons. Therefore the absorption intensities decrease by a factor of about 100 compared to the usual(d-d) absorption band thus, the spectra are not observed in the visible region[16]. The Fe(II) complex (7) gives absorption band at (10466 $\text{cm}^{-1}$ ), which corresponds to ( ${}^5E \rightarrow {}^5T_2$ ) transition in the tetrahedral geometry Complexes(8-12) show absorption bands at the range (11032-12542)  $\text{cm}^{-1}$ , which were assigned to ( ${}^5T_2g \rightarrow {}^5Eg$ ) transition in an octahedral geometry[13].

The Co (II) of complex (13) recorded an absorption bands at (11206,&12461 $\text{cm}^{-1}$ ) in vis spectra, which were assigned to the transition of ( ${}^4A_2(F) \rightarrow {}^4T_1(F)$ ) and ( ${}^4A_2(F) \rightarrow {}^4T_2(P)$ ) respectively in the tetrahedral configuration of

this complex, the absence of ( ${}^4A_2(F) \rightarrow {}^4T_1(F)$ ), is due to the sensitivity of the instrument used. On the other hand, complexes 14-18 show three absorption bands at the range (10324-13425 $\text{cm}^{-1}$ , (13245-17665 $\text{cm}^{-1}$ ) and (20543-23654 $\text{cm}^{-1}$ ), which were specified to ( ${}^4T_1g(F) \rightarrow {}^4T_2g(F)$ ), ( ${}^4T_1g(F) \rightarrow {}^4A_2g(F)$ ) and ( ${}^4T_1g(F) \rightarrow {}^4T_1g(P)$ ) transition in octahedral configuration[17].

The Ni (II) complex (19) shows two absorption bands at (11929  $\text{cm}^{-1}$ ) and (19865 $\text{cm}^{-1}$ ) which were assigned to ( ${}^3T_1(F) \rightarrow {}^3A_2(F)$ ) and ( ${}^3T_1(F) \rightarrow {}^3T_1(P)$ ) transitions respectively in a tetrahedral geometry, at the same time, the complexes( 20-24) exhibit a three absorption bands in the range (10342-14234 $\text{cm}^{-1}$ ), (14432-18734 $\text{cm}^{-1}$ ) and (16564-20743 $\text{cm}^{-1}$ ), in which were corresponded to ( ${}^3A_2g(F) \rightarrow {}^3T_2g(F)$ ), ( ${}^3A_2g(F) \rightarrow {}^3T_1g(F)$ ) and ( ${}^3A_2g(F) \rightarrow {}^3T_1g(P)$ ) octahedral transitions sequentially[18].

The Cu(II) complex( 25) shows absorption band at (11234 $\text{cm}^{-1}$ ), which correlates to ( ${}^2T_2 \rightarrow {}^2E$ ) transition in the tetrahedral geometry, whereas octahedral complexes ( 26-30) exhibited broadband in the region (12475-14454 $\text{cm}^{-1}$ ), which was assigned to ( ${}^2Eg \rightarrow {}^2T_2g$ ) in an octahedral geometry [15].

The Zn (II) complexes show no peak in the visible region ( $d^{10}$ -system). This means there is no (d-d) electronic transition happened. These metal metal complexes do not show (d-d) transition [15].

**Table (2):** Data on the electronic spectra of the ligand and produced compounds (cm<sup>-1</sup>)

NO		U-Vis. bands (cm <sup>-1</sup> )	Assignment	Proposed Structure
L	Cyclopentyl xanthate	44523, 49734	$\pi \rightarrow \pi^*, n \rightarrow \pi$	-----
1	Mn (cyclopentyl xant.) <sub>2</sub>	33406, 34765	Charge transfer	Tetrahedral
2	Mn(cyclopentylxant.) <sub>2</sub> (Q) <sub>2</sub>	32269, 36235	Charge transfer	Octahedral
3	Mn (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	34659, 35465	Charge transfer	Octahedral
4	Mn(cyclopentylxant.) <sub>2</sub> (3-acet.P) <sub>2</sub>	33461, 35241	Charge transfer	Octahedral
5	Mn(cyclopentylxant.) <sub>2</sub> (1,10,phen	30687, 33245	Charge transfer	Octahedral
6	Mn (cyclopentyl xant.) <sub>2</sub> (en)	33245, 33678	Charge transfer	Octahedral
7	Fe (cyclopentyl xant.) <sub>2</sub>	34625, 34967	Charge transfer	Tetrahedral
		10466	( <sup>5</sup> E → <sup>5</sup> T <sub>2</sub> )	
8	Fe (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	33057, 34256	Charge transfer	Octahedral
		12545	( <sup>5</sup> T <sub>2g</sub> → <sup>5</sup> E <sub>g</sub> )	
9	Fe (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	32445, 34445	Charge transfer	Octahedral
		11467	( <sup>5</sup> T <sub>2g</sub> → <sup>5</sup> E <sub>g</sub> )	
10	Fe (cyclopentylxant.) <sub>2</sub> (3-acet.P) <sub>2</sub>	34435, 36564	Charge transfer	Octahedral
		11802	( <sup>5</sup> T <sub>2g</sub> → <sup>5</sup> E <sub>g</sub> )	

11	Fe (cyclopentylxant.) <sub>2</sub> (1,10,phen)	32732, 33367	Charge transfer	Octahedral
		11032	( <sup>5</sup> T <sub>2g</sub> → <sup>5</sup> E <sub>g</sub> )	
12	Fe (cyclopentyl xant.) <sub>2</sub> (en)	34742, 35246	Charge transfer	Octahedral
		12366	( <sup>5</sup> T <sub>2g</sub> → <sup>5</sup> E <sub>g</sub> )	
13	Co (cyclopentyl xant.) <sub>2</sub>	30243 31443	Charge transfer	Tetrahedral
		11206, 12461	( <sup>4</sup> A <sub>2</sub> (F)→ <sup>4</sup> T <sub>1</sub> (F) <sup>4</sup> (A <sub>2</sub> (F) → <sup>4</sup> T <sub>1</sub> (P))	
14	Co (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	34232, 35567	Charge transfer	Octahedral
		11342, 16453, 21415	( <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> T <sub>2g</sub> F <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> A <sub>2g</sub> F <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> T <sub>1g</sub> P	
15	Co (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	35421, 3667	Charge transfer	Octahedral
		10324, 13245, 20543	( <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> T <sub>2g</sub> F <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> A <sub>2g</sub> F <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> T <sub>1g</sub> P	
16	Co (cyclopentyl xant.) <sub>2</sub> (3-acet.P) <sub>2</sub>	32533, 34456	Charge transfer	Octahedral
		11245, 16324, 23654	( <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> T <sub>2g</sub> F <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> A <sub>2g</sub> F <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> T <sub>1g</sub> P	
17	Co (cyclopentylxant.) <sub>2</sub> (1,10,phen)	33734, 35456	Charge transfer	Octahedral
		13425, 17665, 22834	( <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> T <sub>2g</sub> F <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> A <sub>2g</sub> F <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> T <sub>1g</sub> P	
18	Co (cyclopentyl xant.) <sub>2</sub> (en)	30345, 31245	Charge transfer	Octahedral
		11356, 14543, 20976,	( <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> T <sub>2g</sub> F <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> A <sub>2g</sub> F <sup>4</sup> T <sub>1g</sub> (F)→ <sup>4</sup> T <sub>1g</sub> P	
19	Ni (cyclopentyl xant.) <sub>2</sub>	31130, 33456	Charge transfer	Tetrahedral
		11929, 19865	( <sup>3</sup> T <sub>1</sub> (F)→ <sup>3</sup> A <sub>2</sub> (F) <sup>3</sup> T <sub>1</sub> (F)→ <sup>3</sup> T <sub>1</sub> (P)	
20	Ni (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	31652, 34456	Charge transfer	Octahedral
		12654, 15765, 20743,	( <sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>2g</sub> F <sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>1g</sub> F <sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>1g</sub> P	

21	Ni (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	30654, 32456	Charge transfer	Octahedral
		13455, 17342, 19342,	<sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>2g</sub> F <sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>1g</sub> F <sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>1g</sub> P	
22	Ni (cyclopentyl xant.) <sub>2</sub> (3-acet.P) <sub>2</sub>	30522, 31567	Charge transfer	Octahedral
		14234, 15542, 20512,	<sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>2g</sub> F <sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>1g</sub> F F <sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>1g</sub> P	
23	Ni (cyclopentylxant.) <sub>2</sub> (1,10,phen)	32544, 34975	Charge transfer	Octahedral
		11023, 18734, 19532,	<sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>2g</sub> F <sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>1g</sub> F <sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>1g</sub> P	
24	Ni (cyclopentyl xant.) <sub>2</sub> (en)	33556, 35986	Charge transfer	Octahedral
		10342, 14432, 16564,	<sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>2g</sub> F <sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>1g</sub> F <sup>3</sup> A <sub>2g</sub> (F)→ <sup>3</sup> T <sub>1g</sub> P	
25	Cu (cyclopentyl xant.) <sub>2</sub>	32465, 33445	Charge transfer	Tetrahedral
		11234	( <sup>2</sup> T <sub>2</sub> → <sup>2</sup> E)	
26	Cu (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	33345, 34096	Charge transfer	Octahedral
		12475	( <sup>2</sup> E <sub>g</sub> → <sup>2</sup> T <sub>2g</sub> )	
27	Cu (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	32176, 32456	Charge transfer	Octahedral
		14565	( <sup>2</sup> E <sub>g</sub> → <sup>2</sup> T <sub>2g</sub> )	
28	Cu (cyclopentyl xant.) <sub>2</sub> (3-acet.P) <sub>2</sub>	34387, 36567	Charge transfer	Octahedral
		14276	( <sup>2</sup> E <sub>g</sub> → <sup>2</sup> T <sub>2g</sub> )	
29	Cu (cyclopentylxant.) <sub>2</sub> (1,10,phen)	31120, 35654	Charge transfer	Octahedral
		14454	( <sup>2</sup> E <sub>g</sub> → <sup>2</sup> T <sub>2g</sub> )	
30	Cu (cyclopentyl xant.) <sub>2</sub> (en)	33222, 34456	Charge transfer	Octahedral
		12566	( <sup>2</sup> E <sub>g</sub> → <sup>2</sup> T <sub>2g</sub> )	
31	Zn (cyclopentyl xant.) <sub>2</sub>	34652, 35456	Charge transfer	Tetrahedral
32	Zn (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	32933, 33566	Charge transfer	Octahedral
33	Zn (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	30587, 34675	Charge transfer	Octahedral



34	Zn (cyclopentyl xant.) <sub>2</sub> (3-acet.P)2	32445, 33456	Charge transfer	Octahedral
35	Zn (cyclopentylxant.) <sub>2</sub> (1,10,phen)	34766, 35098	Charge transfer	Octahedral
36	Zn (cyclopentyl xant.) <sub>2</sub> (en)	33345, 36678	Charge transfer	Octahedral

### 3.3 Nuclear Magnetic Resonance (NMR) studies-<sup>1</sup>H-NMR

The <sup>1</sup>H correlated NMR analysis was performed to characterize the ligands in order to ensure the synthesis process via the newly generated functional groups displayed in addition to the already existing ones. [19]. Nowadays, substances dissolved in solutions are generally studied using <sup>1</sup>H-NMR spectroscopy since molecules move quickly during the <sup>1</sup>H-NMR experiment, [20].

<sup>1</sup>H-NMR (CDCl<sub>3</sub>; 400 MHz) δH (ppm): 1.43-1.52 (2H, m, CH<sub>2</sub>), 1.58-1.65 (4H, m, CH<sub>2</sub>), 1.76-1.81 (2H, m, CH<sub>2</sub>), 5.56-5.60 (1H, m, CH), The <sup>1</sup>H-NMR spectrum of the xanthate ligand showed three multiplet signals at the respective chemical shift of δ = 1.43 -1.52, 1.58-1.65 and 1.76-1.81 ppm are assigned to the methylene protons of the substituted cycloalkane. Another multiplet signal appearing at δ = 5.56-5.60 ppm is ascribed to the methine proton attached to oxygen atoms. The structure of ligand and their complexes identify by <sup>1</sup>H- NMR instrument (500 & 400 MHz), and

the chemical shift (<sup>1</sup>H-NMR-500MHz; DMSO)δin ppm for Cyclopentylxanthate ligand exhibited the following chemical shifts,

### 3.4 Infra-red spectral studies

The critical IR bands of the ligand (Cyclopentyl xanthate)K and its complexes are listed in (Table 3). The band of FT-IR spectrum at (1180 cm<sup>-1</sup>) was assigned to ν(C – O) in ligand spectra, this band was shifted to a higher frequency and observed in the range(1217-1274) cm<sup>-1</sup>. The band at (1118 cm<sup>-1</sup>) due to ν(C- S) of the ligand which shifted to a lower frequency (1001-1080) cm<sup>-1</sup>[21].

The range (401-440 cm<sup>-1</sup>) of the IR spectra revealed a new band of moderate to strong intensity that provides support for the coordination of metal to sulfur (M-S). This phenomenon could be explained by alcohol's release of electrons, which pushes a high electron density toward the sulfur atoms, where the (M-N) was seen in the (441-525) cm<sup>-1</sup> region. [15].

**Table 3:** FT-IR bands of the most important bonds in the ligand and their complexes  
Stretching vibrations of ν(C-O), ν(C-S), ν (M-S), ν (M-N)

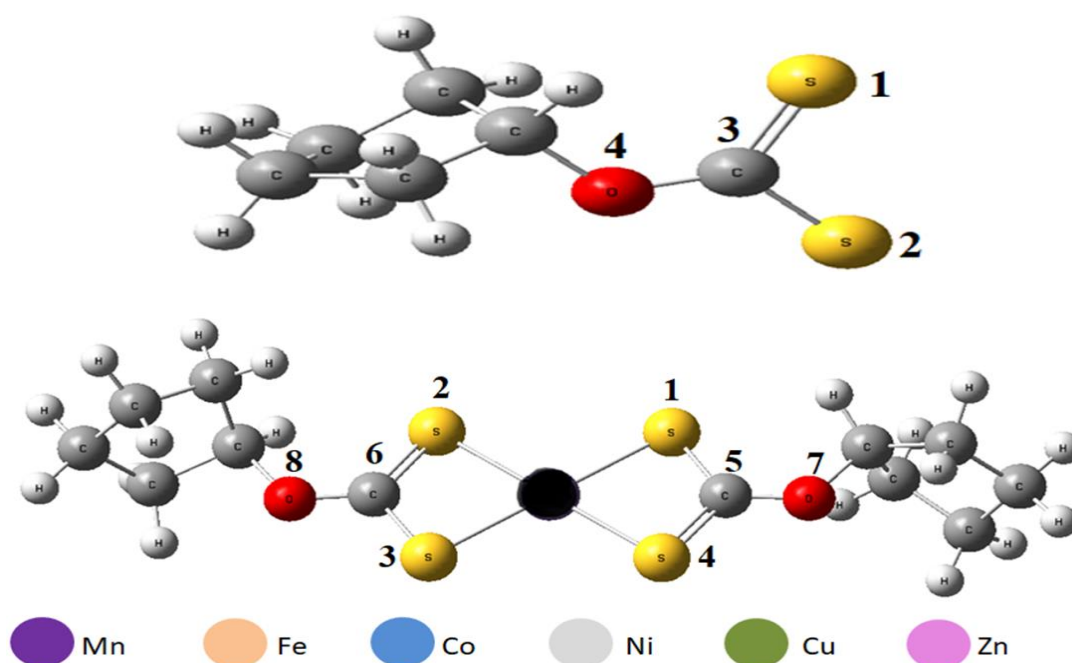
Name of complex	ν(C-O)	ν(C-S)	ν(M-S)	ν(M-N)
L [Cyclopentyl xanthate ligand]	1180	1118	-----	-----
1 Mn (cyclopentyl xant.) <sub>2</sub>	1261	1012	431	-----
2 Fe (cyclopentyl xant.) <sub>2</sub>	1261	1012	432	-----
3 Co (cyclopentyl xant.) <sub>2</sub>	1246	1001	440	-----
4 Ni (cyclopentyl xant.) <sub>2</sub>	1271	1016	436	-----
5 Cu (cyclopentyl xant.) <sub>2</sub>	1217	1014	433	-----
6 Zn (cyclopentyl xant.) <sub>2</sub>	1226	1019	430	-----
7 Mn (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	1261	1024	424	501
8 Fe (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	1263	1022	425	487
9 Co (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	1253	1045	428	490
10 Ni (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	1269	1024	429	515
11 Cu (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	1217	1024	421	500
12 Zn (cyclopentyl xant.) <sub>2</sub> (Q) <sub>2</sub>	1220	1049	418	478
13 Mn (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	1261	1034	430	484
14 Fe (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	1255	1021	426	519
15 Co (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	1249	1044	429	491
16 Ni (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	1271	1026	416	456
17 Cu (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	1218	1024	420	511

18	Zn (cyclopentyl xant.) <sub>2</sub> (Py) <sub>2</sub>	1255	1043	430	507
19	Mn (cyclopentylxant.) <sub>2</sub> (3Acet.P)2	1273	1034	420	498
20	Fe(cyclopentyl xant.) <sub>2</sub> (3-Acet.P)2	1269	1042	417	512
21	Co(cyclopentyl xant.) <sub>2</sub> (3-Acet.P)2	1251	1045	423	515
22	Ni(cyclopentyl xant.) <sub>2</sub> (3-Acet.P)2	1271	1026	401	510
23	Cu(cyclopentyl xant.) <sub>2</sub> (3-Acet.P)2	1273	1044	419	477
24	Zn(cyclopentyl xant.) <sub>2</sub> (3-Acet.P)2	1222	1051	425	425
25	Mn(cyclopentylxant.) <sub>2</sub> (1,10,phen)	1217	1026	423	488
26	Fe (cyclopentylxant.) <sub>2</sub> (1,10,phen)	1242	1049	428	501
27	Co(cyclopentylxant.) <sub>2</sub> (1,10,phen)	1249	1045	426	513
28	Ni (cyclopentylxant.) <sub>2</sub> (1,10,phen)	1271	1026	413	441
29	Cu(cyclopentylxant.) <sub>2</sub> (1,10,phen)	1228	1032	430	505
30	Zn (cyclopentylxant.) <sub>2</sub> (1,10,phen)	1224	1045	424	456
31	Mn (cyclopentyl xant.) <sub>2</sub> (en)	1269	1045	431	511
32	Fe (cyclopentyl xant.) <sub>2</sub> (en)	1259	1033	427	519
33	Co (cyclopentyl xant.) <sub>2</sub> (en)	1273	1080	429	499
34	Ni (cyclopentyl xant.) <sub>2</sub> (en)	1274	1028	431	465
35	Cu (cyclopentyl xant.) <sub>2</sub> (en)	1267	1033	422	525
36	Zn (cyclopentyl xant.) <sub>2</sub> (en)	1223	1045	416	473

### 3.5 Computational studies

The ligand [cyclopentyle xanthate] with their transition metals and non-transition complexes. The DFT Method / B3LYP / 6-311++G (d,p) (DFT) has developed into a useful tool for figuring out structure, bond angles, bond lengths,

thermodynamic parameters, and electronic properties with the use of DFT computations. The quantum chemical computations' optimal molecule structures (with minimal energies) are displayed in (Figuer1)



**Fig. (1):** Optimized structure of Ligand and Complex at B3LYP/6-311G++(d,p) (different color indicated Metal atoms, yellow- sulfur , red-oxygen, gray-carbon, and white -hydrogen.

### 3.6 Thermodynamic Parameters of the four coordinates complexes

Thermodynamic parameters for four coordinates complexes were done, In order to

obtain consistent relationships between the energetic, structural, and reactive properties of complexes, the thermodynamic parameters were also computed using quantum mechanics.

**Table 4:** The thermodynamic parameters of the ligand and their complexes, such as their specific heat capacity, internal energy, and zero-point vibrational energy, (DFT, B3LYP) method at 298.15 K and 1 atm pressure were calculated.

No.	Compounds	Zero-point vibrational energies (a.u)	Gibbs free energy (a.u)	Enthalpy (a.u)	Internal energy (a.u)	Entropy (calmol <sup>-1</sup> K <sup>-1</sup> )	Specific heat, Cv (calmol <sup>-1</sup> K <sup>-1</sup> )
L	[Cyclopentyl xanthate ligand]	-1105.629	-1105.667	-1105.619	95.299	100.442	32.816
1.	Mn (cyclopentyl xant.) <sub>2</sub>	-3362.355	-3362.411	-3362.333	165.276	-3362.334	75.97
2.	Fe (cyclopentyl xant.) <sub>2</sub>	-3475.065	-3475.120	-3475.042	162.325	-3475.043	76.06
3.	Co (cyclopentyl xant.) <sub>2</sub>	-3594.177	-3594.232	-3594.154	163.135	-3594.155	75.79
4.	Ni (cyclopentyl xant.) <sub>2</sub>	-3719.725	-3719.779	-3719.703	161.217	-3719.704	75.72
5.	Cu (cyclopentyl xant.) <sub>2</sub>	-3851.903	-3851.960	-3851.880	167.26	-3851.881	76.26
6.	Zn (cyclopentyl xant.) <sub>2</sub>	-3990.761	-3990.818	-3990.738	167.798	-3990.739	76.25

metal atom of complexes from 1, to 6, is coordinated tetrahedral formed by four S- atoms from two bonds of cyclopentyl xanthate ligand. The computed bond lengths and bond angles assist us in understanding complex's molecules are organized in as shown in table (5 ).The bond length for (M-S1, M-S2, M-S3 and M-S4) fall in the range[ (2.315-2.350), (2.314-2.324), (2.301-2.310), (2.259-2.267), (2.365-2.381), (2.382 – 2.418) ].respectively, which are accepted with

[(1.706- 1.723), (1.713-1.723), (1.706- 2.301), and (1.713- 2.310). Furthermore, the bond length of (C5-O7) and (C6-O8)] for all four coordinate complexes are ranged in [(1.310-1.315).on another side, the computed bond angles for (S1-M-S2), (S3-M-S4), (S1-M-S4), and (S2-M-S3) are found in the range [(100.944-127.050), (101.705- 127.489), (76.257-78.678), and (76.256-78.676)]agreement of [24].

**Table (5):** Geometrical bond length for synthesized ligands and their complexes by B3LYP/6-311++G (d,p).

No.	Compounds	M-S1	M-S2	M-S3	M-S4	C5-S1	C5-S4	C6-S2	C6-S3	C5-O7	C6-O8
1.	Mn (cyclopentyl xant.) <sub>2</sub>	2.315	2.339	2.327	2.350	1.723	1.716	1.709	1.731	1.310	1.310
2.	Fe (cyclopentyl xant.) <sub>2</sub>	2.314	2.315	2.324	2.323	1.711	1.719	1.711	1.719	1.313	1.313
3.	Co (cyclopentyl xant.) <sub>2</sub>	2.301	2.301	2.310	2.310	1.708	1.716	2.301	2.310	1.312	1.312
4.	Ni (cyclopentyl xant.) <sub>2</sub>	2.259	2.259	2.267	2.267	1.706	1.713	1.706	1.713	1.311	1.311
5.	Cu (cyclopentyl xant.) <sub>2</sub>	2.365	2.365	2.381	2.381	1.710	1.716	1.710	1.716	1.313	1.313
6.	Zn (cyclopentyl xant.) <sub>2</sub>	2.382	2.383	2.418	2.418	1.720	1.723	1.721	1.723	1.315	1.315

No.	Compounds	C3-S1	C3-S2	C3-O4	M-S4	C5-S1	C5-S4	C6-S2	C6-S3	C5-O7	C6-O8
L	[Cyclopentyl xanthate ligand]	1.689	1.687	1.314	-----	-----	-----	-----	-----	-----	-----

**Table (6):** Geometrical bond angle for synthesized complexes by B3LYP/6-311++G(d,p).

No.	Compounds	S1-M-S2	S3-M-S4	S1-M-S4	S2-M-S3
1.	Mn (cyclopentyl xant.) <sub>2</sub>	102.632	103.170	77.119	77.079
2.	Fe (cyclopentyl xant.) <sub>2</sub>	102.586	103.201	77.115	77.101
3.	Co (cyclopentyl xant.) <sub>2</sub>	102.188	102.780	77.519	77.517
4.	Ni (cyclopentyl xant.) <sub>2</sub>	100.944	101.705	78.678	78.676
5.	Cu (cyclopentyl xant.) <sub>2</sub>	103.902	103.589	76.257	76.256
6.	Zn (cyclopentyl xant.) <sub>2</sub>	127.050	127.489	77.128	77.123

### 3.8 Quantum mechanics

#### Frontier molecular orbitals (FMO) analysis

Frontier molecular orbitals theory describes HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) For evaluating the energy distribution and energetic behavior of a molecule, it is useful to know the essential factors that determine the electrical transport qualities in the molecule's orbitals. The HOMO and LUMO energies denote the ability of molecules to donate and acquire an electron, respectively. The energy gap (EHOMO-ELUMO) makes it possible to designate the kinetic stability and reactivity of a compound. The HOMO and LUMO orbitals and their energy gap were calculated in the Gaussian09 [25].

Furthermore, the physical calculation parameters of compounds, such as absolute electronegativity ( $\chi$ ), chemical potentials (IP), absolute hardness, ( $\eta$ ) absolute softness ( $\sigma$ ), global electrophilicity ( $\omega$ ), global softness ( $S$ ), were scheduled in Table according to the following equations and optimized via DFT Method / B3LYP / 6-311++G (d,p)[26]. In this study, various parameters such as frontier orbital energies, energy gap, hardness, electronegativity, Fukui indices, electron-donating power, and electro-accepting power are calculated using a series of equations to describe the chemical reactivity and corrosion inhibition effect of studied compounds.

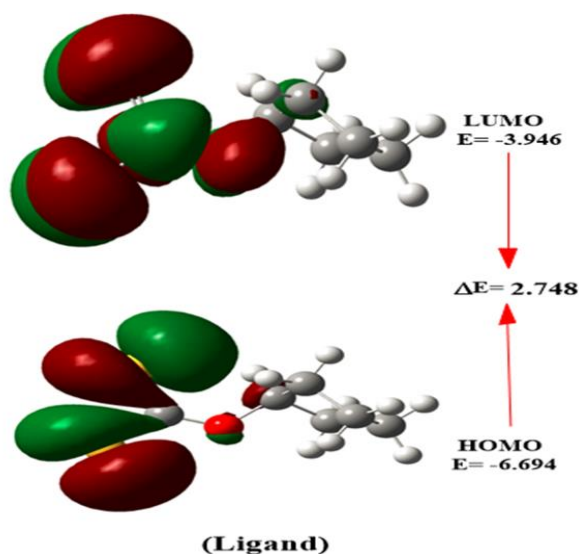
The quantum chemical parameters are calculated through the values of the energies of

the HOMO and the LUMO using the following formulas:

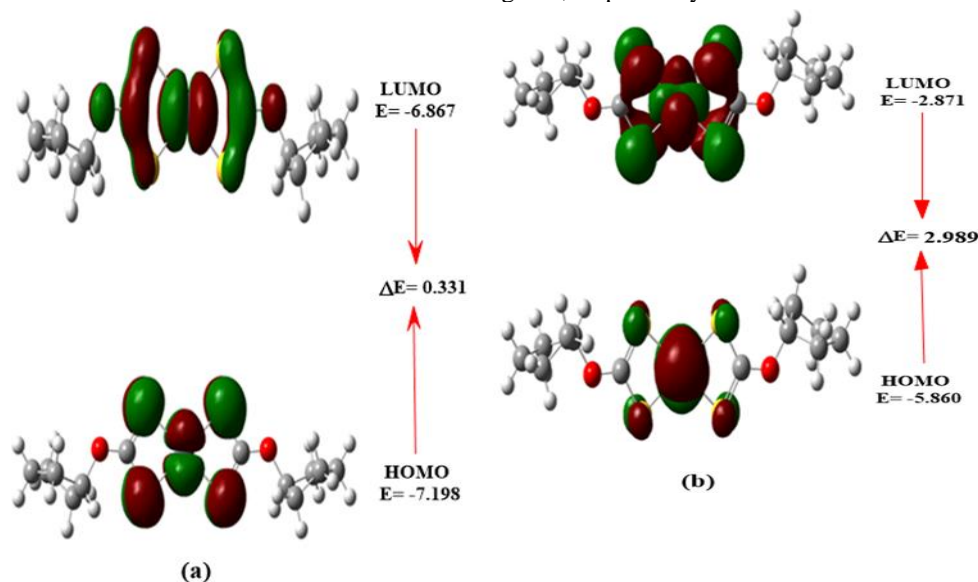
Ionization energy (I):  $I = -E_{HOMO}$   
 Electronic affinity (A):  $A = -E_{LUMO}$   
 Energy Gap ( $\Delta E_{GAP}$ ):  $\Delta E_{GAP} = E_{LUMO} - E_{HOMO}$   
 Global Hardness ( $\eta$ ):  $\eta = \frac{E_{LUMO} - E_{HOMO}}{2}$   
 Absolute Electronegativity ( $\chi$ ):  $\chi = \frac{I + A}{2}$   
 Chemical Softness ( $\sigma$ ):  $\sigma = \frac{1}{\eta}$

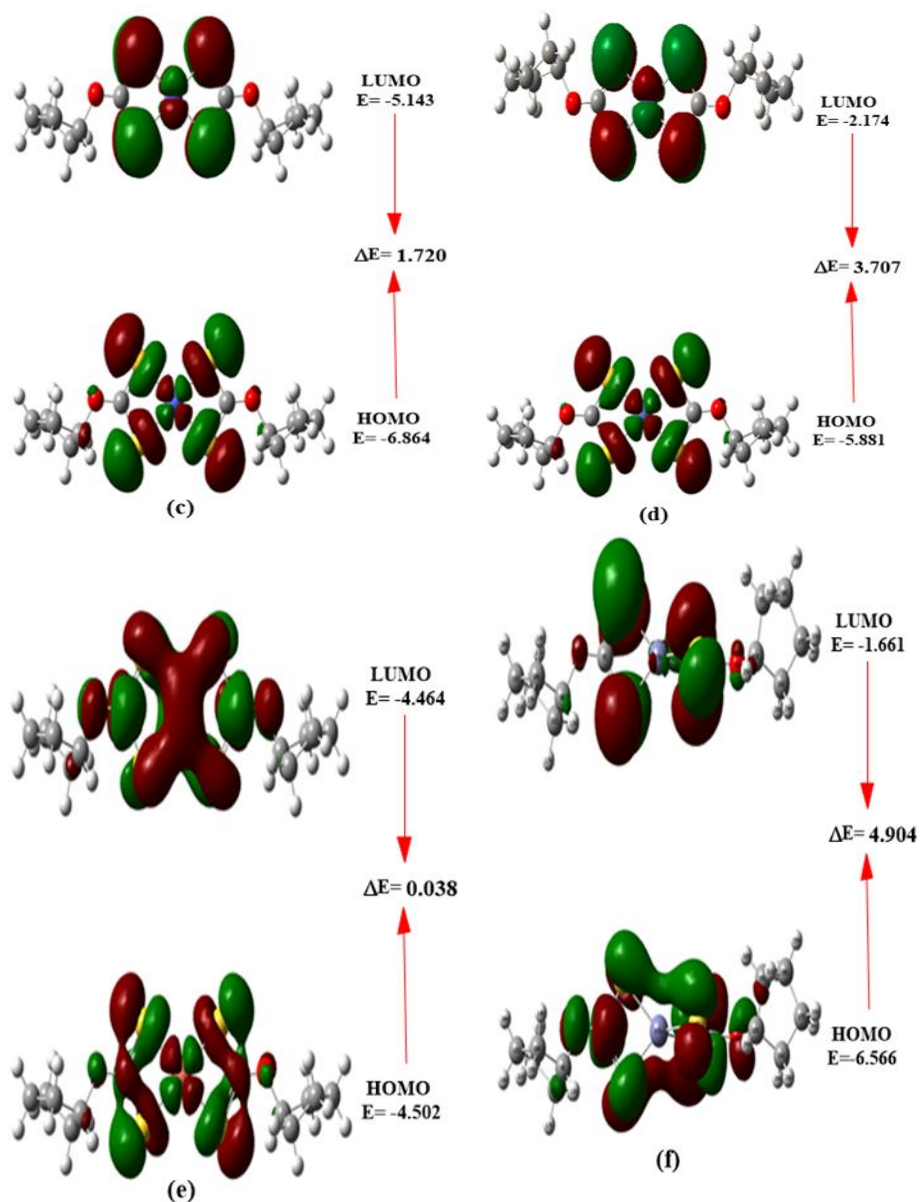
Electrophilicity Index ( $\omega$ ):  $\omega = \frac{\chi^2}{2\eta}$

[27]. Table (7) shows the electronic structure parameters ( $E_{HOMO}$ ,  $E_{LUMO}$ , ( $E_{Gap}$ ), electron affinity (EA), ionization potential (IP), dipole moment (D), hardness ( $\eta$ ), softness (S), absolute electronegativity ( $\chi$ ), Chemical potential ( $\mu$ ), electrophilicity index ( $\omega$ ), which determined using the B3LYP/6-311++G(d,p) technique.



**Fig. (2):** The HOMO and LUMO orbitals for Ligand :Negative and positive sigh of the orbitals are coloured and green, respectively.





**Fig. (3):** The HOMO and LUMO orbitals for complex: (a) L-Mn, (b) L-Fe, (c) L-Co, (d) L-Ni, (e) L-Cu and (f) L-Zn. Negative and positive sign of the orbitals are coloured red and green, respectively.

**Table (7):** Electronic parameters (in a.u., 1 a.u. = 27.211 eV, except dipole moment which is in the units of Debye) calculated of prepared ligand and their complexes at the level of DFT/B3LYP theory.

Symbol	$E_{\text{HOMO}}$	$E_{\text{LUMO}}$	$E_{\text{gap}}$	(IP)	(EA)	( $\eta$ )	(S)	( $\chi$ )	( $\mu$ )	( $\omega$ )	(D)
L [Cyclopentyl xanthate ligand]	-6.694	-3.946	2.748	3.946	6.694	1.3742	0.728	5.320	3.1845	-6.864	3.9187
1.Mn (cyclopentyl xant.) <sub>2</sub>	-5.860	-2.871	2.989	2.871	5.860	1.4943	0.669	4.365	3.1872	-5.860	-2.871
2.Fe (cyclopentyl xant.) <sub>2</sub>	-6.864	-5.143	1.720	5.143	6.864	0.8601	1.163	6.004	3.1845	-6.864	-5.143
3.Co (cyclopentyl xant.) <sub>2</sub>	-5.881	-2.174	3.707	2.174	5.881	1.8534	0.540	4.028	3.1859	-5.881	-2.174
4.Ni (cyclopentyl xant.) <sub>2</sub>	-4.502	-4.464	0.038	4.464	4.502	0.0190	52.499	4.483	3.1479	-4.502	-4.464
5.Cu (cyclopentyl xant.) <sub>2</sub>	-6.566	-1.661	4.904	1.661	6.566	2.4521	0.408	4.113	1.7998	-6.566	-1.661
6.Zn (cyclopentyl xant.) <sub>2</sub>	-7.198	-6.867	0.331	6.867	7.198	0.1656	6.039	7.032	3.2315	-7.198	-6.867

#### 4. CONCLUSION

Even though metal xanthates play a significant role in a variety of industrial processes and since the creation of the applications, there has been no attempt to manufacture the metal xanthate in recent years. Instead, researchers have focused on producing stable four-coordinate xanthate complexes with the CS<sub>2</sub> group because of their many useful properties. The necessary xanthate ligand is produced when cyclopentanol and CS<sub>2</sub> are combined in an alkaline solution. The research data for this study show the existence of four-coordinated complexes with the metal ions MnII, FeII, CoII, NiII, CuII, and ZnII. By different reactions with nitrogenous bases, that four-coordinate grew to a six-coordinate state. Numerous bonding and structural behaviors were discovered after the coordination chemistry of the metal complexes of the new ligand was analyzed. FT-IR, <sup>1</sup>H NMR, elemental analysis, magnetic susceptibility, molar conductivity, melting points, and DFT study were used to prepare and characterize the complexes. Zinc II, xanthate is diamagnetic, whereas the manganese (II), iron

(II), copper (II), nickel (II), and cobalt (II), complexes are paramagnetic. The discovered electronic spectrum bands are distinctive and agree with the ligand's postulated chemical structure and metal complexes. NMR <sup>1</sup>H signal variations also correlate with the coordination-mediated chemical shifts of ligand. Thus, Further research into this strategy may open the door to creating a reaction of xanthate-metal complexes suitable for four-coordinate, DFT studies. Method / B3LYP / 6-311++G (d,p) has been done, DFT has developed into a useful method for figuring out electrical characteristics, bond lengths, bond angles, and structure. Quantum chemical computations yielded the optimum molecule structures (with minimal energy).

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